

*** Applied Machine Learning Fundamentals ***

Bayesian Decision Theory

Daniel Wehner, M.Sc.

SAP SE / DHBW Mannheim

Winter term 2021/2022



Find all slides on [GitHub](https://github.com/DaWe1992/Applied_ML_Fundamentals) (DaWe1992/Applied_ML_Fundamentals)

Lecture Overview

Unit I	Machine Learning Introduction
Unit II	Mathematical Foundations
Unit III	Bayesian Decision Theory
Unit IV	Probability Density Estimation
Unit V	Regression
Unit VI	Classification I
Unit VII	Evaluation
Unit VIII	Classification II
Unit IX	Clustering
Unit X	Dimensionality Reduction

Agenda for this Unit

① Bayesian Decision Theory

- Introduction
- Class Conditional Probabilities
- Class Priors
- Bayes' Theorem
- Bayes' optimal Classifier

② Naïve Bayes Classifier

- Assumptions and Algorithm
- An Example
- Laplace Smoothing

③ Risk Minimization

- Error \neq Risk
- Loss Functions for Risk Minimization
- Handling of continuous Data

④ Wrap-Up

- Summary
- Self-Test Questions
- Lecture Outlook
- Recommended Literature and further Reading
- Meme of the Day

Section:
Bayesian Decision Theory

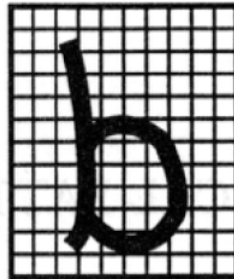
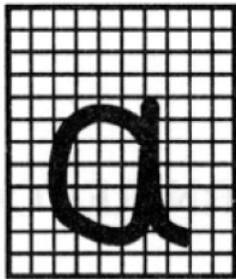


Statistical Methods

- Statistical methods assume that the process that 'generates' the data is governed by the **rules of probability**
- The data is understood to be a set of **random samples** from some underlying **probability distribution**
- This is the reason for the name **statistical machine learning**

The basic assumption about how the data is generated is always there, even if you don't see a single probability distribution!

Running Example: Optical Character Recognition (OCR)



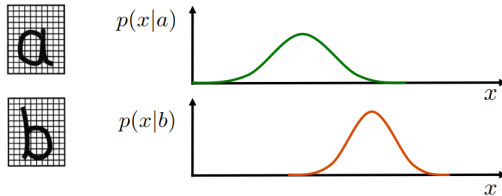
Goal: Classify a new letter so that the probability of a wrong classification is minimized

Class Conditional Probabilities

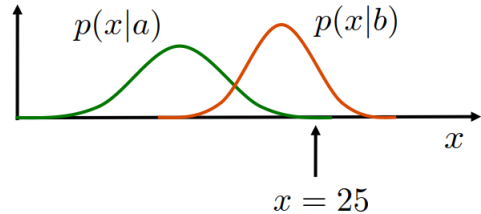
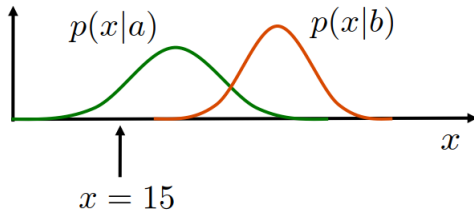
- First concept: **Class conditional probabilities**
- Probability of \mathbf{x} given a specific class \mathcal{C}_k is formally written as:

$$p(\mathbf{x}|\mathcal{C}_k) \in [0, 1] \quad (1)$$

- $\mathbf{x} \in \mathbb{R}^m$ is a feature vector, e. g. # black pixels, height-width ratio, ...



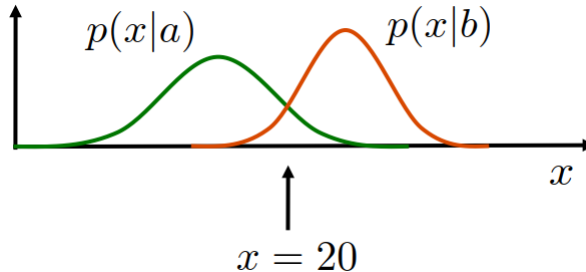
Class Conditional Probabilities (Ctd.)



