

Machine Learning - Lecture 1

Introduction

18.04.2016

Bastian Leibe

RWTH Aachen

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Many slides adapted from B. Schiele



Organization

Lecturer

Prof. Bastian Leibe (<u>leibe@vision.rwth-aachen.de</u>)

Assistants

- Alexander Hermans (<u>hermans@vision.rwth-aachen.de</u>)
- Aljosa Osep (osep@vision.rwth-aachen.de)

Course webpage

- http://www.vision.rwth-aachen.de/teaching/
- Slides will be made available on the webpage
- There is also an L2P electronic repository
- Please subscribe to the lecture on the Campus system!
 - Important to get email announcements and L2P access!



Language

- Official course language will be English
 - If at least one English-speaking student is present.
 - If not... you can choose.

However...

- Please tell me when I'm talking too fast or when I should repeat something in German for better understanding!
- You may at any time ask questions in German!
- You may turn in your exercises in German.
- You may answer exam questions in German.



Organization

- Structure: 3V (lecture) + 1Ü (exercises)
 - 6 EECS credits
 - Part of the area "Applied Computer Science"
- Place & Time

> Lecture: Mon 16:15 - 17:45 room UMIC 025

Lecture/Exercises: Tue 16:15 - 17:45 room UMIC 025

- Exam
 - Written exam

> 1st Try Thu 18.08. 14:00 - 17:30

> 2nd Try Fri 16.09. 14:00 - 17:30

Exercises and Supplementary Material

Exercises

- Typically 1 exercise sheet every 2 weeks.
- Pen & paper and Matlab based exercises
- Hands-on experience with the algorithms from the lecture.
- Send your solutions the night before the exercise class.
- Need to reach ≥ 50% of the points to qualify for the exam!

Teams are encouraged!

- You can form teams of up to 3 people for the exercises.
- Each team should only turn in one solution.
- But list the names of all team members in the submission.



Course Webpage

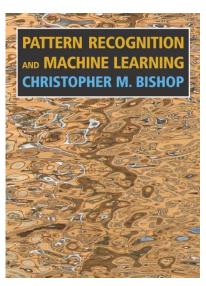
Course Schedule			
Date	Title	Content	Material
Mon, 2016-04-18	Introduction	Introduction, Probability Theory, Bayes Decision Theory, Minimizing Expected Loss	
Tue, 2016-04-19	Exercise 0	Intro Matlab	
Mon, 2016-04-25	Prob. Density Estimation I	Parametric Methods, Gaussian Distribution, Maximum Likelihood	Exercise
Mon, 2016-04-25	Prob. Density Estimation II	Bayesian Learning, Nonparametric Methods, Histograms, Kernel Density Estimation	on Tuesday
Tue, 2016-04-26	Prob. Density Estimation III	Mixture of Gaussians, k-Means Clustering, EM- Clustering, EM Algorithm	
Mon, 2016-05-02	Linear Discriminant Functions I	Linear Discriminant Functions, Least-squares Classification, Generalized Linear Models	
Mon, 2016-05-09	Exercise 1	Probability Density, GMM, EM	
Tue, 2016-05-10	Linear Discriminant Functions II	Fisher Linear Discriminants, Logistic Regression, Iteratively Reweighted Least Squares	
Thu, 2016-05-12	Linear SVMs	Linear SVMs, Soft-margin classifiers, nonlinear basis functions	

http://www.vision.rwth-aachen.de/teaching/



Textbooks

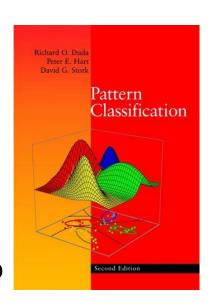
- Most lecture topics will be covered in Bishop's book.
- Some additional topics can be found in Duda & Hart.



Christopher M. Bishop Pattern Recognition and Machine Learning Springer, 2006

(available in the library's "Handapparat")

R.O. Duda, P.E. Hart, D.G. Stork Pattern Classification 2nd Ed., Wiley-Interscience, 2000



- Research papers will be given out for some topics.
 - Tutorials and deeper introductions.
 - Application papers



How to Find Us

Office:

- UMIC Research Centre
- Mies-van-der-Rohe-Strasse 15, room 124



Office hours

- If you have questions to the lecture, come to Alex or Aljosa.
- My regular office hours will be announced (additional slots are available upon request)
- Send us an email before to confirm a time slot.

