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Machine Learning - Lecture 1

Introduction

09.04.2015

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Many slides adapted from B. Schiele

Machine Learning Summer '15

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Organization

- Lecturer
 - Prof. Bastian Leibe (leibe@vision.rwth-aachen.de)
- Assistants
 - Ishrat Badami (badami@vision.rwth-aachen.de)
 - Michael Kramp (kramp@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!

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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 take the oral exam in German.

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Organization

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

➢ Lecture:	Tue 14:15 - 15:45	room UMIC 025
➢ Lecture/Exercises:	Thu 14:15 - 15:45	room UMIC 025
- Exam
 - Written exam
 - Towards the end of the semester, there will be a proposed date

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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.

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Course Webpage

Tentative Schedule

Date	Topic	Content	Slides	Related Material
07.04.15	no class	-	-	-
09.04.15	Introduction	Introduction, Probability Theory, Bayes Decision Theory, Minimizing Expected Loss	pdf, fullpage	Bishop Ch. 1.1, 1.2.1-1.2.3, 1.5, 1.1-1.5.4
14.04.15	Exercise 0	Intro Matlab	-	-
16.04.15	Prob. Density Estimation I	Nonparametric Methods, Histograms, Kernel Density Estimation, Parametric Methods, Gaussian Distribution, Maximum Likelihood, Bayesian Learning, Bias-Variance Problem	-	Exercise on Tuesday Bishop Ch. 2.5, 1.2.4, 2.3.1-2.3.4
21.04.15	Prob. Density Estimation II	Mixture of Gaussians, k-Means Clustering, EM-Clustering, EM Algorithm	-	Bishop chapter 9, original Dempster/Laird EM paper, Bilmes' EM tutorial
23.04.15	Linear Discriminant Functions	Linear Discriminant Functions, Least-squares Classification, Generalized Linear Models	-	Bishop chapter 4.1

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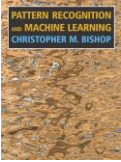
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Textbooks

- 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

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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 Ishrat or Michael.
 - 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!

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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. speed-dialing)
 - 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 (e.g. prediction of battery lifetime)

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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

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Machine Learning: Core Questions

- *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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Machine Learning: Core Questions

- *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
 - Regression: continuous y
 - Classification: discrete y
 - E.g. class membership, sometimes also posterior probability

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Example: Regression

- Automatic control of a vehicle

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Examples: Classification

- Email filtering $x \in [a-z]^+ \rightarrow y \in [\text{important, spam}]$
- Character recognition $x \rightarrow y \in [a, b, c, \dots, z]$
- Speech recognition $x \rightarrow y \in [\text{apple}, \dots, \text{zebra}]$

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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.

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Machine Learning: Core Questions

- 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"

Slide adapted from Bernt Schiele

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Machine Learning: Core Questions

- 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

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Machine Learning: Core Questions

- 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
 - $y = [0.0, 0.0, 1.0, 0.0, 0.0, 0.0, 0.0, 0.0]^T$, $L_2 = 1.02$
 - $y = [0.0, 0.0, 1.0, 0.0, 0.0, 0.0, 0.0, 0.0]^T$, $L_2 = 1.00$

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Machine Learning: Core Questions

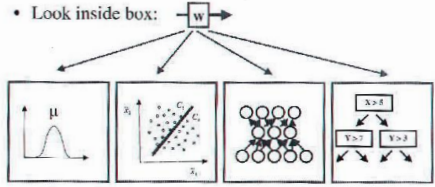
- **Learning to perform a task from experience**
- What data is available?
 - Data with labels: **supervised learning**
 - Images / speech with target labels
 - Car sensor data with target steering signal
 - Data without labels: **unsupervised learning**
 - Automatic clustering of sounds and phonemes
 - 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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Machine Learning: Core Questions

- $y = f(x; w)$
 - w : characterizes the family of functions
 - w : indexes the space of hypotheses
 - w : vector, connection matrix, graph, ...
- Look inside box:
 

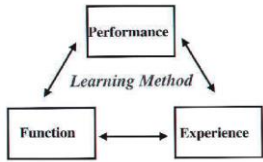
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Machine Learning: Core Questions

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



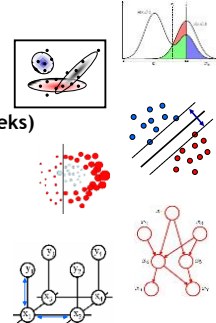
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Course Outline

- **Fundamentals (2 weeks)**
 - Bayes Decision Theory
 - Probability Density Estimation
- **Discriminative Approaches (5 weeks)**
 - Linear Discriminant Functions
 - Support Vector Machines
 - Ensemble Methods & Boosting
 - Randomized Trees, Forests & Ferns
- **Generative Models (4 weeks)**
 - Bayesian Networks
 - Markov Random Fields
 - Probabilistic Inference



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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

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Probability Theory



“Probability theory is nothing but common sense reduced to calculation.”