If $x = 15$ we would predict class a , since $p(15|a) > p(15|b)$.

If $x = 25$ we would output class b , since $p(25|b) > p(25|a)$.

Class Conditional Probabilities (Ctd.)



We have a problem!

- Which class should be chosen now?
- The conditional probabilities are the same... ☠

Class Prior Probabilities

- Second concept: **Class priors**
- The prior probability of a data point belonging to a particular class \mathcal{C}_k

$$\mathcal{C}_1 \equiv a \quad p(\mathcal{C}_1) = 0.75$$

$$\mathcal{C}_2 \equiv b \quad p(\mathcal{C}_2) = 0.25$$

- By definition:

How would you decide now?

- $0 \leq p(\mathcal{C}_k) \leq 1, \forall k$
- The sum of all probabilities equals one: $\sum_{k=1}^{|\mathcal{C}|} p(\mathcal{C}_k) = 1$

- **The class prior is equivalent to a prior belief in the class label**

How to get the Prior Probabilities?

Count Count's advice:

Simply count the
number of instances
in each class!



Bayes' Theorem

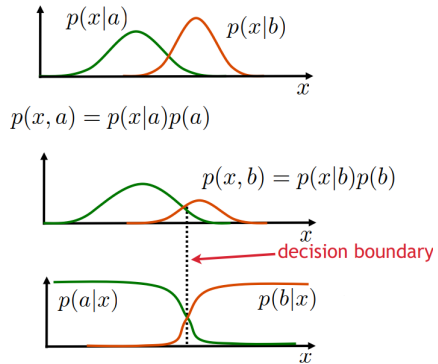
- What we actually want to compute: $p(\mathcal{C}_k|\mathbf{x}) \Rightarrow$ **Posterior probability**
- We can compute it by applying **Bayes' theorem**
- This is one of the **most important formulas (!!!)**

$$\begin{array}{c} \text{Class posterior} \\ \overbrace{p(\mathcal{C}_k|\mathbf{x})} \end{array} = \frac{\overbrace{p(\mathbf{x}|\mathcal{C}_k)}^{\text{Class cond.}} \cdot \overbrace{p(\mathcal{C}_k)}^{\text{Class prior}}}{\underbrace{p(\mathbf{x})}_{\text{Normalization term}}} = \frac{p(\mathbf{x}|\mathcal{C}_k) \cdot p(\mathcal{C}_k)}{\sum_{j=1}^{|\mathcal{C}|} p(\mathbf{x}|\mathcal{C}_j) \cdot p(\mathcal{C}_j)} \quad (2)$$

Calculation of the Posterior Probability

- By applying Bayes' theorem we can compute the posterior
- Simply plug ❶ and ❷ into Bayes' theorem
 - ❶ Class prior probabilities
 - ❷ Class conditional probabilities

We get the final **decision boundary**



a Priori vs. a Posteriori

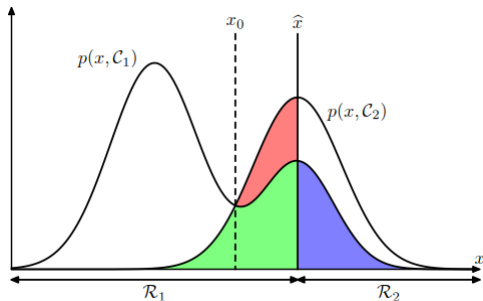
a Priori

A **belief** or conclusion **based on assumptions** or reasoning of some sort rather than actual experience or empirical evidence. Before actually encountering, experiencing, or observing a fact.

a Posteriori

A fact, belief, or argument that is **based on actual experience**, experiment, or observation.

Error Minimization



$$p(\text{error}) = p(x \in \mathcal{R}_1, \mathcal{C}_2) + p(x \in \mathcal{R}_2, \mathcal{C}_1)$$

$$= \overbrace{\int_{\mathcal{R}_1} p(x|\mathcal{C}_2) \cdot p(\mathcal{C}_2) dx}^{\text{red + green area}} + \underbrace{\int_{\mathcal{R}_2} p(x|\mathcal{C}_1) \cdot p(\mathcal{C}_1) dx}_{\text{blue area}}$$

