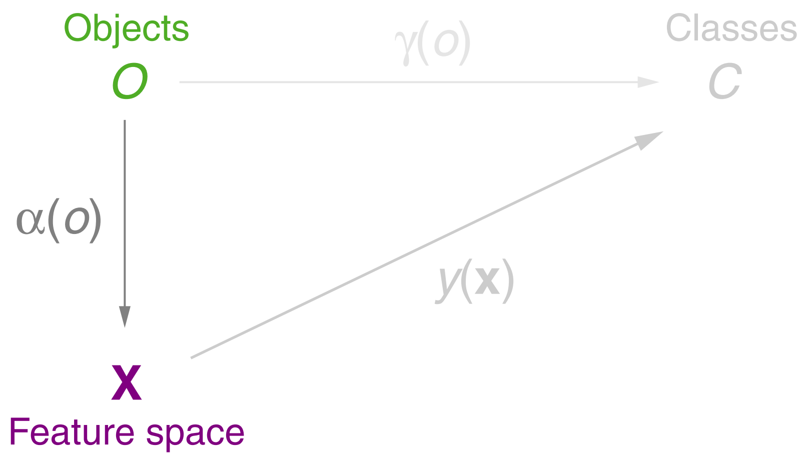
Chapter ML:I

I. Introduction

- Examples of Learning Tasks
- Specification of Learning Tasks
- Elements of Machine Learning
- Notation Overview
- Classification Approaches Overview

Elements of Machine Learning

(1) Model Formation: Real World → Model World



Related questions:

- From what kind of experience should be learned?
- Which level of fidelity is sufficient to solve a certain task?

Elements of Machine Learning

(2) Design Choices in the Machine Learning Stack: LMS

Optimization approach

Optimization objective

Loss function [+ Regularization]

Model function $\rightsquigarrow$ Hypothesis space

Task

Data

Elements of Machine Learning

(2) Design Choices in the Machine Learning Stack: LMS (continued)

Optimization approach

Optimization objective
Loss function [+ Regularization]

Model function $\rightsquigarrow$ Hypothesis space

Task

Data

Binary classification

$$D = \{(\mathbf{x}_1, c_1), \ldots, (\mathbf{x}_n, c_n)\} \subseteq X \times \{-1, 1\}$$

Elements of Machine Learning

(2) Design Choices in the Machine Learning Stack: LMS (continued)

Optimization approach

Optimization objective
Loss function [+ Regularization]

Model function $\rightsquigarrow$ Hypothesis space

- Hypothesis space: $\mathbf{w} \in \mathbf{R}^{p+1}$
- Linear model: $y(\mathbf{x}) = w_0 + \sum_{i=1}^{p} w_i x_i$

Task

Binary classification

Data

$D = \{(\mathbf{x}_1, c_1), \ldots, (\mathbf{x}_n, c_n)\} \subseteq X \times \{-1, 1\}$

Elements of Machine Learning

(2) Design Choices in the Machine Learning Stack: LMS (continued)

Optimization approach	
Optimization objective Loss function [+ Regularization]	❑ Objective: minimize squared loss (RSS) ❑ Regularization: none ❑ Loss: $l_2(c, y(\mathbf{x})) = (c - y(\mathbf{x}))^2, \;\; (\mathbf{x}, c) \in D$
Model function ⇝ Hypothesis space	❑ Hypothesis space: $\mathbf{w} \in \mathbf{R}^{p+1}$ ❑ Linear model: $y(\mathbf{x}) = w_0 + \sum_{i=1}^{p} w_i x_i$
Task	Binary classification
Data	$D = \{(\mathbf{x}_1, c_1), \ldots, (\mathbf{x}_n, c_n)\} \subseteq X \times \{-1, 1\}$

Elements of Machine Learning

(2) Design Choices in the Machine Learning Stack: LMS (continued)

Optimization approach	Stochastic gradient descent (SGD)
Optimization objective Loss function [+ Regularization]	❑ Objective: minimize squared loss (RSS) ❑ Regularization: none ❑ Loss: $l_2(c, y(\mathbf{x})) = (c - y(\mathbf{x}))^2, \;\; (\mathbf{x}, c) \in D$
Model function $\rightsquigarrow$ Hypothesis space	❑ Hypothesis space: $\mathbf{w} \in \mathbf{R}^{p+1}$ ❑ Linear model: $y(\mathbf{x}) = w_0 + \sum_{i=1}^{p} w_i x_i$
Task	Binary classification
Data	$D = \{(\mathbf{x}_1, c_1), \ldots, (\mathbf{x}_n, c_n)\} \subseteq X \times \{-1, 1\}$

Related questions:

- What are useful classes of model functions?
- What are methods to fit (= learn) model functions?
- What are measures to assess the goodness of fit?