Questions are welcome!



Machine Learning

Statistical Machine Learning

Principles, methods, and algorithms for learning and prediction on the basis of past evidence

Already everywhere

- Speech recognition (e.g. Siri)
- Computer vision (e.g. face detection)
- Hand-written character recognition (e.g. letter delivery)
- Information retrieval (e.g. image & video indexing)
- Operation systems (e.g. caching)
- Fraud detection (e.g. credit cards)
- Text filtering (e.g. email spam filters)
- Game playing (e.g. strategy prediction)
- Robotics (everywhere)

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Machine Learning

Goal

> Machines that learn to perform a task from experience

Why?

- Crucial component of every intelligent/autonomous system
- Important for a system's adaptability
- Important for a system's generalization capabilities
- Attempt to understand human learning



Learning to perform a task from experience

Learning

- Most important part here!
- We do not want to encode the knowledge ourselves.
- > The machine should learn the relevant criteria automatically from past observations and adapt to the given situation.

Tools

- Statistics
- Probability theory
- Decision theory
- Information theory
- Optimization theory

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Learning to perform a task from experience

- Task
 - > Can often be expressed through a mathematical function

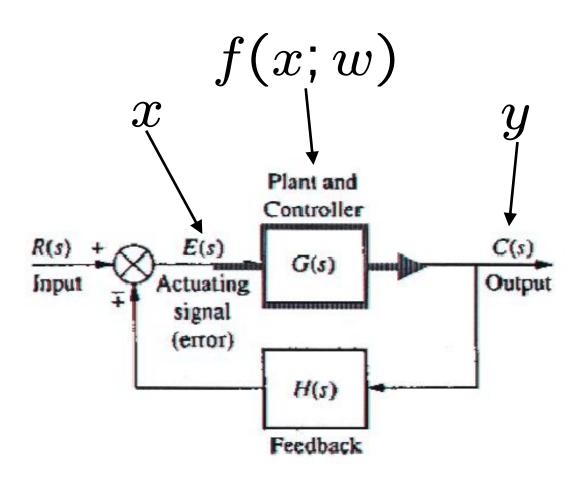
$$y = f(x; w)$$

- > x: Input
- > y: Output
- > w: Parameters (this is what is "learned")
- Classification vs. Regression
 - \triangleright Regression: continuous y
 - Classification: discrete y
 - E.g. class membership, sometimes also posterior probability



Example: Regression

Automatic control of a vehicle



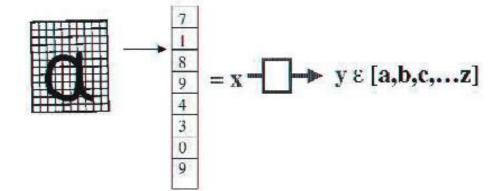


Examples: Classification

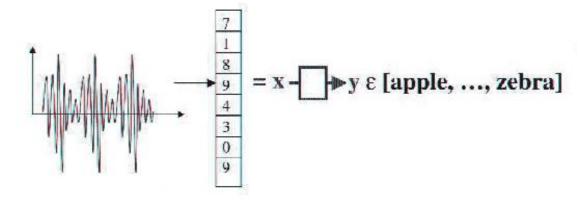
Email filtering

$$x \in [a-z]^+ \longrightarrow y \in [\text{important, spam}]$$

Character recognition



Speech recognition

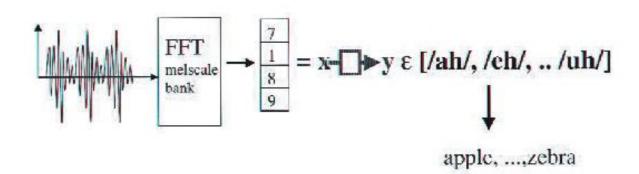


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Machine Learning: Core Problems

Input x:



Features

- Invariance to irrelevant input variations
- Selecting the "right" features is crucial
- Encoding and use of "domain knowledge"
- Higher-dimensional features are more discriminative.
- Curse of dimensionality
 - Complexity increases exponentially with number of dimensions.



