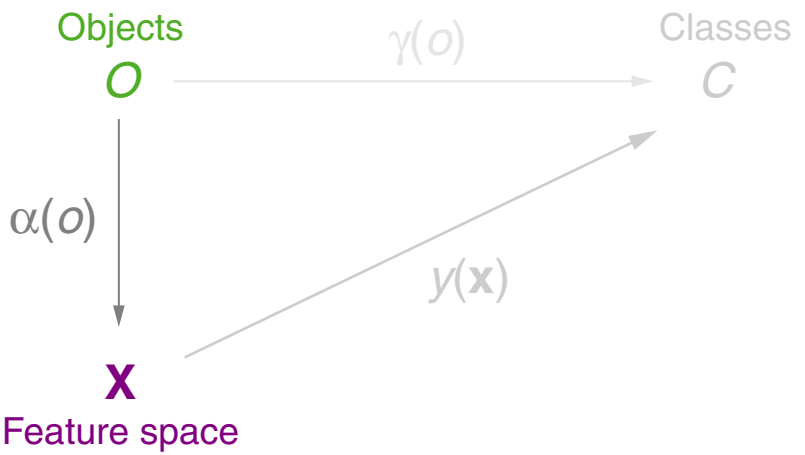
Chapter ML:I

Elements of Machine Learning

(1) Model Formation: Real World → Model World

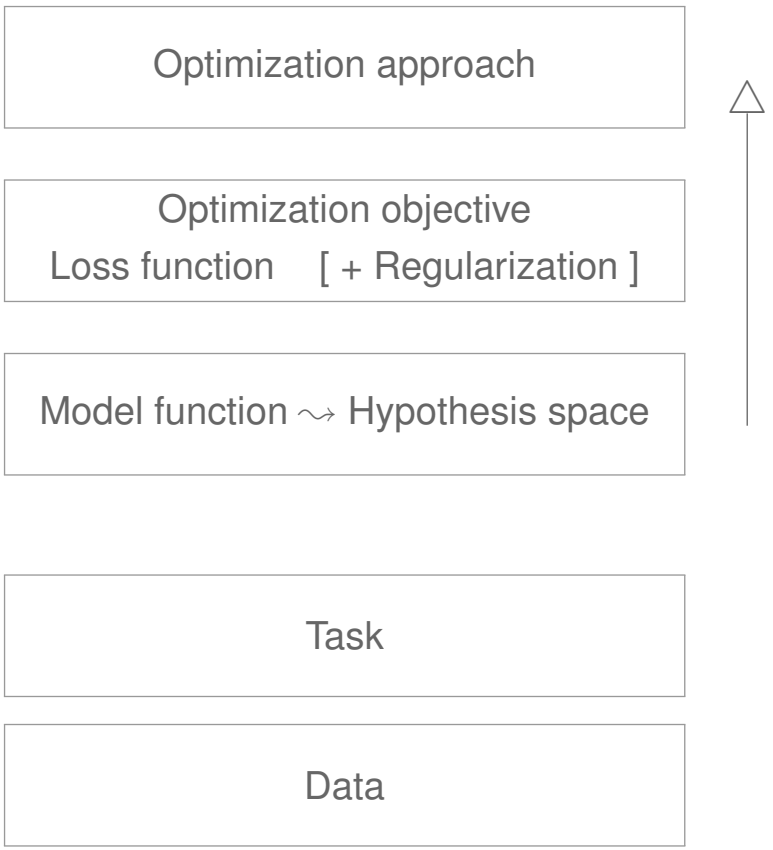


Related questions:

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

Elements of Machine Learning

(2) ML Stack: LMS [ML stack: LMS, log. regression, loss comp., regularization, GD]



