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

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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
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Agenda for this Unit

Section:

Bayesian Decision Theory

Bayesian Decision Theory
Naïve Bayes Classifier
Risk Minimization
Wrap-Up

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

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!

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Running Example: Optical Character Recognition (OCR)
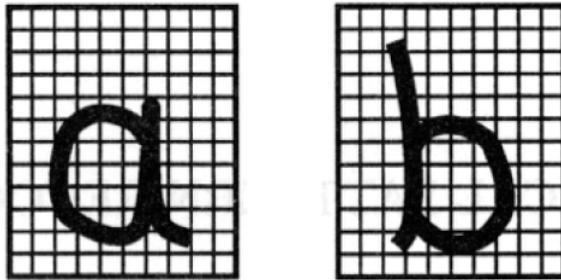
Goal: Classify a new letter so that the probability of a wrong classification is minimized

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Class Conditional Probabilities

- First concept: **Class conditional probabilities**

- Probability of x given a specific class $\mathcal{C}_k$ is formally written as:

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

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

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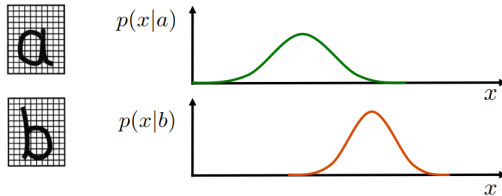
Class Conditional Probabilities (Ctd.)
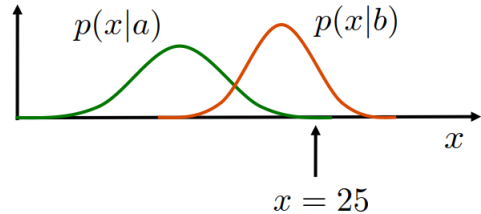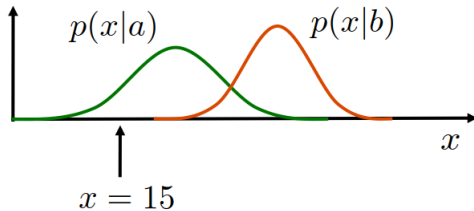
If $x = 15$ we would predict class a, since $p(15|a) > p(15|b)$.

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

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Class Conditional Probabilities (Ctd.)

$p(x|a)$ $\qquad$ $p(x|b)$

We have a problem!

x

$x = 20$
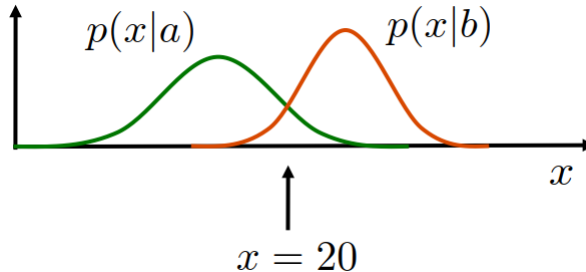
- **Which class should be chosen now?**
- The conditional probabilities are the same... ☠

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Class Prior Probabilities

- Second concept: **Class priors**

- The prior probability of a data point belonging to a particular class $\mathcal{C}_k$

$$\mathcal{C}_1 \equiv a \qquad p(\mathcal{C}_1) = 0.75$$
$$\mathcal{C}_2 \equiv b \qquad p(\mathcal{C}_2) = 0.25$$

- By definition:

  How would you decide now?

  - $0 \leqslant p(\mathcal{C}_k) \leqslant 1, \ \forall k$
  - 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**

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How to get the Prior Probabilities?

Count Count's advice:

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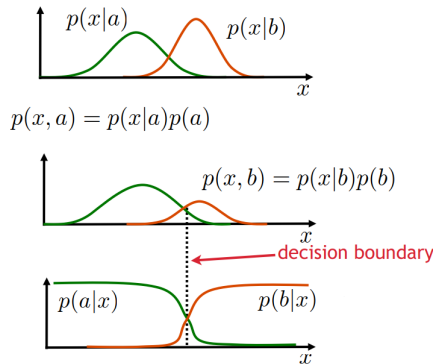
Important

Bayes' Theorem

- What we actually want to compute: $p(\mathcal{C}_k|\boldsymbol{x}) \Rightarrow$ **Posterior probability**