Bayes' optimal Classifier

- Decision rule:
 - Decide \mathcal{C}_1 , if $p(\mathcal{C}_1|\mathbf{x}) > p(\mathcal{C}_2|\mathbf{x})$
 - This is equivalent to: *(we don't need the normalization)*

$$p(\mathbf{x}|\mathcal{C}_1) \cdot p(\mathcal{C}_1) > p(\mathbf{x}|\mathcal{C}_2) \cdot p(\mathcal{C}_2) \quad (3)$$

- Which is in turn equivalent to:

$$\frac{p(\mathbf{x}|\mathcal{C}_1)}{p(\mathbf{x}|\mathcal{C}_2)} > \frac{p(\mathcal{C}_2)}{p(\mathcal{C}_1)} \quad (4)$$

- A classifier obeying this rule is called **Bayes' optimal Classifier**

Section:
Naïve Bayes Classifier



A naïve Assumption

- We want to compute $p(\mathcal{C}_k|\mathbf{x})$. Recall Bayes' theorem:

Our first classification algorithm!

$$p(\mathcal{C}_k|\mathbf{x}) = \frac{p(\mathbf{x}|\mathcal{C}_k) \cdot p(\mathcal{C}_k)}{p(\mathbf{x})} \quad (5)$$

- Assumptions:
 - All features x_j are **pairwise conditionally independent** (\Rightarrow naïve)

$$p(\mathbf{x}|\mathcal{C}_k) = p(x_1|\mathcal{C}_k) \cdot p(x_2|\mathcal{C}_k, x_1) \cdot p(x_3|\mathcal{C}_k, x_1, x_2) \cdot \dots = \prod_{j=1}^m p(x_j|\mathcal{C}_k) \quad (6)$$

- $p(\mathbf{x})$ is constant w. r. t. class label \Rightarrow **It is omitted**

How to get the most probable Class?

- **Given:**
 - New instance $\mathbf{x} = \langle x_1, x_2, \dots, x_m \rangle$ to be classified
 - Finite set of κ classes $\{\mathcal{C}_1, \mathcal{C}_2, \dots, \mathcal{C}_\kappa\}$
 - **Labeled** training data (\Rightarrow supervised learning)
- **Wanted:** Most probable class \mathcal{C}_{MAP} (maximum a posteriori) for \mathbf{x} :

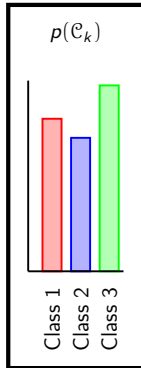
$$\mathcal{C}_{MAP} = \arg \max_{\mathcal{C}_k \in \{\mathcal{C}_1, \dots, \mathcal{C}_\kappa\}} \hat{p}(\mathcal{C}_k | \mathbf{x}) \quad (7)$$

\hat{p} denotes an
approximated probability

$$= \arg \max_{\mathcal{C}_k \in \{\mathcal{C}_1, \dots, \mathcal{C}_\kappa\}} \hat{p}(\mathcal{C}_k) \prod_{j=1}^m \hat{p}(x_j | \mathcal{C}_k) \quad (8)$$

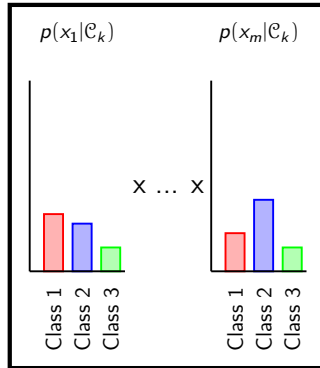
How to get the most probable Class? (Ctd.)

Apriori Probabilities



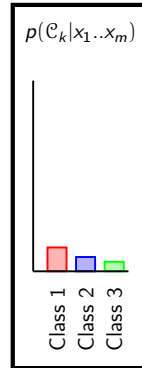
x

Feature Contributions



Aposteriori Probabilities

=



Example Data Set

Outlook	Temperature	Humidity	Wind	PlayGolf
sunny	hot	high	weak	no
sunny	hot	high	strong	no
overcast	hot	high	weak	yes
rainy	mild	high	weak	yes
rainy	cool	normal	weak	yes
rainy	cool	normal	strong	no
overcast	cool	normal	strong	yes
sunny	mild	high	weak	no
sunny	cool	normal	weak	yes
rainy	mild	normal	weak	yes
sunny	mild	normal	strong	yes
overcast	mild	high	strong	yes
overcast	hot	normal	weak	yes
rainy	mild	high	strong	no
sunny	cool	high	strong	???