Elements of Machine Learning

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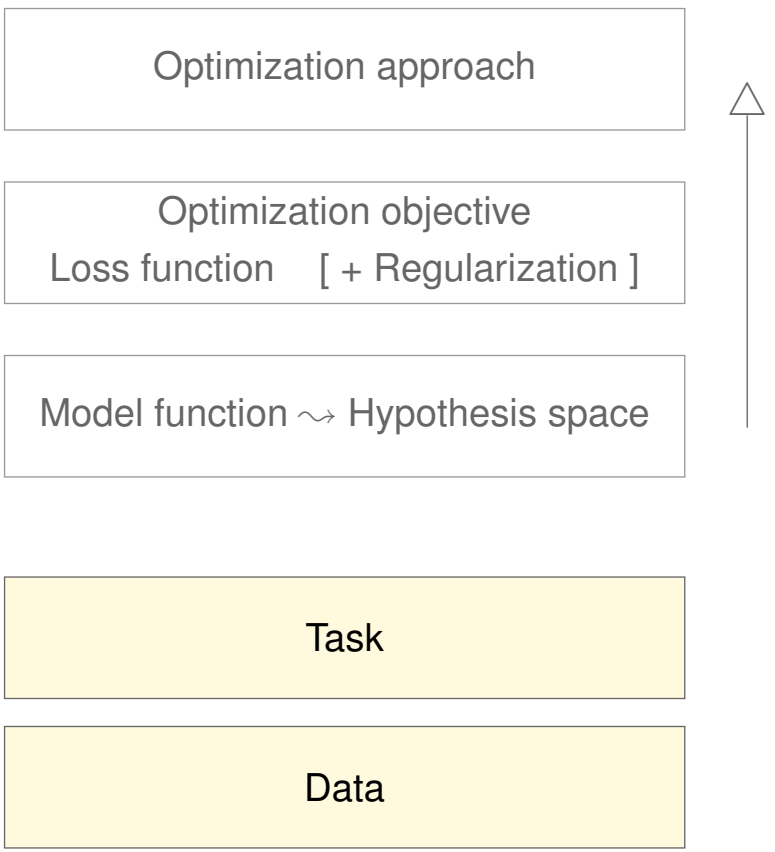

Binary classification

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

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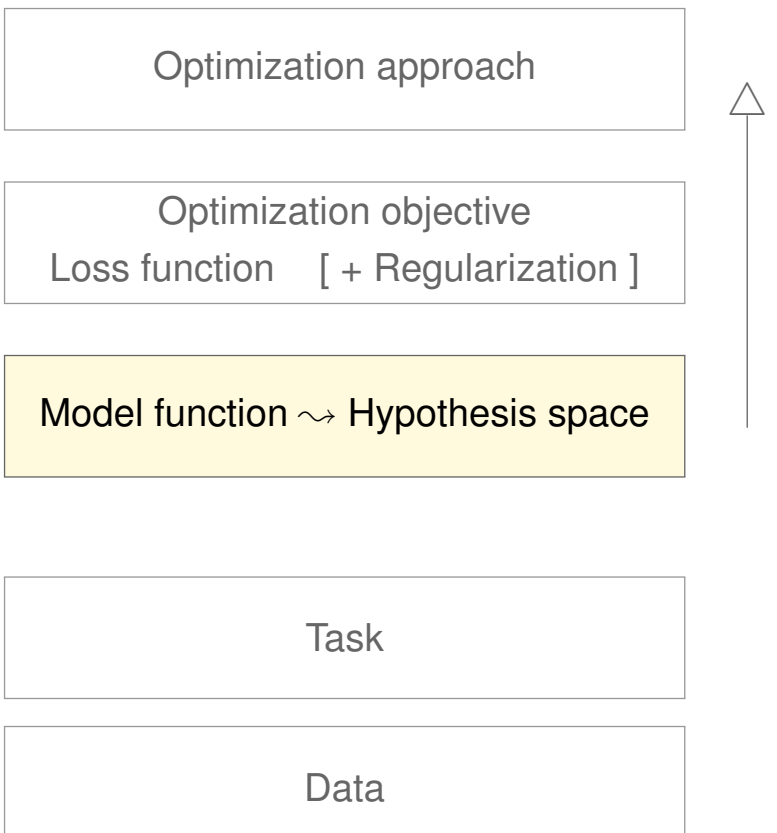

