

Machine Learning – Lecture 2

Probability Density Estimation

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Announcements: Reminders

- L2P electronic repository
 - Slides, exercises, and supplementary material will be made available here
 - Lecture recordings will be uploaded 2-3 days after the lecture
 - L2P access should now be fixed for all registered participants!
- Course webpage
 - http://www.vision.rwth-aachen.de/courses/
 - Slides will also be made available on the webpage
- Please subscribe to the lecture on rwth online!
 - Important to get email announcements and L2P access!

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Course Outline

Fundamentals

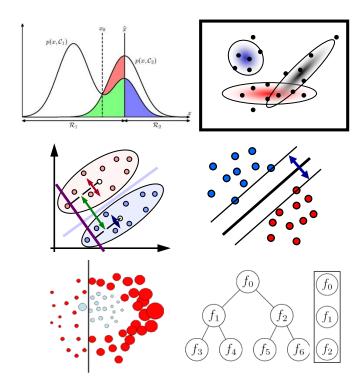
- Bayes Decision Theory
- Probability Density Estimation

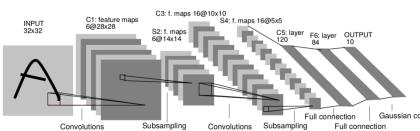
Classification Approaches

- Linear Discriminants
- Support Vector Machines
- Ensemble Methods & Boosting
- Randomized Trees, Forests & Ferns

Deep Learning

- Foundations
- Convolutional Neural Networks
- Recurrent Neural Networks







Topics of This Lecture

- Bayes Decision Theory
 - Basic concepts
 - Minimizing the misclassification rate
 - Minimizing the expected loss
 - Discriminant functions
- Probability Density Estimation
 - General concepts
 - Gaussian distribution
- Parametric Methods
 - Maximum Likelihood approach
 - Bayesian vs. Frequentist views on probability





Recap: The Rules of Probability

We have shown in the last lecture

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

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

5





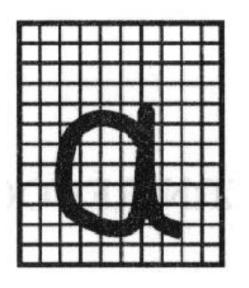
Thomas Bayes, 1701-1761

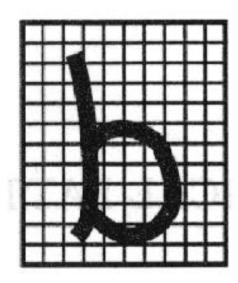
"The theory of inverse probability is founded upon an error, and must be wholly rejected."

R.A. Fisher, 1925



Example: handwritten character recognition





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

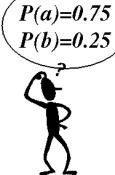


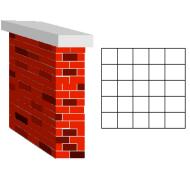
Concept 1: Priors (a priori probabilities)

$$p(C_k)$$

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

a a b a b a a b a baaaabaaba abaaaabba babaabaa





$$C_1 = a$$
$$C_2 = b$$

$$C_2 = b$$

$$p(C_1) = 0.75$$

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

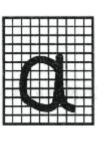
• In general:
$$\sum_{k} p(C_k) = 1$$



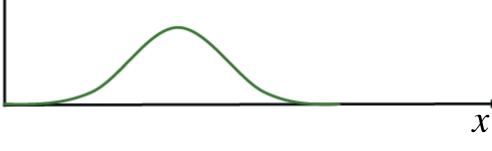
Concept 2: Conditional probabilities

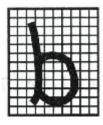


- Let x be a feature vector.
- x measures/describes certain properties of the input.
 - E.g. number of black pixels, aspect ratio, ...
- $p(x|C_k)$ describes its likelihood for class C_k .