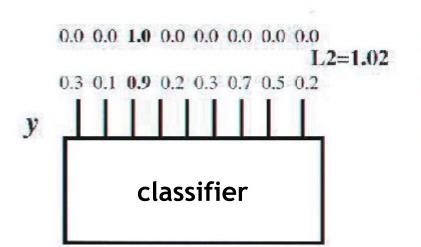
- Learning to perform a task from experience
- Performance: "99% correct classification"
 - Of what???
 - Characters? Words? Sentences?
 - Speaker/writer independent?
 - Over what data set?
 - **>** ...
- "The car drives without human intervention 99% of the time on country roads"

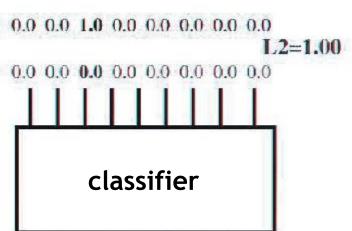


- Learning to perform a task from experience
- Performance measure: Typically one number
 - % correctly classified letters
 - Average driving distance (until crash...)
 - % games won
 - % correctly recognized words, sentences, answers
- Generalization performance
 - Training vs. test
 - "All" data



- Learning to perform a task from experience
- Performance measure: more subtle problem
 - Also necessary to compare partially correct outputs.
 - How do we weight different kinds of errors?
 - Example: L2 norm





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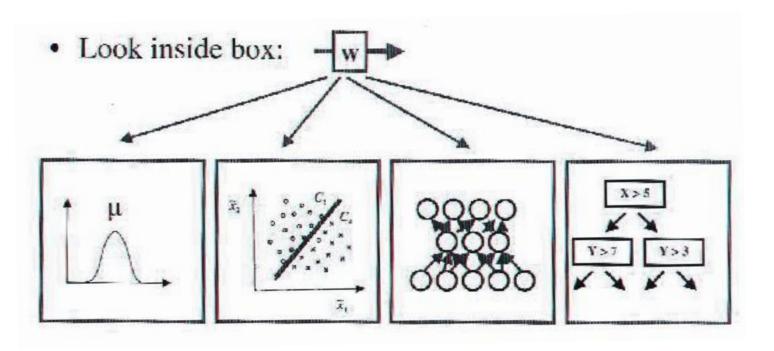
- Learning to perform a task from experience
- What data is available?
 - Data with labels: supervised learning
 - Images / speech with target labels
 - Car sensor data with target steering signal
 - Data without labels: unsupervised learning
 - Automatic clustering of sounds and phonemes
 - Automatic clustering of web sites
 - Some data with, some without labels: semi-supervised learning
 - No examples: learning by doing
 - Feedback/rewards: reinforcement learning

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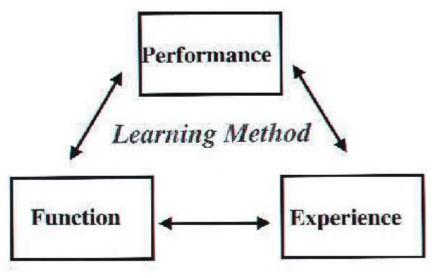


- y = f(x; w)
 - > w: characterizes the family of functions
 - > w: indexes the space of hypotheses
 - \rightarrow w: vector, connection matrix, graph, ...





- Learning to perform a task from experience
- Learning
 - Most often learning = optimization
 - Search in hypothesis space
 - ightarrow Search for the "best" function / model parameter w
 - I.e. maximize $y=f(x;w)\,$ w.r.t. the performance measure

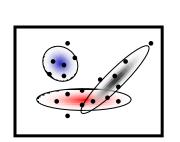


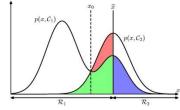
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Course Outline

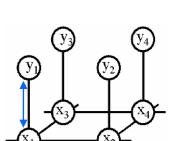
- Fundamentals (2 weeks)
 - Bayes Decision Theory
 - Probability Density Estimation





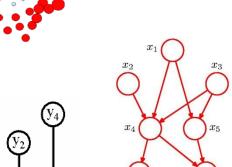


- Linear Discriminant Functions
- Support Vector Machines
- Ensemble Methods & Boosting
- Randomized Trees, Forests & Ferns
- Outlook: Deep Learning





- Bayesian Networks
- Markov Random Fields
- Probabilistic Inference





Topics of This Lecture

- (Re-)view: Probability Theory
 - Probabilities
 - Probability densities
 - Expectations and covariances
- Bayes Decision Theory
 - Basic concepts
 - Minimizing the misclassification rate
 - Minimizing the expected loss
 - Discriminant functions



Probability Theory



"Probability theory is nothing but common sense reduced to calculation."