- Hypothesis space: $\mathbf{w} \in \mathbf{R}^{p+1}$
- Linear model: $y(\mathbf{x}) = w_0 + \sum_{i=1}^{p} w_i x_i$

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Optimization approach

Optimization objective
Loss function [+ Regularization]

Model function $\rightsquigarrow$ Hypothesis space

Task

Data

- Objective: minimize squared loss (RSS)
- Regularization: none
- Loss: $l_2(c, y(\mathbf{x})) = (c - y(\mathbf{x}))^2, \ (\mathbf{x}, c) \in D$

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(2) ML Stack: LMS [ML stack: LMS, log. regression, loss comp., regularization, GD]

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 operation called “inner product”.
- Example: Euclidean vector space equipped with the dot product.
- Enables algorithms such as gradient descent and support vector machines.

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

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

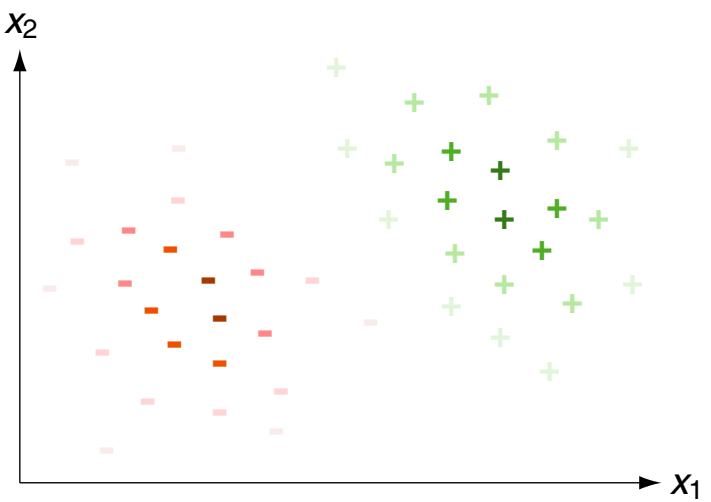
Remarks:

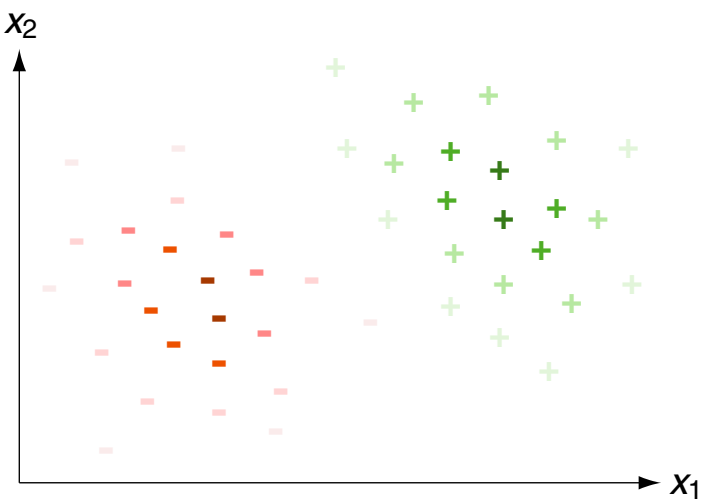
- The aforementioned examples of feature spaces are not meant to be complete. But, they illustrate a broad range of structures underlying the example sets we want to learn from.
- The structure of a feature space constrains the applicable learning algorithm. Usually, this structure is inherently determined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