- How does (label) noise affect the learning process?
- How does the example number affect the learning process?
- How to deal with extreme class imbalance?

Elements of Machine Learning

(3) Feature Space Structure

The feature space is an inner product space.

- An inner product space (also called pre-Hilbert space) is a vector space with an additional structure called “inner product”.
- Example: Euclidean vector space equipped with the dot product.
- Enables algorithms such as gradient descent and support vector machines.

Elements of Machine Learning

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The feature space is a σ-algebra.

- A σ-algebra on a set Ω is a collection of subsets of Ω that includes Ω itself, is closed under complement, and is closed under countable unions.
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Elements of Machine Learning

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The feature space is a finite set of vectors with nominal dimensions.

- Requires concept learning via set splitting as done by decision trees.

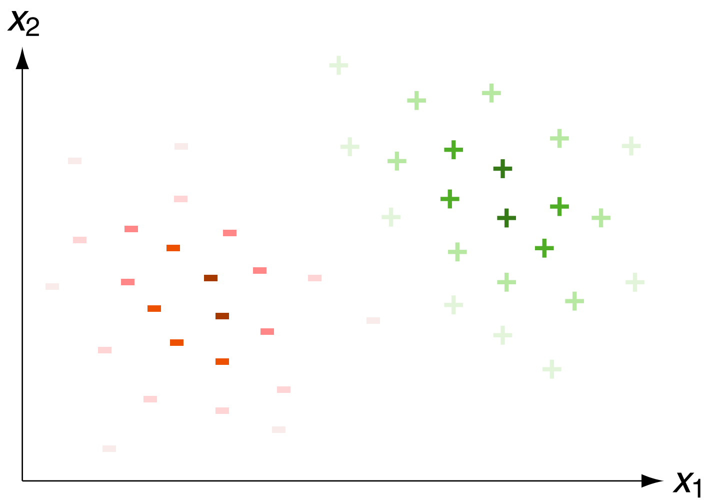
Remarks:

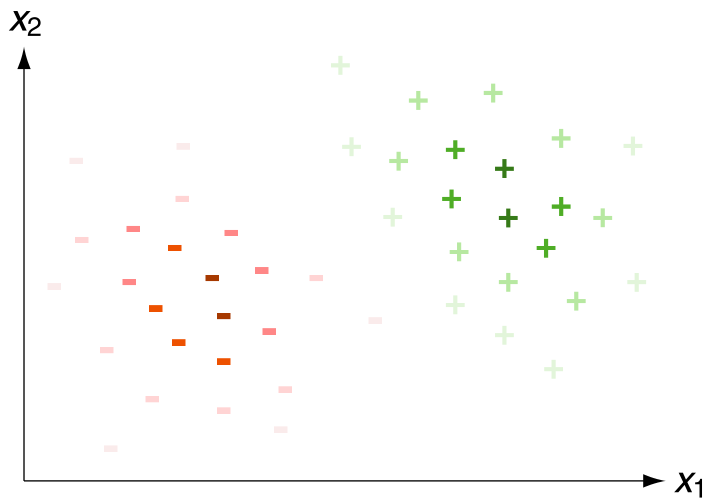
- The aforementioned examples of feature spaces are not meant to be complete. However, they illustrate a broad range of structures underlying the example sets we want to learn from.
- The structure of a feature space constrains the applicable learning algorithm. Usually, this structure is inherently determined by the application domain and cannot be chosen.

Elements of Machine Learning

(4) Discriminative versus Generative Approach to Classification

- Discriminative classifiers (models) learn a boundary between classes.
- Generative classifiers exploit the distributions underlying the classes.





