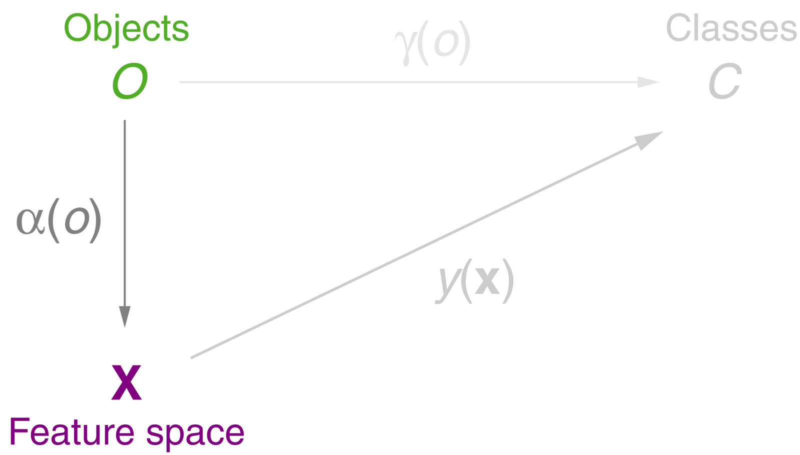
Chapter ML:I (continued)

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 $\rightarrow$ 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?

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.

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.

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.
- Enables probability spaces and statistical learning, such as naive Bayes.

Elements of Machine Learning

(3) Feature Space Structure (continued)

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.

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.
- Enables probability spaces and statistical learning, such as naive Bayes.

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

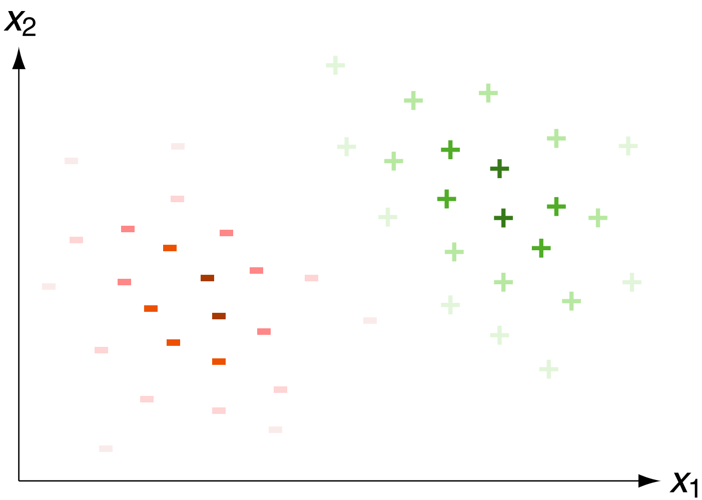
- Requires concept learning via set splitting as done by decision trees.

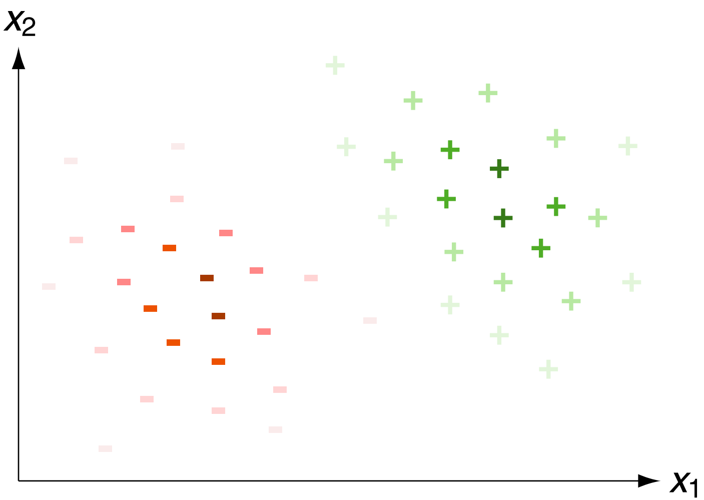
Remarks:

- 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.