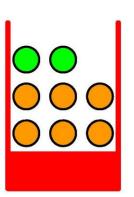
Pierre-Simon de Laplace, 1749-1827

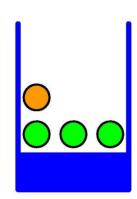
Image source: Wikipedia



Probability Theory

- Example: apples and oranges
 - We have two boxes to pick from.
 - > Each box contains both types of fruit.
 - What is the probability of picking an apple?





Formalization

- Let $B \in \{r, b\}$ be a random variable for the box we pick.
- Let $F \in \{a, o\}$ be a random variable for the type of fruit we get.
- > Suppose we pick the red box 40% of the time. We write this as

$$p(B = r) = 0.4$$

$$p(B=b) = 0.6$$

The probability of picking an apple *given* a choice for the box is $p(F = a \mid B = r) = 0.25$ $p(F = a \mid B = b) = 0.75$

What is the probability of picking an apple?

$$p(F = a) = ?$$

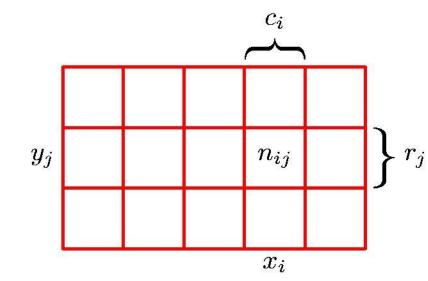
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Probability Theory

More general case

- > Consider two random variables $X \in \{x_i\}$ and $Y \in \{y_i\}$
- Consider N trials and let

$$n_{ij} = \#\{X = x_i \land Y = y_j\}$$
 $c_i = \#\{X = x_i\}$
 $r_j = \#\{Y = y_j\}$



Then we can derive

- > Joint probability
- Marginal probability
- Conditional probability

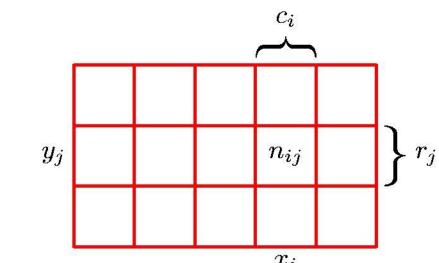
$$p(X = x_i, Y = y_j) = \frac{n_{ij}}{N}$$
$$p(X = x_i) = \frac{c_i}{N}.$$

$$p(Y = y_j | X = x_i) = \frac{n_{ij}}{c_i}$$

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Probability Theory



Rules of probability

> Sum rule

$$p(X = x_i) = \frac{c_i}{N} = \frac{1}{N} \sum_{i=1}^{L} n_{ij} = \sum_{i=1}^{L} p(X = x_i, Y = y_j)$$

> Product rule

$$p(X = x_i, Y = y_j) = \frac{n_{ij}}{N} = \frac{n_{ij}}{c_i} \cdot \frac{c_i}{N}$$
$$= p(Y = y_i | X = x_i) p(X = x_i)$$



The Rules of Probability

Thus we have

Sum Rule

$$p(X) = \sum_{Y} p(X, Y)$$

Product Rule

$$p(X,Y) = p(Y|X)p(X)$$

From those, we can derive

Bayes' Theorem
$$p(Y|X) = \frac{p(X|Y)p(Y)}{p(X)}$$

where

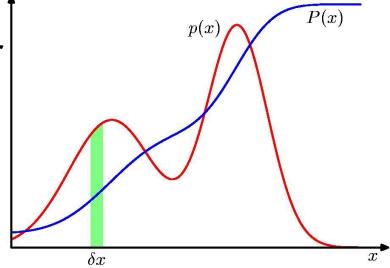
$$p(X) = \sum_{Y} p(X|Y)p(Y)$$



Probability Densities

• Probabilities over continuous variables are defined over their probability density function (pdf) p(x).

$$p(x \in (a,b)) = \int_a^b p(x) \, \mathrm{d}x$$



• The probability that x lies in the interval $(-\infty, z)$ is given by the cumulative distribution function

$$P(z) = \int_{-\infty}^{z} p(x) \, \mathrm{d}x$$



Expectations

• The average value of some function f(x) under a probability distribution p(x) is called its expectation

$$\mathbb{E}[f] = \sum_x p(x) f(x) \qquad \qquad \mathbb{E}[f] = \int p(x) f(x) \, \mathrm{d}x$$
 discrete case continuous case