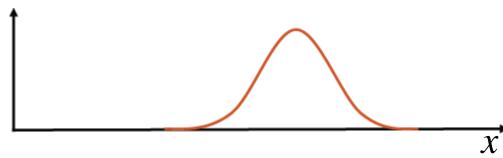


p(x|a)



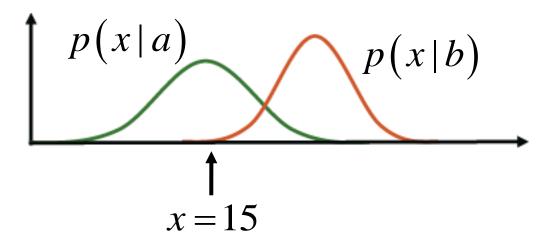


p(x|b)





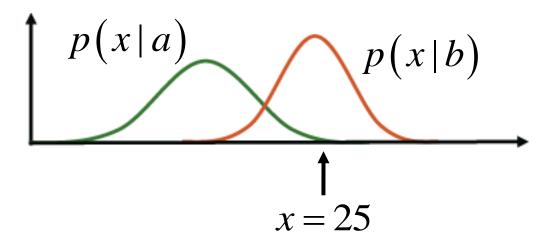
Example:



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



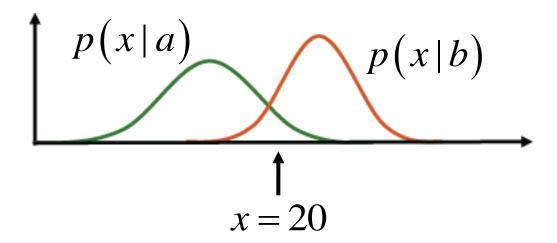
Example:



- 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

$$p(C_k | x)$$

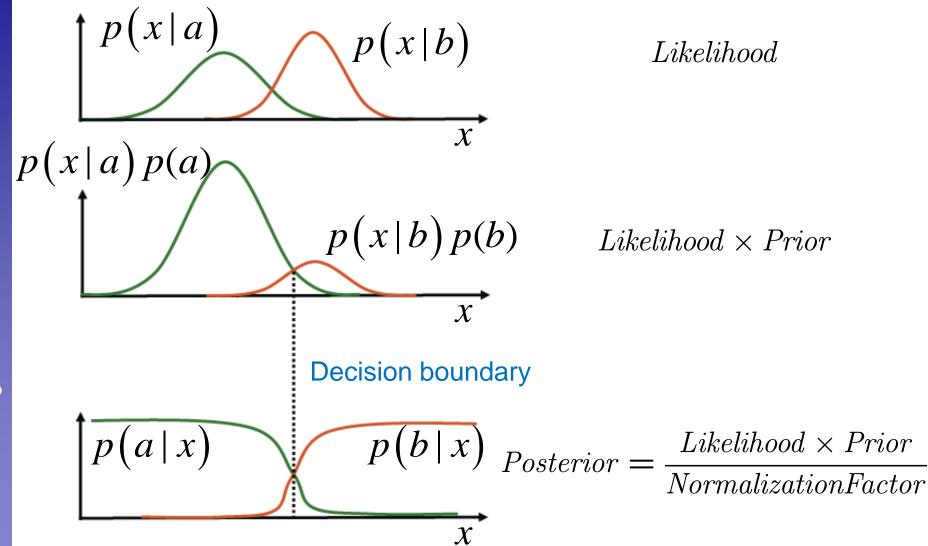
- We are typically interested in the *a posteriori* probability, i.e., the probability of class C_k given the measurement vector x.
- Bayes' Theorem:

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

Interpretation

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





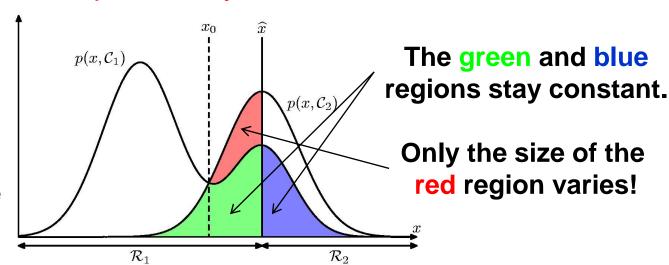


Goal: Minimize the probability of a misclassification

Decision rule:

$$x < \hat{x} \Rightarrow \mathcal{C}_1$$
$$x \ge \hat{x} \Rightarrow \mathcal{C}_2$$

How does p(mistake) change when we move \hat{x} ?