(4) Discriminative versus Generative Approach to Classification

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

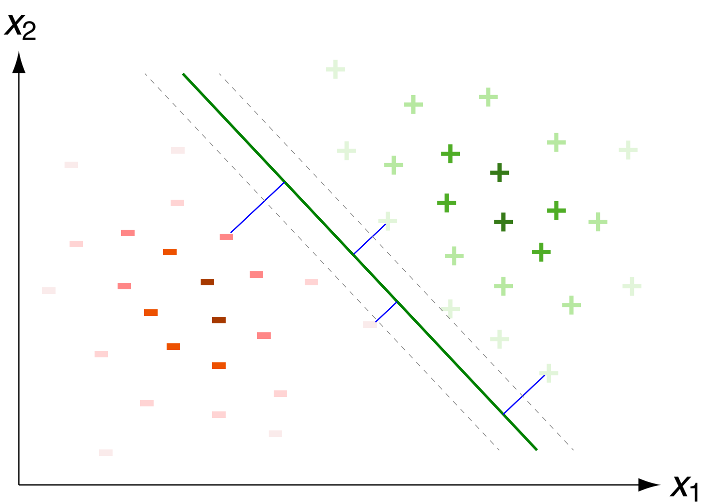




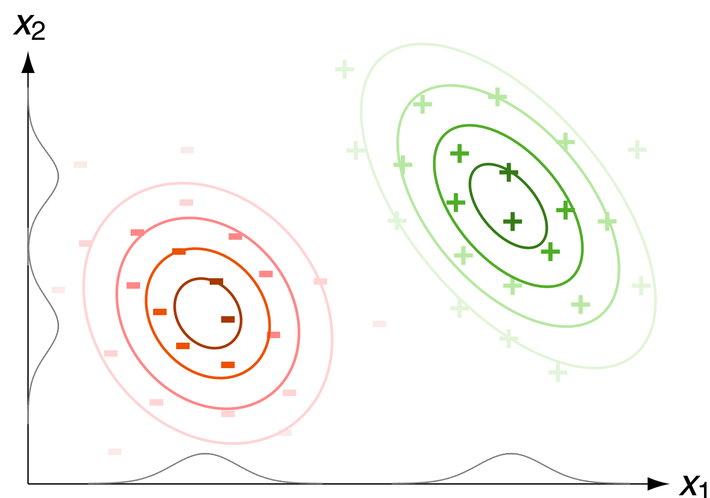
Elements of Machine Learning

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

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



discriminative
$\rightsquigarrow$ classification rule

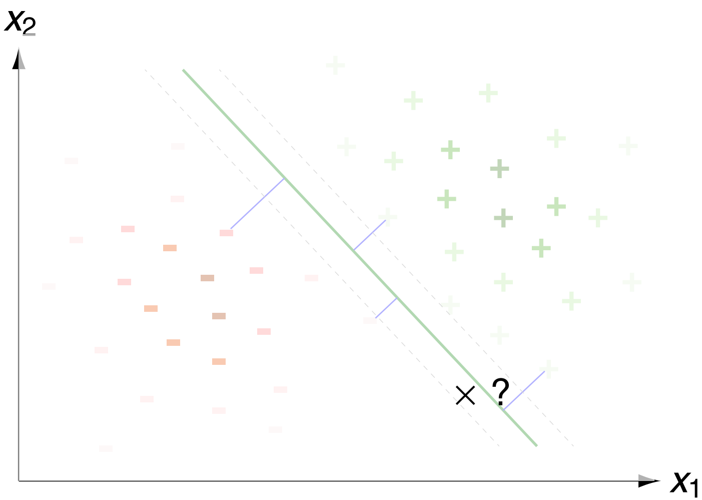


generative
$\rightsquigarrow$ class membership probability

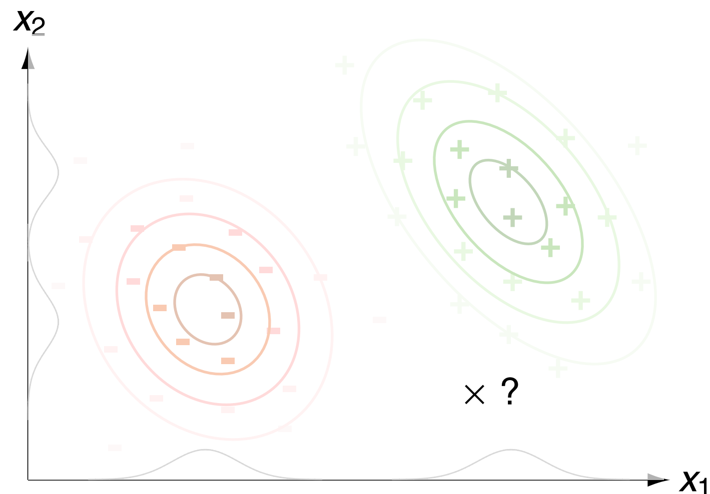
Elements of Machine Learning

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

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



discriminative
⇝ classification rule



generative
⇝ class membership probability

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 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)

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.

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

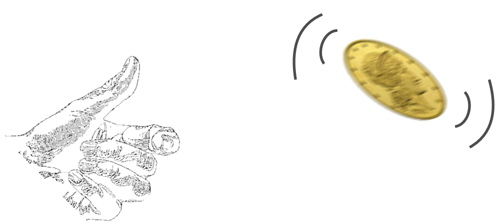
Elements of Machine Learning

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

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.

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



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

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, $p(D;h)$.

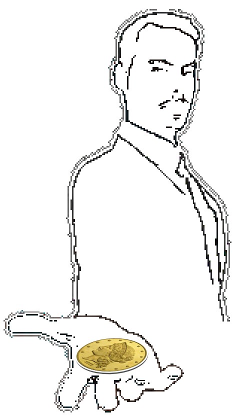