• If we have a finite number N of samples drawn from a pdf, then the expectation can be approximated by

$$\mathbb{E}[f] \simeq \frac{1}{N} \sum_{n=1}^{N} f(x_n)$$

We can also consider a conditional expectation

$$\mathbb{E}_{x}[f|y] = \sum_{\substack{x \\ \text{B. Leibe}}} p(x|y)f(x)$$



Variances and Covariances

• The variance provides a measure how much variability there is in f(x) around its mean value $\mathbb{E}[f(x)]$.

$$var[f] = \mathbb{E}\left[\left(f(x) - \mathbb{E}[f(x)]\right)^2\right] = \mathbb{E}[f(x)^2] - \mathbb{E}[f(x)]^2$$

 For two random variables x and y, the covariance is defined by

$$cov[x,y] = \mathbb{E}_{x,y} [\{x - \mathbb{E}[x]\} \{y - \mathbb{E}[y]\}]$$
$$= \mathbb{E}_{x,y} [xy] - \mathbb{E}[x]\mathbb{E}[y]$$

If x and y are vectors, the result is a covariance matrix

$$cov[\mathbf{x}, \mathbf{y}] = \mathbb{E}_{\mathbf{x}, \mathbf{y}} [\{\mathbf{x} - \mathbb{E}[\mathbf{x}]\} \{\mathbf{y}^{\mathrm{T}} - \mathbb{E}[\mathbf{y}^{\mathrm{T}}]\}]$$
$$= \mathbb{E}_{\mathbf{x}, \mathbf{y}} [\mathbf{x}\mathbf{y}^{\mathrm{T}}] - \mathbb{E}[\mathbf{x}] \mathbb{E}[\mathbf{y}^{\mathrm{T}}]$$





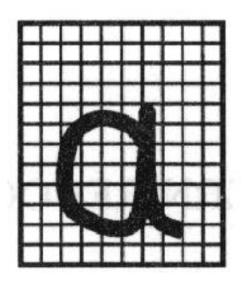
Thomas Bayes, 1701-1761

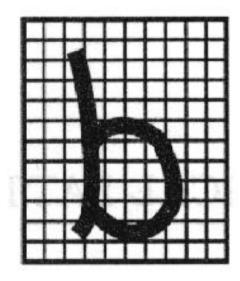
"The theory of inverse probability is founded upon an error, and must be wholly rejected."

R.A. Fisher, 1925



Example: handwritten character recognition





- Goal:
 - Classify a new letter such that the probability of misclassification is minimized.

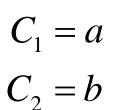


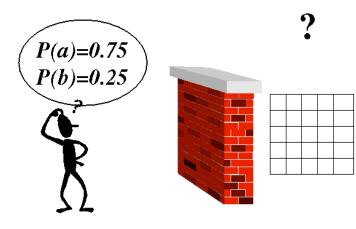
Concept 1: Priors (a priori probabilities)

$$p(C_k)$$

- > What we can tell about the probability before seeing the data.
- > Example:







$$p(C_1) = 0.75$$
$$p(C_2) = 0.25$$

• In general:
$$\sum_{k} p(C_k) = 1$$

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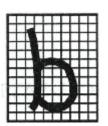


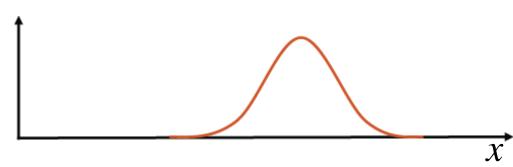
Concept 2: Conditional probabilities

 $p(x|C_k)$

- Let x be a feature vector.
- > x measures/describes certain properties of the input.
 - E.g. number of black pixels, aspect ratio, ...
- $p(x|C_k)$ describes its likelihood for class C_k .

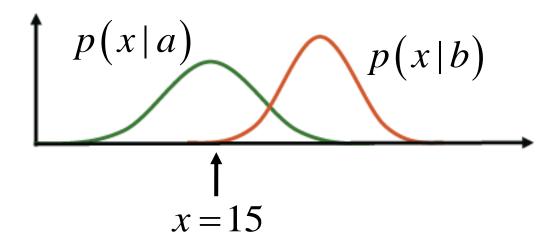








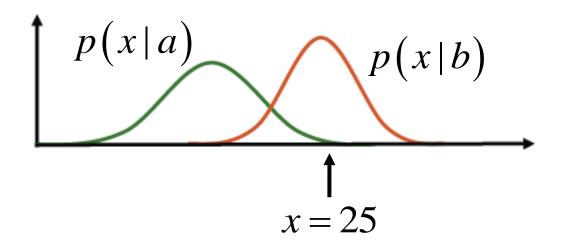
Example:



- Question:
 - Which class?
 - Since p(x|b) is much smaller than p(x|a), the decision should be 'a' here.