How to estimate the Probabilities?

- How to estimate the probabilities $\hat{p}(\mathcal{C}_k)$ and $\hat{p}(x_j|\mathcal{C}_k)$?
- **Solution:** Simply count the occurrences



$$\hat{p}(\mathcal{C}_k) = \frac{\sum_{i=1}^n \mathbb{1}\{y^{(i)} = \mathcal{C}_k\}}{n} \quad (9)$$

$$\hat{p}(x_j = v|\mathcal{C}_k) = \frac{\sum_{i=1}^n \mathbb{1}\{x_j^{(i)} = v \wedge y^{(i)} = \mathcal{C}_k\}}{\sum_{i=1}^n \mathbb{1}\{y^{(i)} = \mathcal{C}_k\}} \quad (10)$$

- $\mathbb{1}\{bool\}$ is the **indicator function**
 (returns 1, if *bool* is true, 0 otherwise. E. g.: $\mathbb{1}\{1 + 1 = 2\} = 1$, $\mathbb{1}\{3 = 2\} = 0$)

Let's compute some Probabilities

- New instance $\mathbf{x} = \langle \text{sunny}, \text{cool}, \text{high}, \text{strong} \rangle$
- What is its class?
- Let's compute some of the probabilities needed:

$$\hat{p}(\text{Golf} = \text{yes}) = 9/14 = 0.64$$

$$\hat{p}(\text{Golf} = \text{no}) = 5/14 = 0.36$$

$$\hat{p}(\text{Outlook} = \text{sunny} | \text{Golf} = \text{yes}) = 2/9 = 0.22$$

$$\hat{p}(\text{Outlook} = \text{sunny} | \text{Golf} = \text{no}) = 3/5 = 0.60$$

...

Class Prediction

$$\begin{aligned}\hat{p}(\text{yes}|\mathbf{x}) &= \overbrace{\hat{p}(\text{sunny}|\text{yes})}^{=0.22} \cdot \overbrace{\hat{p}(\text{cool}|\text{yes}) \cdot \hat{p}(\text{high}|\text{yes}) \cdot \hat{p}(\text{strong}|\text{yes})}^{\text{calculate probabilities accordingly}} \cdot \overbrace{\hat{p}(\text{yes})}^{=0.64} \\ &= 0.0053\end{aligned}$$

$$\begin{aligned}\hat{p}(\text{no}|\mathbf{x}) &= \overbrace{\hat{p}(\text{sunny}|\text{no})}^{=0.60} \cdot \overbrace{\hat{p}(\text{cool}|\text{no}) \cdot \hat{p}(\text{high}|\text{no}) \cdot \hat{p}(\text{strong}|\text{no})}^{\text{calculate probabilities accordingly}} \cdot \overbrace{\hat{p}(\text{no})}^{=0.36} \\ &= 0.0206\end{aligned}$$

Classification: $\mathcal{C}_{MAP} = \text{no}$ (no golf today...)

Scaling the Output

- **But wait!** These probabilities don't sum up to one!?!?
- This is because we dropped the normalization term $p(\mathbf{x})$
- **Scaling** can fix this:

$$\hat{p}(\text{yes}|\mathbf{x})_{\text{norm}} = \frac{0.0053}{0.0053 + 0.0206} = 0.205$$

$$\hat{p}(\text{no}|\mathbf{x})_{\text{norm}} = \frac{0.0206}{0.0053 + 0.0206} = 0.795$$

- Scaling does **not** change the prediction

Laplace Smoothing

- **Problem:** A feature value v^* in the test data not seen during training
- $\hat{p}(v^*|\mathcal{C}_k) = 0$: The whole product becomes zero...
- **Solution:** **Laplace smoothing**

$$\hat{p}(\mathcal{C}_k) = \frac{\sum_{i=1}^n \mathbb{1}\{y^{(i)} = \mathcal{C}_k\} + 1}{n + \kappa} \quad (11)$$

$$\hat{p}(x_j = v|\mathcal{C}_k) = \frac{\sum_{i=1}^n \mathbb{1}\{x_j^{(i)} = v \wedge y^{(i)} = \mathcal{C}_k\} + 1}{\sum_{i=1}^n \mathbb{1}\{y^{(i)} = \mathcal{C}_k\} + \kappa} \quad (12)$$