Pierre-Simon de Laplace, 1749-1827

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Image source: Wikipedia

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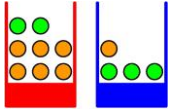
Probability Theory

- 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

$$p(B=r)=0.4 \quad p(B=b)=0.6$$
 - The probability of picking an apple given a choice for the box is

$$p(F=a|B=r)=0.25 \quad p(F=a|B=b)=0.75$$
 - What is the probability of picking an apple?

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



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Image source: C. M. Bishop, 2006

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Probability Theory

- More general case
 - Consider two random variables $X \in \{x_i\}$ and $Y \in \{y_j\}$
 - Consider N trials and let

$$n_{ij} = \#\{X = x_i \wedge Y = y_j\}$$

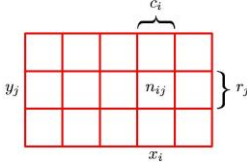
$$c_i = \#\{X = x_i\}$$

$$r_j = \#\{Y = y_j\}$$
- Then we can derive
 - Joint probability

$$p(X = x_i, Y = y_j) = \frac{n_{ij}}{N}$$
 - Marginal probability

$$p(X = x_i) = \frac{c_i}{N}$$
 - Conditional probability

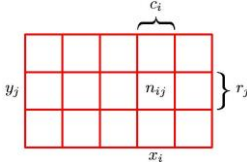
$$p(Y = y_j | X = x_i) = \frac{n_{ij}}{c_i}$$



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Image source: C. M. Bishop, 2006

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Probability Theory



- Rules of probability
 - Sum rule

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

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

$$= p(Y = y_j | X = x_i) p(X = x_i)$$

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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 $p(X) = \sum_Y p(X|Y)p(Y)$

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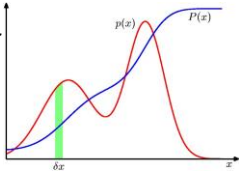
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Probability Densities

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

$$p(x \in (a, b)) = \int_a^b p(x) dx$$
- The probability that x lies in the interval $(-\infty, z)$ is given by the **cumulative distribution function**

$$P(z) = \int_{-\infty}^z p(x) dx$$



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Expectations

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

$$\mathbb{E}[f] = \sum_x p(x)f(x) \quad \mathbb{E}[f] = \int p(x)f(x) dx$$

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

$$\mathbb{E}[f] \approx \frac{1}{N} \sum_{n=1}^N f(x_n)$$
- We can also consider a **conditional expectation**

$$\mathbb{E}_x[f|y] = \sum_x p(x|y)f(x)$$

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Variations and Covariances

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

$$\text{var}[f] = \mathbb{E} \left[(f(x) - \mathbb{E}[f(x)])^2 \right] = \mathbb{E}[f(x)^2] - \mathbb{E}[f(x)]^2$$
- For two random variables x and y , the **covariance** is defined by


$$\begin{aligned} \text{cov}[x, y] &= \mathbb{E}_{x,y} \{ (x - \mathbb{E}[x]) \cdot (y - \mathbb{E}[y]) \} \\ &= \mathbb{E}_{x,y} [xy] - \mathbb{E}[x]\mathbb{E}[y] \end{aligned}$$
- If \mathbf{x} and \mathbf{y} are vectors, the result is a **covariance matrix**

$$\begin{aligned} \text{cov}[\mathbf{x}, \mathbf{y}] &= \mathbb{E}_{\mathbf{x}, \mathbf{y}} \{ (\mathbf{x} - \mathbb{E}[\mathbf{x}]) (\mathbf{y}^T - \mathbb{E}[\mathbf{y}^T]) \} \\ &= \mathbb{E}_{\mathbf{x}, \mathbf{y}} [\mathbf{x} \mathbf{y}^T] - \mathbb{E}[\mathbf{x}] \mathbb{E}[\mathbf{y}^T] \end{aligned}$$

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Bayes Decision Theory



Thomas Bayes, 1701-1761

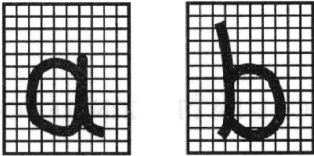
"The theory of inverse probability is founded upon an error, and must be wholly rejected."
R.A. Fisher, 1925

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Bayes Decision Theory

- Example: handwritten character recognition



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

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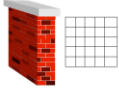
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Bayes Decision Theory