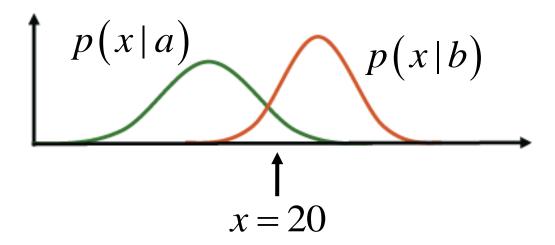
Example:



- Question:
 - Which class?
 - Since p(x|a) is much smaller than p(x|b), the decision should be 'b' here.



Example:



Question:

- Which class?
- > Remember that p(a) = 0.75 and p(b) = 0.25...
- I.e., the decision should be again 'a'.
- ⇒ How can we formalize this?



Concept 3: Posterior probabilities

$$p(C_k \mid x)$$

- We are typically interested in the *a posteriori* probability, i.e. the probability of class C_k given the measurement vector x.
- Bayes' Theorem:

$$p(C_k | x) = \frac{p(x | C_k) p(C_k)}{p(x)} = \frac{p(x | C_k) p(C_k)}{\sum_i p(x | C_i) p(C_i)}$$

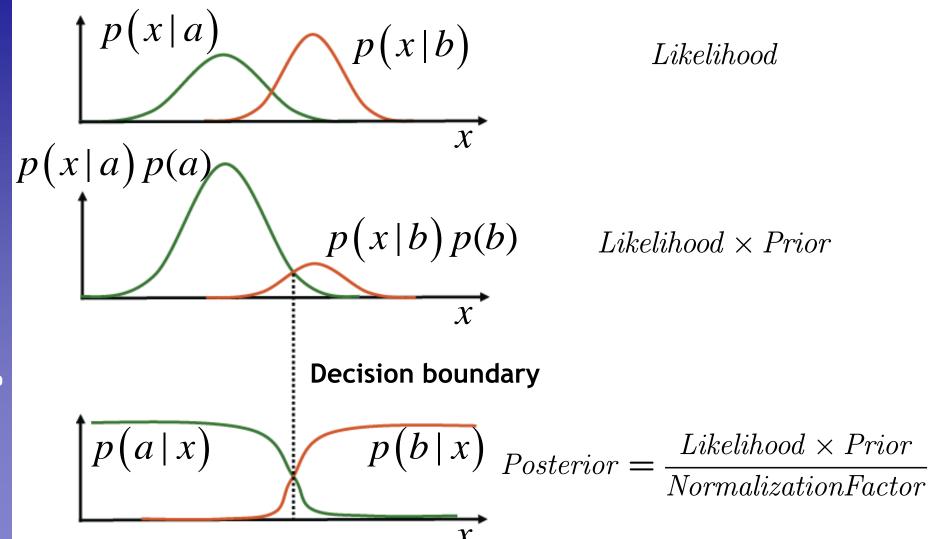
Interpretation

$$Posterior = \frac{Likelihood \times Prior}{Normalization \ Factor}$$

Slide credit: Bernt Schiele



Bayes Decision Theory

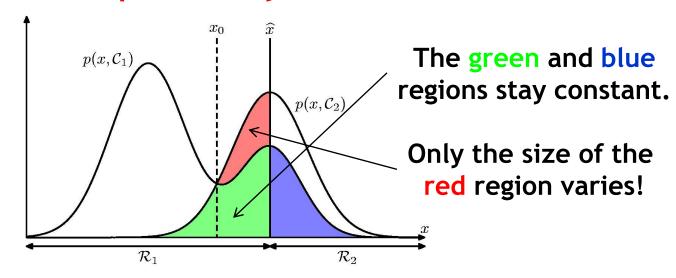


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Goal: Minimize the probability of a misclassification