Elements of Machine Learning

(4) Discriminative versus Generative Approach to Classification (continued)

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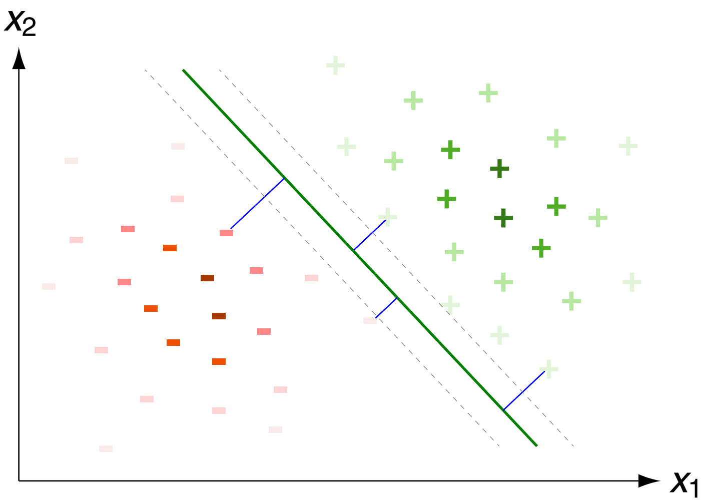
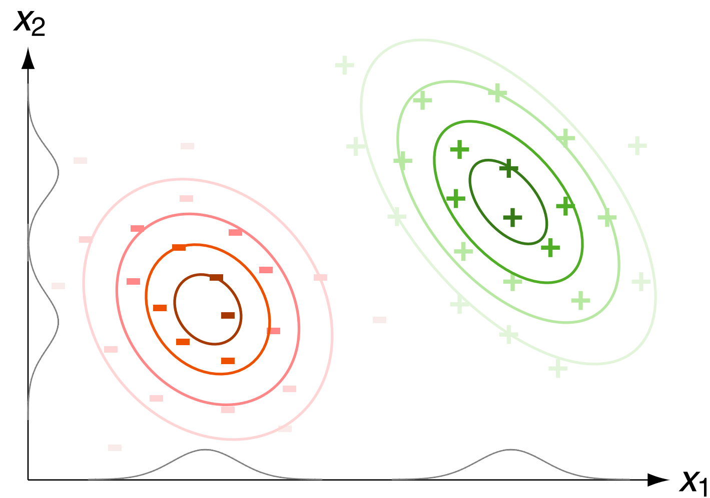


discriminative
$\rightsquigarrow$ classification rule



generative
$\rightsquigarrow$ class membership probability

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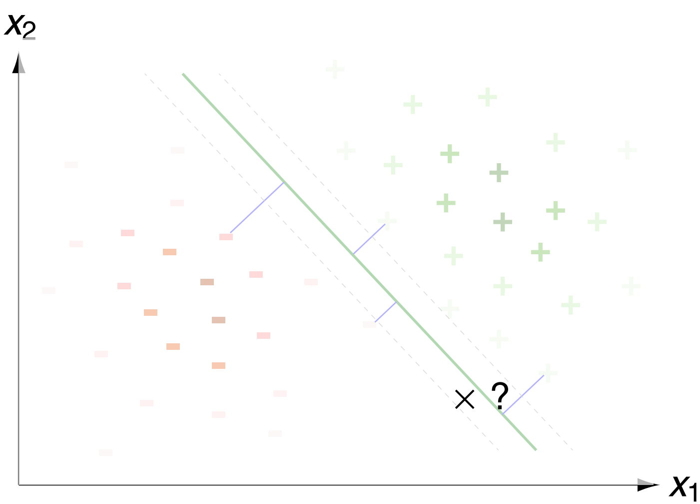
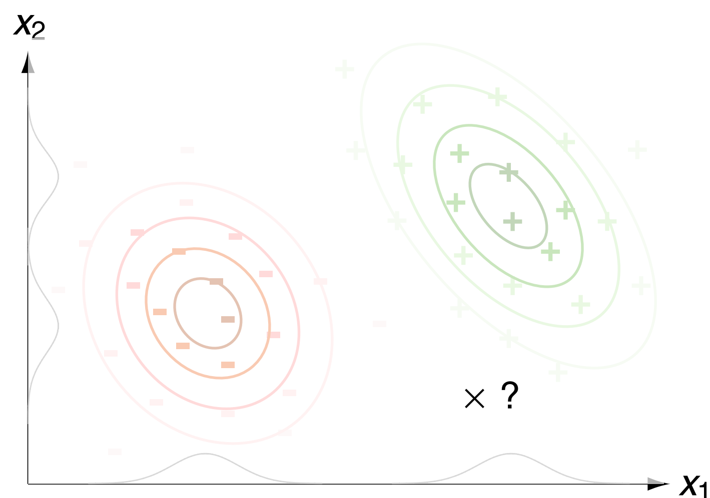


discriminative
⇝ classification rule



generative
⇝ class membership probability

Remarks:

- When classifying a new example, then

  (1) discriminative classifiers apply a decision rule that was learned via minimizing the misclassification rate given training examples D, while

  (2) generative classifiers maximize the probability of the combined event $p(\mathbf{x}, y)$, or, similarly, the posterior probability $p(y \mid \mathbf{x})$, $y \in \{\ominus, \oplus\}$.