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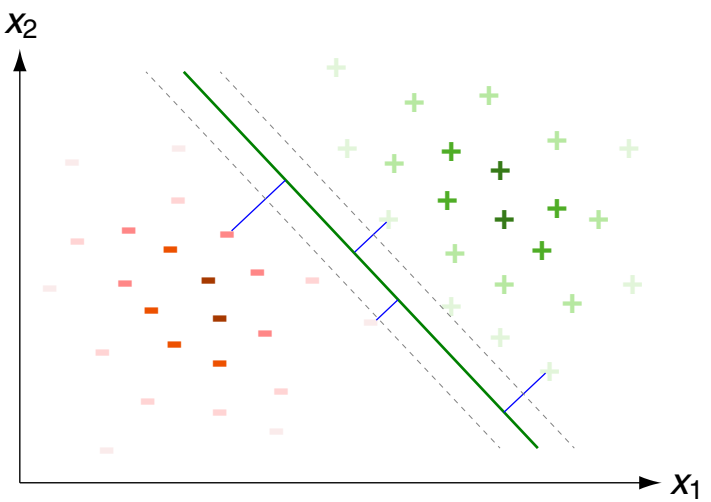
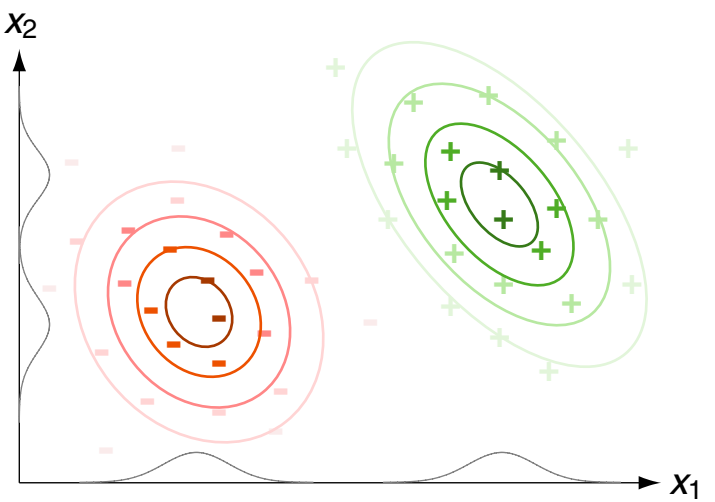


discriminative
$\rightsquigarrow$ classification rule



generative
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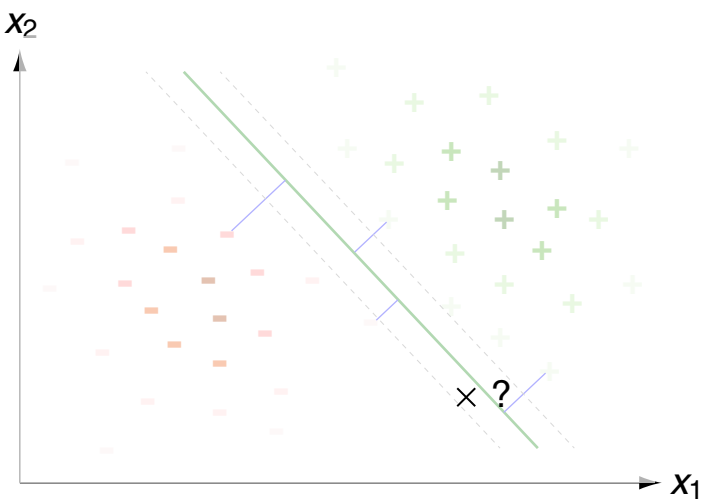