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

$$= \int_{\mathcal{R}_1} p(\mathbf{x}, \mathcal{C}_2) d\mathbf{x} + \int_{\mathcal{R}_2} p(\mathbf{x}, \mathcal{C}_1) d\mathbf{x}.$$

$$= \int_{\mathcal{R}_1} p(\mathcal{C}_2 | \mathbf{x}) p(\mathbf{x}) d\mathbf{x} + \int_{\mathcal{R}_2} p(\mathcal{C}_1 | \mathbf{x}) p(\mathbf{x}) d\mathbf{x}$$

Image source: C.M. Bishop, 2006



- Optimal decision rule
 - ▶ Decide for C₁ if

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

> This is equivalent to

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

Which is again equivalent to (Likelihood-Ratio test)

$$\frac{p(x|\mathcal{C}_1)}{p(x|\mathcal{C}_2)} > \underbrace{\frac{p(\mathcal{C}_2)}{p(\mathcal{C}_1)}}$$

Decision threshold θ



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Generalization to More Than 2 Classes

Decide for class k whenever it has the greatest posterior probability of all classes:

$$p(\mathcal{C}_k|x) > p(\mathcal{C}_j|x) \quad \forall j \neq k$$

$$p(x|\mathcal{C}_k)p(\mathcal{C}_k) > p(x|\mathcal{C}_j)p(\mathcal{C}_j) \quad \forall j \neq k$$

Likelihood-ratio test

$$\frac{p(x|\mathcal{C}_k)}{p(x|\mathcal{C}_j)} > \frac{p(\mathcal{C}_j)}{p(\mathcal{C}_k)} \quad \forall j \neq k$$



Classifying with Loss Functions

- Generalization to decisions with a loss function
 - Differentiate between the possible decisions and the possible true classes.
 - Example: medical diagnosis
 - Decisions: sick or healthy (or: further examination necessary)
 - Classes: patient is *sick* or *healthy*
 - The cost may be asymmetric:

$$loss(decision = healthy|patient = sick) >>$$

 $loss(decision = sick|patient = healthy)$



Decision

Classifying with Loss Functions

• In general, we can formalize this by introducing a loss matrix ${\cal L}_{ki}$

$$L_{kj} = loss for decision C_j if truth is C_k$$
.

Example: cancer diagnosis

$L_{cancer\ diagnosis} = \mathbf{\Xi}_{normal}^{cancer} \begin{pmatrix} 0 & 1000 \\ 1 & 0 \end{pmatrix}$



Classifying with Loss Functions

- Loss functions may be different for different actors.
 - Example:

$$L_{stocktrader}(subprime) = \begin{pmatrix} -\frac{1}{2}c_{gain} & 0\\ 0 & 0 \end{pmatrix}$$



$$L_{bank}(subprime) = \begin{pmatrix} -\frac{1}{2}c_{gain} & 0\\ 0 \end{pmatrix}$$



⇒ Different loss functions may lead to different Bayes optimal strategies.



Minimizing the Expected Loss

- Optimal solution is the one that minimizes the loss.
 - > But: loss function depends on the true class, which is unknown.
- Solution: Minimize the expected loss

$$\mathbb{E}[L] = \sum_{k} \sum_{j} \int_{\mathcal{R}_{j}} L_{kj} p(\mathbf{x}, \mathcal{C}_{k}) d\mathbf{x}$$

• This can be done by choosing the regions \mathcal{R}_j such that

$$\mathbb{E}[L] = \sum_{k} L_{kj} p(\mathcal{C}_k | \mathbf{x})$$

which is easy to do once we know the posterior class probabilities $p(C_k|\mathbf{x})$.



Minimizing the Expected Loss

Example:

- > 2 Classes: C_1 , C_2
- > 2 Decision: $\alpha_{\scriptscriptstyle 1}$, $\alpha_{\scriptscriptstyle 2}$
- Loss function: $L(\alpha_j|\mathcal{C}_k) = L_{kj}$
- Expected loss (= risk R) for the two decisions:

$$\mathbb{E}_{\alpha_1}[L] = R(\alpha_1|\mathbf{x}) = L_{11}p(\mathcal{C}_1|\mathbf{x}) + L_{21}p(\mathcal{C}_2|\mathbf{x})$$

$$\mathbb{E}_{\alpha_2}[L] = R(\alpha_2|\mathbf{x}) = L_{12}p(\mathcal{C}_1|\mathbf{x}) + L_{22}p(\mathcal{C}_2|\mathbf{x})$$