Section:
Risk Minimization



Error \neq Risk

- So far, we have tried to minimize the misclassification rate
- Nevertheless, there are cases where not every misclassification is equally bad
- Some classical examples:
 - **Smoke detector**
 - If there is a fire, we must make sure to detect it
 - If there is not, an occasional false alarm may be acceptable
 - **Medical diagnosis**
 - If the patient is sick, we have to detect the disease
 - If they are healthy, it can be okay to classify them as sick (order further tests)
- **Minimizing the error is not necessarily equal to minimizing the risk**

Loss Functions

- **Key idea:** We have to create a loss function which expresses what we want:

$$\begin{aligned} \text{loss}(\text{decision} = \text{healthy} \mid \text{patient} = \text{sick}) &\gg \\ \text{loss}(\text{decision} = \text{sick} \mid \text{patient} = \text{healthy}) \end{aligned}$$

- We can decide for one of the κ possible classes...
- ...and we have a loss function $\ell(\mathcal{C}_i|\mathcal{C}_k)$ which returns the cost for deciding for \mathcal{C}_i given \mathcal{C}_k (**depends on the weighting of false positives and false negatives**)
- Expected loss (risk) of making a decision for class \mathcal{C}_i :

$$R(\mathcal{C}_i|\mathbf{x}) = \sum_k \ell(\mathcal{C}_i|\mathcal{C}_k)p(\mathcal{C}_k|\mathbf{x}) \quad (13)$$

Risk Minimization

- Consider two classes: \mathcal{C}_1 and \mathcal{C}_2
- Therefore, we have two possibilities: Deciding for class \mathcal{C}_1 or class \mathcal{C}_2
- Let ℓ_{ik} be a shorthand notation for $\ell(\mathcal{C}_i|\mathcal{C}_k)$
- Risk of both decisions:

$$R(\mathcal{C}_1|\mathbf{x}) = \ell_{11}p(\mathcal{C}_1|\mathbf{x}) + \ell_{12}p(\mathcal{C}_2|\mathbf{x})$$

$$R(\mathcal{C}_2|\mathbf{x}) = \ell_{21}p(\mathcal{C}_1|\mathbf{x}) + \ell_{22}p(\mathcal{C}_2|\mathbf{x})$$

- **Goal:** Create a decision rule so that the overall risk is minimized
- Decide for \mathcal{C}_1 , iff $R(\mathcal{C}_2|\mathbf{x}) > R(\mathcal{C}_1|\mathbf{x})$

Risk Minimization (Ctd.)

$$R(\mathcal{C}_2|\mathbf{x}) > R(\mathcal{C}_1|\mathbf{x})$$

$$\ell_{21}p(\mathcal{C}_1|\mathbf{x}) + \ell_{22}p(\mathcal{C}_2|\mathbf{x}) > \ell_{11}p(\mathcal{C}_1|\mathbf{x}) + \ell_{12}p(\mathcal{C}_2|\mathbf{x})$$

$$(\ell_{21} - \ell_{11})p(\mathcal{C}_1|\mathbf{x}) > (\ell_{12} - \ell_{22})p(\mathcal{C}_2|\mathbf{x})$$

$$\frac{\ell_{21} - \ell_{11}}{\ell_{12} - \ell_{22}} > \frac{p(\mathcal{C}_2|\mathbf{x})}{p(\mathcal{C}_1|\mathbf{x})} = \frac{p(\mathbf{x}|\mathcal{C}_2)p(\mathcal{C}_2)}{p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1)}$$

$$\frac{p(\mathbf{x}|\mathcal{C}_1)}{p(\mathbf{x}|\mathcal{C}_2)} > \frac{\ell_{12} - \ell_{22}}{\ell_{21} - \ell_{11}} \frac{p(\mathcal{C}_2)}{p(\mathcal{C}_1)}$$