- Concept 1: **Priors** (a priori probabilities) $p(C_k)$
 - What we can tell about the probability *before seeing the data*.
 - Example:

a a b a a a b a
 b a a a a a b a
 a b a a a b b a
 b a b a a b a a

$P(a)=0.75$
 $P(b)=0.25$



$C_1 = a$
 $C_2 = b$


$p(C_1) = 0.75$
 $p(C_2) = 0.25$
- In general: $\sum_k p(C_k) = 1$

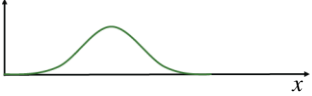
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
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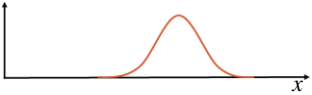
Bayes Decision Theory

- 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 .



$p(x|a)$




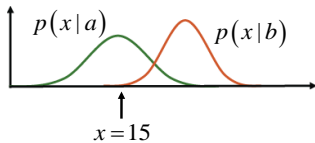
$p(x|b)$


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Bayes Decision Theory

- Example:


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

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Bayes Decision Theory

- Example:

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

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Bayes Decision Theory

- 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?

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Bayes Decision Theory

- Concept 3: **Posterior probabilities** $p(C_k | x)$
 - > 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

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

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Bayes Decision Theory

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Bayesian Decision Theory

- Goal: **Minimize the probability of a misclassification**

The green and blue regions stay constant.
Only the size of the red region varies!

$$\begin{aligned}
 p(\text{mistake}) &= p(x \in \mathcal{R}_1, C_2) + p(x \in \mathcal{R}_2, C_1) \\
 &= \int_{\mathcal{R}_1} p(x, C_2) dx + \int_{\mathcal{R}_2} p(x, C_1) dx \\
 &= \int_{\mathcal{R}_1} p(C_2|x)p(x) dx + \int_{\mathcal{R}_2} p(C_1|x)p(x) dx
 \end{aligned}$$

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Bayes Decision Theory

- Optimal decision rule
 - > Decide for C_1 if

$$p(C_1|x) > p(C_2|x)$$
 - > This is equivalent to

$$p(x|C_1)p(C_1) > p(x|C_2)p(C_2)$$
 - > Which is again equivalent to (Likelihood-Ratio test)

$$\frac{p(x|C_1)}{p(x|C_2)} > \underbrace{\frac{p(C_2)}{p(C_1)}}_{\text{Decision threshold } \theta}$$

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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

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

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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:

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

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Classifying with Loss Functions

- In general, we can formalize this by introducing a loss matrix L_{kj}

$$L_{kj} = \text{loss for decision } \mathcal{C}_j \text{ if truth is } \mathcal{C}_k.$$
- Example: cancer diagnosis

		Decision	
		cancer	normal
Truth	cancer	0	1000
	normal	1	0

$$L_{\text{cancer diagnosis}} =$$

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Classifying with Loss Functions

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

		"invest"	"don't invest"
		$-\frac{1}{2}c_{\text{gain}}$	0
Stocktrader (subprime)	$=$	$\begin{pmatrix} -\frac{1}{2}c_{\text{gain}} & 0 \\ 0 & 0 \end{pmatrix}$	

		c_{gain}	0
Bank (subprime)	$=$	$\begin{pmatrix} -\frac{1}{2}c_{\text{gain}} & 0 \\ \text{skull} & 0 \end{pmatrix}$	
- ⇒ Different loss functions may lead to different Bayes optimal strategies.

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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 $p(\mathcal{C}_k | \mathbf{x})$.

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Minimizing the Expected Loss

- Example:
 - 2 Classes: $\mathcal{C}_1, \mathcal{C}_2$
 - 2 Decision: α_1, α_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 $R(\alpha_2 | \mathbf{x}) > R(\alpha_1 | \mathbf{x})$

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Minimizing the Expected Loss

$$R(\alpha_2|\mathbf{x}) > R(\alpha_1|\mathbf{x})$$

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

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

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

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

⇒ Adapted decision rule taking into account the loss.

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The Reject Option

- Classification errors arise from regions where the largest posterior probability $p(\mathcal{C}_k|\mathbf{x})$ 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.

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Discriminant Functions

- Formulate classification in terms of comparisons
 - Discriminant functions

$$y_1(x), \dots, y_K(x)$$
 - Classify x as class \mathcal{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.
 - ⇒ *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.
 - ⇒ *Discriminative methods*
- Alternative
 - Directly find a discriminant function $y_k(x)$ which maps each input x directly onto a class label.

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Next Lectures...

- 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
- Discriminant functions
 - Linear discriminants
 - Support vector machines

⇒ Next lectures...

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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

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