- Goal: Decide such that expected loss is minimized
 - I.e. decide α_1 if $R(\alpha_2|\mathbf{x}) > R(\alpha_1|\mathbf{x})$



Minimizing the Expected Loss

$$R(\alpha_{2}|\mathbf{x}) > R(\alpha_{1}|\mathbf{x})$$

$$L_{12}p(C_{1}|\mathbf{x}) + L_{22}p(C_{2}|\mathbf{x}) > L_{11}p(C_{1}|\mathbf{x}) + L_{21}p(C_{2}|\mathbf{x})$$

$$(L_{12} - L_{11})p(C_{1}|\mathbf{x}) > (L_{21} - L_{22})p(C_{2}|\mathbf{x})$$

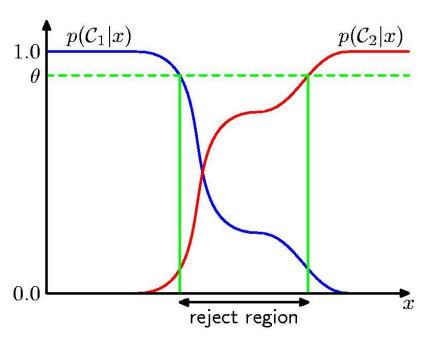
$$\frac{(L_{12} - L_{11})}{(L_{21} - L_{22})} > \frac{p(C_{2}|\mathbf{x})}{p(C_{1}|\mathbf{x})} = \frac{p(\mathbf{x}|C_{2})p(C_{2})}{p(\mathbf{x}|C_{1})p(C_{1})}$$

$$\frac{p(\mathbf{x}|C_{1})}{p(\mathbf{x}|C_{2})} > \frac{(L_{21} - L_{22})}{(L_{12} - L_{11})} \frac{p(C_{2})}{p(C_{1})}$$

⇒ Adapted decision rule taking into account the loss.



The Reject Option



- Classification errors arise from regions where the largest posterior probability $p(C_k|\mathbf{x})$ is significantly less than 1.
 - These are the regions where we are relatively uncertain about class membership.
 - For some applications, it may be better to reject the automatic decision entirely in such a case and e.g. consult a human expert.



Discriminant Functions

- Formulate classification in terms of comparisons
 - Discriminant functions

$$y_1(x),\ldots,y_K(x)$$

ightharpoonup Classify x as class C_k if

$$y_k(x) > y_j(x) \quad \forall j \neq k$$

Examples (Bayes Decision Theory)

$$y_k(x) = p(\mathcal{C}_k|x)$$

$$y_k(x) = p(x|\mathcal{C}_k)p(\mathcal{C}_k)$$

$$y_k(x) = \log p(x|\mathcal{C}_k) + \log p(\mathcal{C}_k)$$

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Different Views on the Decision Problem

- $y_k(x) \propto p(x|\mathcal{C}_k)p(\mathcal{C}_k)$
 - First determine the class-conditional densities for each class individually and separately infer the prior class probabilities.
 - > Then use Bayes' theorem to determine class membership.
 - \Rightarrow Generative methods
- $y_k(x) = p(\mathcal{C}_k|x)$
 - First solve the inference problem of determining the posterior class probabilities.
 - > Then use decision theory to assign each new x to its class.
 - \Rightarrow Discriminative methods
- Alternative
 - Directly find a discriminant function $y_k(x)$ which maps each input x directly onto a class label.



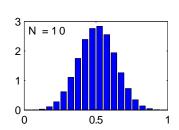
Next Lectures...

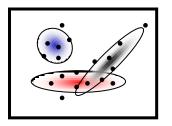
- ullet Ways how to estimate the probability densities $\,p(x|\mathcal{C}_k)\,$
 - Non-parametric methods
 - Histograms
 - k-Nearest Neighbor
 - Kernel Density Estimation
 - Parametric methods
 - Gaussian distribution
 - Mixtures of Gaussians

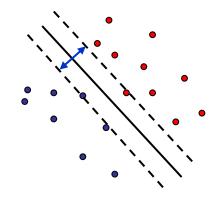


- Linear discriminants
- Support vector machines











References and Further Reading

 More information, including a short review of Probability theory and a good introduction in Bayes Decision Theory can be found in Chapters 1.1, 1.2 and 1.5 of

Christopher M. Bishop
Pattern Recognition and Machine Learning
Springer, 2006