It is reasonable to assume that **the loss of a correct decision is smaller than that of a wrong decision**:

$$\ell_{ik} > \ell_{ii} \quad \forall k \neq i$$

Risk Minimization 0-1 Loss

$$\frac{p(\mathbf{x}|\mathcal{C}_1)}{p(\mathbf{x}|\mathcal{C}_2)} > \frac{\ell_{12} - \ell_{22}}{\ell_{21} - \ell_{11}} \frac{p(\mathcal{C}_2)}{p(\mathcal{C}_1)}$$

- **0-1 loss:** Decide for \mathcal{C}_1 , if:

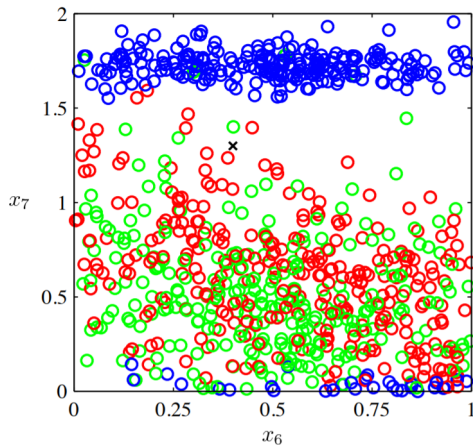
$$\frac{p(\mathbf{x}|\mathcal{C}_1)}{p(\mathbf{x}|\mathcal{C}_2)} > \frac{p(\mathcal{C}_2)}{p(\mathcal{C}_1)} \quad \text{with} \quad \ell(\mathcal{C}_i|\mathcal{C}_k) = \begin{cases} 0 & i = k \\ 1 & i \neq k \end{cases} \quad (14)$$

- **0-1 loss leads to the same decision rule which minimizes the misclassification rate**

Are we done?

- **Question:** Are we done with classification?
 - We have decision rules for simple and general loss functions
 - They are even **Bayes' optimal**
 - We can deal with two or more classes
 - We can deal with high dimensional feature vectors
 - We can incorporate prior knowledge about the class distribution
- We have seen how to get the probabilities for the discrete case (cf. naïve Bayes classifier)
- **But: What about continuous data?**

Continuous Data



Section:
Wrap-Up



Summary

- Statistical methods assume that the process that ‘generates’ the data is **governed by the rules of probability**
- We need class **conditional probabilities** and **class priors**
- Use **Bayes’ theorem** to get the **class posteriors**
- **Bayes’ optimal classifier**: Decide for the most probable class
- Naïve Bayes assumes all **features to be pairwise conditionally independent**
- **Error minimization is not equal to risk minimization**



Self-Test Questions

- 1 What are class conditional probabilities?
- 2 What does *Bayes optimal* mean?
- 3 How can we incorporate prior knowledge about the class distribution into the classification?
- 4 What is the naïve assumption which naïve Bayes makes? When is this a problem?
- 5 Explain what maximum a posteriori is!
- 6 What is misclassification and risk? Are they the same?

What's next...?

Unit I	Machine Learning Introduction
Unit II	Mathematical Foundations
Unit III	Bayesian Decision Theory
Unit IV	Probability Density Estimation
Unit V	Regression
Unit VI	Classification I
Unit VII	Evaluation
Unit VIII	Classification II
Unit IX	Clustering
Unit X	Dimensionality Reduction

Recommended Literature and further Reading I

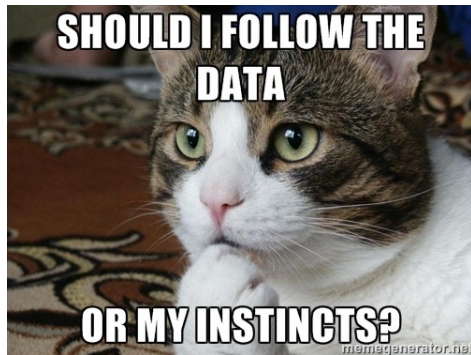


[1] Pattern Recognition and Machine Learning

Christopher Bishop. Springer. 2006.

→ [Link](#), cf. chapter 1.5

Meme of the Day



Thank you very much for the attention!

Topic: *** Applied Machine Learning Fundamentals *** Bayesian Decision Theory

Term: Winter term 2021/2022

Contact:

Daniel Wehner, M.Sc.

SAP SE / DHBW Mannheim

daniel.wehner@sap.com

Do you have any questions?