  The fact that h is a given, unique parameter (though it needs to be searched) and *not* a random variable is reflected by the notation, which uses a »;« instead of a »|« in $p()$.

- 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]

Subjectivist:

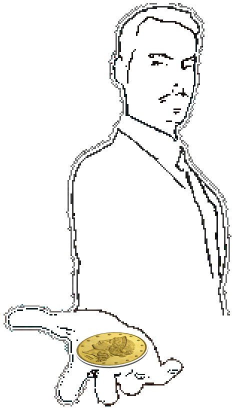
- There is a hidden but ambiguous mechanism that generated the data D.
- As before, consider a model for this mechanism. In addition, we have beliefs (subjective prior probabilities) $p(h)$ for all elements in the hypothesis space H.
- Select the most probable hypothesis $h_{\text{MAP}} \in H$ by weighting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



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.

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

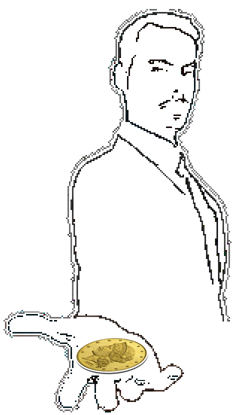


Belief/Prior 2: $P(\Theta{=}\underbrace{0.75}_{\theta_2}) = 0.05$

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.

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



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

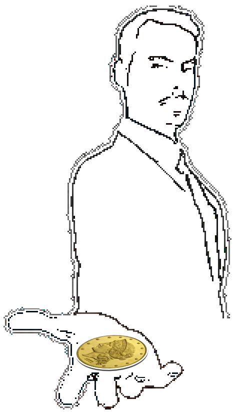
$$\theta_1 + D \rightarrow p(D \mid \theta_1)$$

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

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.

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



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

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

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]