- We can compute it by applying **Bayes' theorem**

- This is one of the **most important formulas (!!!)**

$$
\overbrace{p(\mathcal{C}_k|\boldsymbol{x})}^{\textbf{Class posterior}} = \frac{\overbrace{p(\boldsymbol{x}|\mathcal{C}_k)}^{\textbf{Class cond.}} \cdot \overbrace{p(\mathcal{C}_k)}^{\textbf{Class prior}}}{\underbrace{p(\boldsymbol{x})}_{\textbf{Normalization term}}} = \frac{p(\boldsymbol{x}|\mathcal{C}_k) \cdot p(\mathcal{C}_k)}{\sum_{j=1}^{|\mathcal{C}|} p(\boldsymbol{x}|\mathcal{C}_j) \cdot p(\mathcal{C}_j)} \qquad (2)
$$

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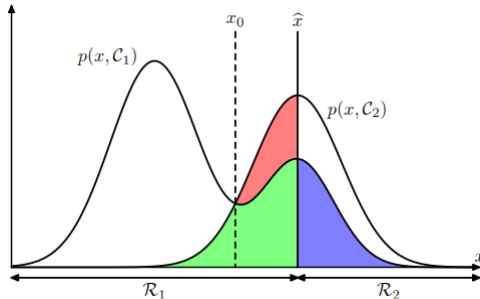# Calculation of the Posterior Probability

- 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**

$p(x|a)$ $p(x|b)$

x

$p(x, a) = p(x|a)p(a)$

$p(x, b) = p(x|b)p(b)$

x

decision boundary

$p(a|x)$ $p(b|x)$

x

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Error Minimization

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

$$\overbrace{\qquad\qquad\qquad\qquad}^{\text{red + green area}}$$

$$= \int_{\mathcal{R}_1} p(x|\mathcal{C}_2) \cdot p(\mathcal{C}_2) \, dx \; +$$

$$\underbrace{\int_{\mathcal{R}_2} p(x|\mathcal{C}_1) \cdot p(\mathcal{C}_1) \, dx}_{\text{blue area}}$$

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Bayes' optimal Classifier

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

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

  - Which is in turn equivalent to:

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

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

Section:

Naïve Bayes Classifier

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Assumptions and Algorithm
An Example
Laplace Smoothing

A naïve Assumption

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

Our first classification algorithm!

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

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

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

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

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How to get the most probable Class?

- **Given**:
  - New instance $\boldsymbol{x} = \langle x_1, x_2, \ldots, x_m \rangle$ to be classified
  - Finite set of κ classes $\{\mathcal{C}_1, \mathcal{C}_2, \ldots, \mathcal{C}_\kappa\}$
  - Labeled training data ($\Rightarrow$ supervised learning)

- **Wanted**: Most probable class $\mathcal{C}_{MAP}$ (maximum aposteriori) for $\boldsymbol{x}$:

$$\mathcal{C}_{MAP} = \underset{\mathcal{C}_k \in \{\mathcal{C}_1, \ldots, \mathcal{C}_\kappa\}}{\arg\max} \widehat{p}(\mathcal{C}_k | \boldsymbol{x}) \tag{7}$$

$$= \underset{\mathcal{C}_k \in \{\mathcal{C}_1, \ldots, \mathcal{C}_\kappa\}}{\arg\max} \widehat{p}(\mathcal{C}_k) \prod_{j=1}^{m} \widehat{p}(x_j | \mathcal{C}_k) \tag{8}$$
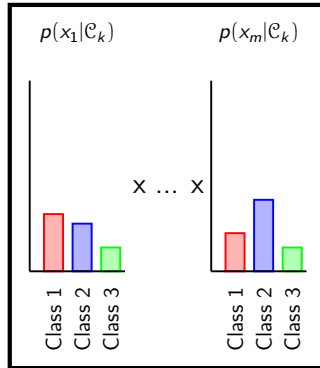
$\widehat{p}$ denotes an
approximated probability

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

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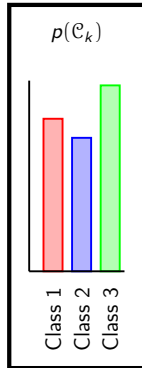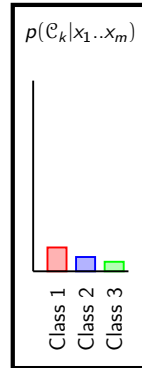
Example Data Set

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	**???**

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How to estimate the Probabilities?

- How to estimate the probabilities $\widehat{p}(\mathcal{C}_k)$ and $\widehat{p}(x_j|\mathcal{C}_k)$?