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

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

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

Z3



- 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



Generalization to More Than 2 Classes

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

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

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

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:

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

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



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

Decision

cancer

normal

$$L_{cancer\ diagnosis} =$$
 $=$ $\begin{bmatrix} \text{cancer} \\ \text{normal} \end{bmatrix} \begin{pmatrix} 0 & 1000 \\ 1 & 0 \end{pmatrix}$



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:
 - \triangleright 2 Classes: C_1, 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
 - Le. decide α_1 if $R(\alpha_2|\mathbf{x}) > R(\alpha_1|\mathbf{x})$



Minimizing the Expected Loss

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

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

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

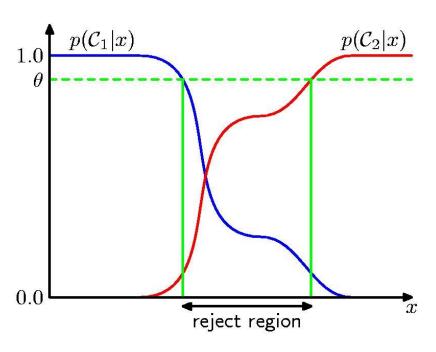
$$\frac{(L_{12} - L_{11})}{(L_{21} - L_{22})} > \frac{p(C_{2}|\mathbf{x})}{p(C_{1}|\mathbf{x})} = \frac{p(\mathbf{x}|C_{2})p(C_{2})}{p(\mathbf{x}|C_{1})p(C_{1})}$$

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

⇒ 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)

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

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

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



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.
 - \triangleright 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.



Topics of This Lecture

- Bayes Decision Theory
 - Basic concepts
 - Minimizing the misclassification rate
 - Minimizing the expected loss
 - Discriminant functions
- Probability Density Estimation
 - General concepts
 - Gaussian distribution
- Parametric Methods
 - Maximum Likelihood approach
 - Bayesian vs. Frequentist views on probability
 - Bayesian Learning



Probability Density Estimation

- Up to now
 - Bayes optimal classification
 - $_{ imes}$ Based on the probabilities $p(\mathbf{x}|\mathcal{C}_k)p(\mathcal{C}_k)$
- How can we estimate (= learn) those probability densities?
 - Supervised training case: data and class labels are known.
 - \succ Estimate the probability density for each class \mathcal{C}_k separately:

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

ightharpoonup (For simplicity of notation, we will drop the class label \mathcal{C}_k in the following.)

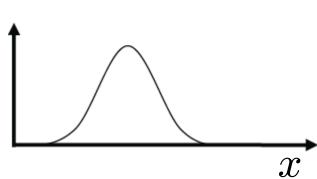


Probability Density Estimation

• Data: $x_1, x_2, x_3, x_4, \dots$



• Estimate: p(x)



- Methods
 - Parametric representations
 - Non-parametric representations
 - Mixture models

(today)

(lecture 3)

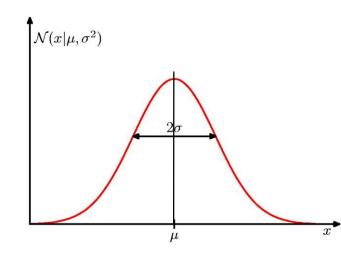
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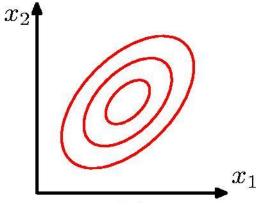
The Gaussian (or Normal) Distribution

- One-dimensional case
 - \triangleright Mean μ
 - ightharpoonup Variance σ^2

$$\mathcal{N}(x|\mu,\sigma^2) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left\{-\frac{(x-\mu)^2}{2\sigma^2}\right\}$$



- Multi-dimensional case
 - \triangleright Mean μ
 - \triangleright Covariance Σ



$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{D/2}|\boldsymbol{\Sigma}|^{1/2}} \exp\left\{-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^{\mathrm{T}} \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu})\right\}$$

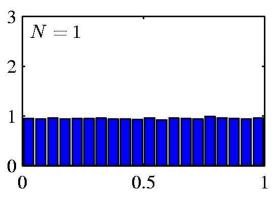
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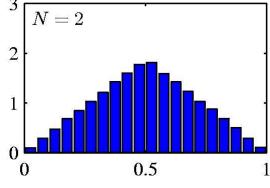


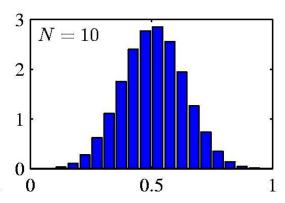
Gaussian Distribution – Properties

Central Limit Theorem

- \succ "The distribution of the sum of N i.i.d. random variables becomes increasingly Gaussian as N grows."
- In practice, the convergence to a Gaussian can be very rapid.
- This makes the Gaussian interesting for many applications.
- Example: N uniform [0,1] random variables.