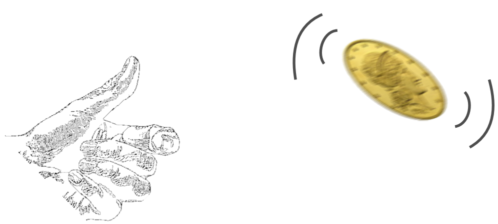
- The LMS algorithm computes “only” a decision boundary, i.e., it constructs a discriminative classifier. A Bayes classifier is an example for a generative model.

- Yoav Freund provides an excellent video illustrating the pros and cons of discriminative and generative models respectively. [YouTube]

- Discriminative models may be further differentiated in models that also determine the posterior class probabilities $p(y \mid \mathbf{x})$ (without computing the joint probabilities $p(\mathbf{x}, y)$) and those that do not. In the latter case, only a so-called “discriminant function” is computed.

Frequentist:

- There is a hidden but unique mechanism that generated the data D.
- Consider a model for this mechanism, such as a family of distributions or a model function, parameterized by θ, $\boldsymbol{\theta}$, $\mathbf{w}$, or similar. The considered parameter values (or vectors) form the hypothesis space H.
- Select for the unknown parameter (vector) that element from H such that the observed data D becomes most probable. The chosen element (our hypothesis), h_{ML}, is called maximum likelihood hypothesis.



Elements of Machine Learning

(5) Frequentist versus Subjectivist Paradigm to Learning (continued)

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$$\theta^*, \boldsymbol{\theta}^* \text{ or } \mathbf{w}^* \rightsquigarrow D, \qquad h_{\text{ML}} = \underset{h \in H}{\operatorname{argmax}}\ p(D; h)$$

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$$\theta^*, \boldsymbol{\theta}^* \text{ or } \mathbf{w}^* \leadsto D, \qquad h_{\text{ML}} = \underset{h \in H}{\text{argmax}}\ p(D; h)$$

$$\theta_{\text{ML}} = \underset{\theta \in [0;1]}{\text{argmax}}\ p(D; \theta) = \underset{\theta \in [0;1]}{\text{argmax}} \binom{n}{k} \cdot \theta^k \cdot (1-\theta)^{n-k}$$

Remarks:

- Likelihood is the hypothetical probability that an event that has already occurred (here: a coin flip experiment parameterized by θ) would yield a specific outcome (here: a sequence D of heads and tails).

  The concept differs from that of a probability in that a probability refers to the occurrence of future events, while a likelihood refers to past events with known outcomes. I.e., $p(D)$ is called likelihood since we reason about a past coin flip experiment. [Mathworld]

- By definition, the unknown parameter value (vector) of the data generation mechanism, θ^*, $\boldsymbol{\theta}^*$, $\mathbf{w}^*$, etc., is considered as unique and has some value from H.

  This means that θ, $\boldsymbol{\theta}$, or h in the argmax-expression is not the realization of a random variable or random vector—which would come along with a distribution and an expected value—but an *exogenous parameter (vector), which we vary* to find the maximum of $p(D;\theta)$, $p(D;\boldsymbol{\theta})$, $p(D;\mathbf{w})$, or, in general, $p(D;h)$.

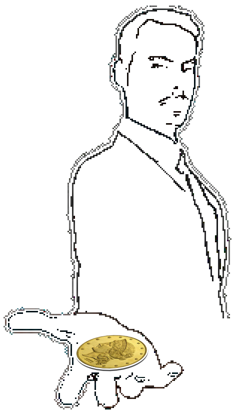
  The fact that h is a given, unique parameter (though it need to be searched) and *not* a random variable is reflected by the notation, which uses a »;« instead of a »|« in $p()$.

- In the experiment of flipping a coin, we assume a Laplace experiment and apply the binomial distribution, $B(n,p)$, with exactly k successes in n independent Bernoulli trials.