- **Solution**: Simply count the occurrences

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

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

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

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Let's compute some Probabilities

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

$$\widehat{p}(Golf = yes) = {}^9/{}_{14} = 0.64$$

$$\widehat{p}(Golf = no) = {}^5/{}_{14} = 0.36$$

$$\widehat{p}(Outlook = sunny | Golf = yes) = {}^2/{}_9 = 0.22$$

$$\widehat{p}(Outlook = sunny | Golf = no) = {}^3/{}_5 = 0.60$$

$$\ldots$$

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Class Prediction

$$\widehat{p}(yes|\boldsymbol{x}) = \overbrace{\widehat{p}(sunny|yes)}^{=0.22} \cdot \overbrace{\widehat{p}(cool|yes) \cdot \widehat{p}(high|yes) \cdot \widehat{p}(strong|yes)}^{\text{calculate probabilities accordingly}} \cdot \overbrace{\widehat{p}(yes)}^{=0.64}$$

$$= 0.0053$$

$$\widehat{p}(no|\boldsymbol{x}) = \underbrace{\widehat{p}(sunny|no)}_{=0.60} \cdot \underbrace{\widehat{p}(cool|no) \cdot \widehat{p}(high|no) \cdot \widehat{p}(strong|no)}_{\text{calculate probabilities accordingly}} \cdot \underbrace{\widehat{p}(no)}_{=0.36}$$

$$= 0.0206$$

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

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Scaling the Output

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

$$\widehat{p}(yes|\boldsymbol{x})_{norm} = \frac{0.0053}{0.0053 + 0.0206} = 0.205$$

$$\widehat{p}(no|\boldsymbol{x})_{norm} = \frac{0.0206}{0.0053 + 0.0206} = 0.795$$

- Scaling does **not** change the prediction

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Laplace Smoothing

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

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

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

Section:
Risk Minimization

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Error ≠ Risk
Loss Functions for Risk Minimization
Handling of continuous Data

Error ≠ 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**

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Loss Functions

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

$$\text{loss(decision = healthy } | \text{ patient = sick)} \gg$$

$$\text{loss(decision = sick } | \text{ patient = healthy)}$$

- 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 $\mathcal{C}_i$:

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

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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:

$$R(\mathcal{C}_1|\boldsymbol{x}) = \ell_{11}p(\mathcal{C}_1|\boldsymbol{x}) + \ell_{12}p(\mathcal{C}_2|\boldsymbol{x})$$
$$R(\mathcal{C}_2|\boldsymbol{x}) = \ell_{21}p(\mathcal{C}_1|\boldsymbol{x}) + \ell_{22}p(\mathcal{C}_2|\boldsymbol{x})$$

- **Goal**: Create a decision rule so that the overall risk is minimized

- Decide for $\mathcal{C}_1$, iff $R(\mathcal{C}_2|\boldsymbol{x}) > R(\mathcal{C}_1|\boldsymbol{x})$

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Risk Minimization (Ctd.)

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

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

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

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

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

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

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

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Risk Minimization 0-1 Loss

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

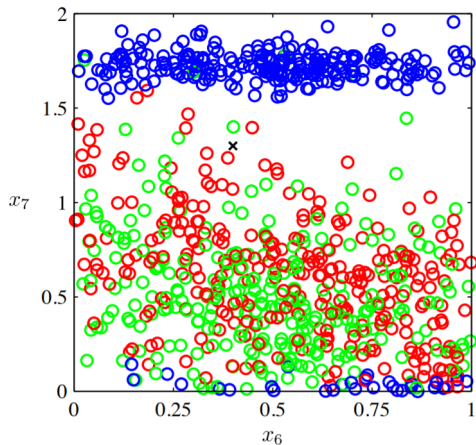- **0-1 loss:** Decide for $\mathcal{C}_1$, if:

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

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

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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?

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Continuous Data

Section:

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Recommended Literature and further Reading
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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**

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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 aposteriori is!

6. What is misclassification and risk? Are they the same?

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Recommended Literature and further Reading I

📕 **[1] Pattern Recognition and Machine Learning**
Christopher Bishop. Springer. 2006.
→ <u>Link</u>, cf. chapter 1.5

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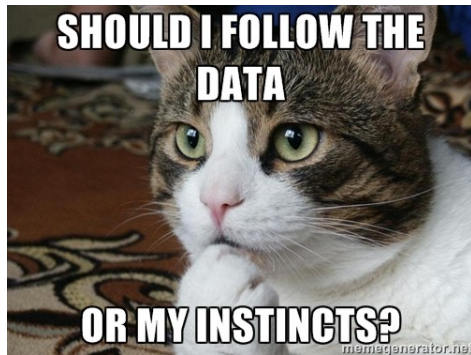
Thank you very much for the attention!

Topic: *** Applied Machine Learning Fundamentals *** Bayesian Decision Theory
Term: Winter term 2020/2021

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Do you have any questions?