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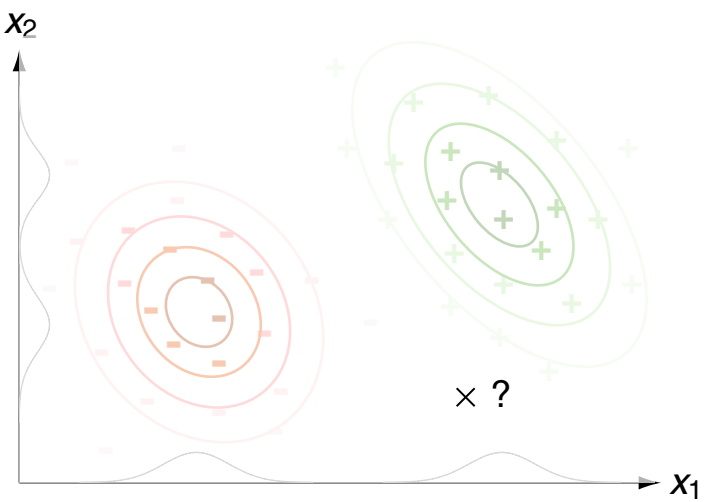

generative
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Remarks:

- When classifying a new example $\mathbf{x}$, 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.

Elements of Machine Learning

(5) Frequentist versus Subjectivist Paradigm to Learning

Frequentist:

- There is a hidden, 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.

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

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

Remarks:

- Frequentist = Let the (large amount of) data speak.
- 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., $p(D;\theta)$ is called likelihood since we reason about a past coin flip experiment. [Mathworld]
- The unknown parameter value (vector) of the data generation mechanism, θ^*, $\boldsymbol{\theta}^*$, $\mathbf{w}^*$, etc., has some value from H. In particular, 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, $p(D;h)$.

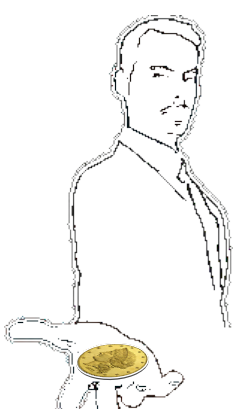
  The fact that h is a given, unique parameter (though it needs to be searched) and *not* a random variable is reflected by the notation, which uses a »;« instead of a »|« in $p()$.
- In the experiment of flipping a coin, we assume a Laplace experiment and apply the binomial distribution, $B(n,p)$, with 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]

Elements of Machine Learning

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

Subjectivist:

- We consider alternative mechanisms that could have generated the data D.
- As before, consider a model for the mechanisms. Moreover, we have beliefs (prior probabilities) $p(h)$ for the elements (alternative mechanisms) in 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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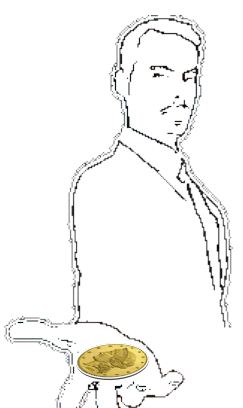
Belief/Prior 1: $P(\Theta = \underbrace{0.5}_{\theta_1}) = 0.95$



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

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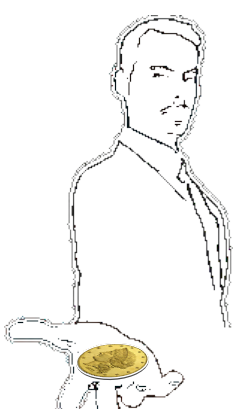

Belief/Prior 2: $P(\Theta = \underbrace{0.75}_{\theta_2}) = 0.05$

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

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

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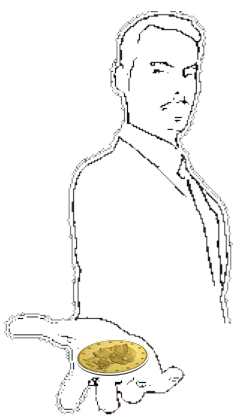

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Remarks:

- Subjectivist = Let (also) the knowledge (about priors, prevalences) speak.
- The elements in H (here: θ_1, θ_2) are realizations of a random variable Θ, and there is (subjective) knowledge about the distribution of Θ (= the prior probability model). 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 can consider knowledge about H in combination with data D. The subjectivist paradigm is necessary, if we have no data D at all 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]