- A general method for finding the maximum likelihood estimate of the parameters of an underlying distribution from a given data set D (even if the data is incomplete) is the Expectation-Maximization (EM) algorithm. [Bilmes 1998]

Subjectivist:

- There is a hidden but ambiguous mechanism that generated the data D.
- As before, consider a model for this mechanism. In addition, we have beliefs (subjective prior probabilities) $p(h)$ for all elements in the hypothesis space H.
- Select the most probable hypothesis $h_{\text{MAP}} \in H$ by weighting the likelihoods $p(D \mid h), h \in H$, with the priors. h_{MAP} is called maximum posterior hypothesis.



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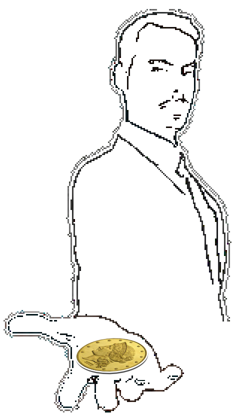
Belief/Prior 1: $P(\Theta = \underbrace{0.5}_{\theta_1})$ = 0.95



Belief/Prior 2: $P(\Theta = \underbrace{0.75}_{\theta_2})$ = 0.05

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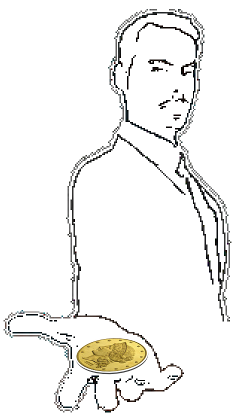

Belief/Prior 2: $P(\Theta = \underbrace{0.75}_{\theta_2}) = 0.05$

$$\theta_1 + D \;\rightarrow\; p(D \mid \theta_1)$$

$$\theta_2 + D \;\rightarrow\; p(D \mid \theta_2)$$

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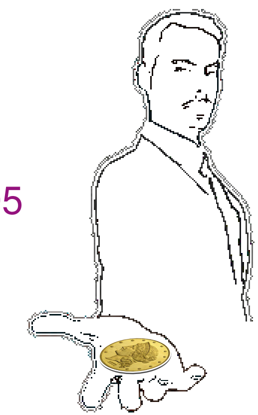

Belief/Prior 2: $P(\Theta = \underbrace{0.75}_{\theta_2}) = 0.05$

$$\left.\begin{array}{l} \theta_1 + D \;\rightarrow\; p(D \mid \theta_1) \\ \theta_2 + D \;\rightarrow\; p(D \mid \theta_2) \end{array}\right\} \quad \theta_{\text{MAP}} = \underset{\theta \in \{\theta_1, \theta_2\}}{\text{argmax}}\; p(\theta \mid D) = \underset{\theta \in \{\theta_1, \theta_2\}}{\text{argmax}}\; \frac{p(D \mid \theta) \cdot p(\theta)}{p(D)}$$

Remarks:

- By definition, the elements in H (here: θ_1, θ_2) are considered as realizations of the random variable Θ. There is (subjective) prior knowledge about the distribution of Θ. Here, Θ models the parameter p of the binomial distribution and defines the success probability for each trial.
  - Belief in θ_1 ($\Theta{=}0.5$): With probability 0.95 the coin is fair, i.e., sides are equally likely.
  - Belief in θ_2 ($\Theta{=}0.75$): With probability 0.05 the odds of preferring one side is 3:1.

  We compute for each element in H the likelihood of the observed data D, i.e., $p(D \mid \theta_1)$ and $p(D \mid \theta_2)$ under the binomial distribution. We then compute the respective values for $p(\theta_1 \mid D)$ and $p(\theta_2 \mid D)$ with Bayes's rule, and finally select θ_{MAP}.

  The fact that h is the realization of a random variable (and not an exogenous parameter) is reflected by the notation, which uses a »|« in $p()$ (and not a »;«).

- The subjectivist paradigm is powerful, if we want to consider knowledge about H that we cannot get from D by maximizing the likelihood. The subjectivist paradigm is necessary, if we have no data D to optimize, e.g., if we reason about "one time events". If all hypotheses are equally likely (a uniform prior), ML optimization and MAP optimization are equivalent.

  If the prior probabilities (here: $p(\theta_1)$, $p(\theta_2)$) are estimated from D as well, we still apply the Bayes calculation rule for a "MAP hypothesis". However, we are not subjective anymore but follow the frequentist paradigm.

- The subjectivist paradigm is also called Bayesian interpretation of probability. It enables by design the integration of prior knowledge or human expertise about alternative mechanisms one of which generated D. [Wikipedia: Bayesian interpretation, probability interpretations]