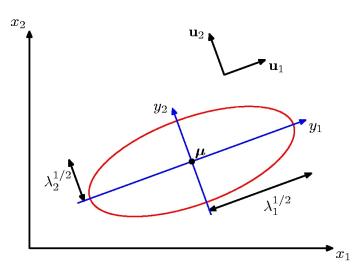
Gaussian Distribution - Properties

Quadratic Form

 $ightarrow \mathcal{N}$ depends on \mathbf{x} through the exponent

$$\Delta^2 = (\mathbf{x} - \boldsymbol{\mu})^{\mathrm{T}} \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu})$$

> Here, \triangle is often called the Mahalanobis distance from \mathbf{x} to μ .



Shape of the Gaussian

- Σ is a real, symmetric matrix.
- We can therefore decompose it into its eigenvectors

$$\boldsymbol{\Sigma} = \sum_{i=1}^D \lambda_i \mathbf{u}_i \mathbf{u}_i^{\mathrm{T}} \qquad \boldsymbol{\Sigma}^{-1} = \sum_{i=1}^D \frac{1}{\lambda_i} \mathbf{u}_i \mathbf{u}_i^{\mathrm{T}}$$
 and thus obtain $\Delta^2 = \sum_{i=1}^D \frac{y_i^2}{\lambda_i}$ with $y_i = \mathbf{u}_i^{\mathrm{T}}(\mathbf{x} - \boldsymbol{\mu})$

 \Rightarrow Constant density on ellipsoids with main directions along the eigenvectors \mathbf{u}_i and scaling factors $\sqrt{\lambda_i}$



Gaussian Distribution - Properties

- Special cases
 - Full covariance matrix

$$\mathbf{\Sigma} = [\sigma_{ij}]$$

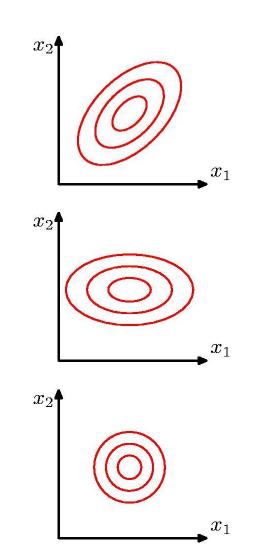
- ⇒ General ellipsoid shape
- Diagonal covariance matrix

$$\Sigma = diag\{\sigma_i\}$$

- ⇒ Axis-aligned ellipsoid
- Uniform variance

$$\Sigma = \sigma^2 \mathbf{I}$$

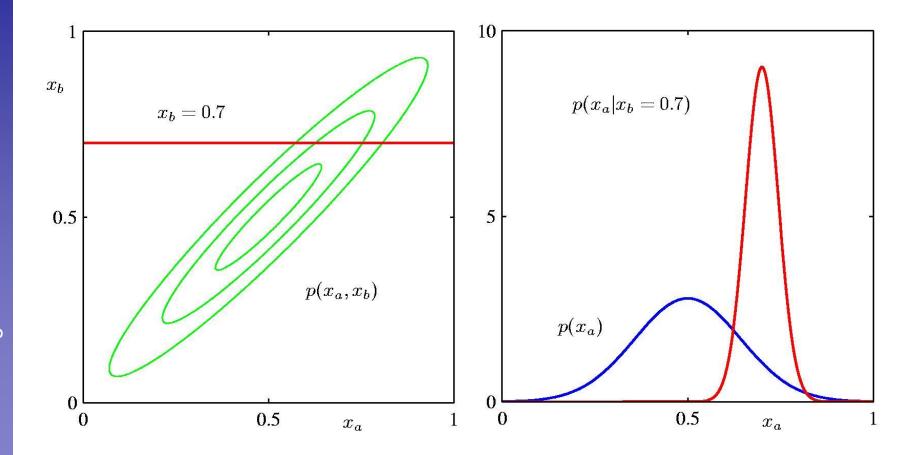
⇒ Hypersphere





Gaussian Distribution – Properties

The marginals of a Gaussian are again Gaussians:





Topics of This Lecture

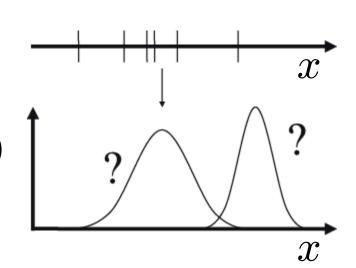
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 - Minimizing the misclassification rate
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 - Maximum Likelihood approach
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Parametric Methods

Given

- \rightarrow Data $X=\{x_1,x_2,\ldots,x_N\}$
- Parametric form of the distribution with parameters θ
- E.g. for Gaussian distrib.: $\, \theta = (\mu, \sigma) \,$



Learning

 \triangleright Estimation of the parameters θ

Likelihood of heta

Probability that the data X have indeed been generated from a probability density with parameters θ

$$L(\theta) = p(X|\theta)$$



- Computation of the likelihood Single data point: $p(x_n|\theta) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left\{-\frac{(x-\mu)^2}{2\sigma^2}\right\}$
 - Assumption: all data points are independent

$$L(\theta) = p(X|\theta) = \prod_{n=1}^{N} p(x_n|\theta)$$

Log-likelihood

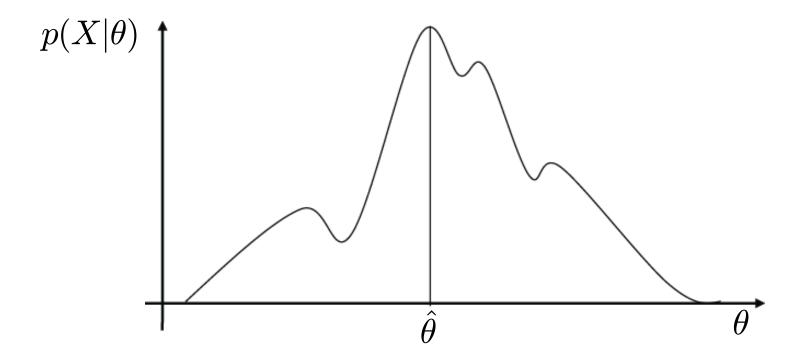
$$E(\theta) = -\ln L(\theta) = -\sum_{n=1}^{N} \ln p(x_n|\theta)$$

- Estimation of the parameters θ (Learning)
 - Maximize the likelihood
 - Minimize the negative log-likelihood





- Likelihood: $L(\theta) = p(X|\theta) = \prod_{n=1}^{\infty} p(x_n|\theta)$
- We want to obtain $\hat{ heta}$ such that $L(\hat{ heta})$ is maximized.





- Minimizing the log-likelihood
 - How do we minimize a function?
 - ⇒ Take the derivative and set it to zero.

$$\frac{\partial}{\partial \theta} E(\theta) = -\frac{\partial}{\partial \theta} \sum_{n=1}^{N} \ln p(x_n | \theta) = -\sum_{n=1}^{N} \frac{\frac{\partial}{\partial \theta} p(x_n | \theta)}{p(x_n | \theta)} \stackrel{!}{=} 0$$

Log-likelihood for Normal distribution (1D case)

$$E(\theta) = -\sum_{n=1}^{N} \ln p(x_n | \mu, \sigma)$$

$$= -\sum_{n=1}^{N} \ln \left(\frac{1}{\sqrt{2\pi}\sigma} \exp\left\{ -\frac{||x_n - \mu||^2}{2\sigma^2} \right\} \right)$$



Minimizing the log-likelihood

$$\frac{\partial}{\partial \mu} E(\mu, \sigma) = -\sum_{n=1}^{N} \frac{\frac{\partial}{\partial \mu} p(x_n | \mu, \sigma)}{p(x_n | \mu, \sigma)}$$

$$= -\sum_{n=1}^{N} -\frac{2(x_n - \mu)}{2\sigma^2}$$

$$= \frac{1}{\sigma^2} \sum_{n=1}^{N} (x_n - \mu)$$

$$= \frac{1}{\sigma^2} \left(\sum_{n=1}^{N} x_n - N\mu\right)$$

$$\frac{\partial}{\partial \mu} E(\mu, \sigma) \stackrel{!}{=} 0 \qquad \Leftrightarrow \qquad \hat{\mu} = \frac{1}{N} \sum_{n=1}^{N} x_n$$

$$p(x_n|\mu,\sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{||x_n-\mu||^2}{2\sigma^2}}$$



We thus obtain

$$\hat{\mu} = \frac{1}{N} \sum_{n=1}^{N} x_n$$

"sample mean"

In a similar fashion, we get

$$\hat{\sigma}^2 = \frac{1}{N} \sum_{n=1}^{N} (x_n - \hat{\mu})^2$$

"sample variance"

- $\hat{\theta} = (\hat{\mu}, \hat{\sigma})$ is the Maximum Likelihood estimate for the parameters of a Gaussian distribution.
- This is a very important result.
- Unfortunately, it is wrong...



- Or not wrong, but rather biased...
- Assume the samples $x_1, x_2, ..., x_N$ come from a true Gaussian distribution with mean μ and variance σ^2
 - We can now compute the expectations of the ML estimates with respect to the data set values. It can be shown that

$$\mathbb{E}(\mu_{\mathrm{ML}}) = \mu$$

$$\mathbb{E}(\sigma_{\mathrm{ML}}^2) = \left(\frac{N-1}{N}\right)\sigma^2$$

- ⇒ The ML estimate will underestimate the true variance.
- Corrected estimate:

$$\tilde{\sigma}^2 = \frac{N}{N-1}\sigma_{\rm ML}^2 = \frac{1}{N-1}\sum_{n=1}^{N}(x_n - \hat{\mu})^2$$



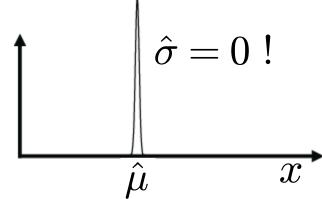
Maximum Likelihood – Limitations

- Maximum Likelihood has several significant limitations
 - It systematically underestimates the variance of the distribution!
 - E.g. consider the case

$$N = 1, X = \{x_1\}$$

-

⇒ Maximum-likelihood estimate:

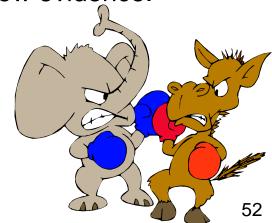


- We say ML overfits to the observed data.
- We will still often use ML, but it is important to know about this effect.



Deeper Reason

- Maximum Likelihood is a Frequentist concept
 - In the Frequentist view, probabilities are the frequencies of random, repeatable events.
 - These frequencies are fixed, but can be estimated more precisely when more data is available.
- This is in contrast to the Bayesian interpretation
 - In the Bayesian view, probabilities quantify the uncertainty about certain states or events.
 - This uncertainty can be revised in the light of new evidence.
- Bayesians and Frequentists do not like each other too well...





Bayesian vs. Frequentist View

- To see the difference...
 - Suppose we want to estimate the uncertainty whether the Arctic ice cap will have disappeared by the end of the century.
 - This question makes no sense in a Frequentist view, since the event cannot be repeated numerous times.
 - In the Bayesian view, we generally have a prior, e.g., from calculations how fast the polar ice is melting.
 - If we now get fresh evidence, e.g., from a new satellite, we may revise our opinion and update the uncertainty from the prior.

$Posterior \propto Likelihood \times Prior$

This generally allows to get better uncertainty estimates for many situations.

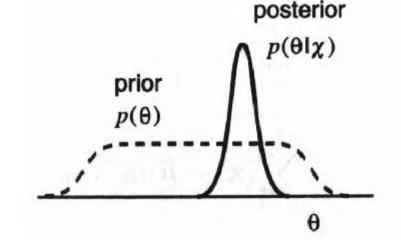
Main Frequentist criticism

The prior has to come from somewhere and if it is wrong, the result will be worse.

53

Bayesian Approach to Parameter Learning

- Conceptual shift
 - Maximum Likelihood views the true parameter vector θ to be unknown, but fixed.
 - \succ In Bayesian learning, we consider heta to be a random variable.
- This allows us to use knowledge about the parameters heta
 - \succ i.e. to use a prior for heta
 - > Training data then converts this prior distribution on θ into a posterior probability density.



The prior thus encodes knowledge we have about the type of distribution we expect to see for θ .



Bayesian Learning

- Bayesian Learning is an important concept
 - However, it would lead to far here.
 - ⇒ I will introduce it in more detail in the Advanced ML lecture.



References and Further Reading

More information in Bishop's book

Gaussian distribution and ML: Ch. 1.2.4 and 2.3.1-2.3.4.

Bayesian Learning: Ch. 1.2.3 and 2.3.6.

Nonparametric methods: Ch. 2.5.

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

