# Machine Learning – Lecture 2

## Probability Density Estimation

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Many slides adapted from B. Schiele

# Announcements

- Course webpage
  - http://www.vision.rwth-aachen.de/teaching/
  - Slides will be made available on the webpage
- L2P electronic repository
  - Exercises and supplementary materials will be posted on the L2P
- Please subscribe to the lecture on the Campus system!
  - Important to get email announcements and L2P access!

# Announcements

- Exercise sheet 1 is now available on L2P
  - Bayes decision theory
  - Maximum Likelihood
  - Kernel density estimation / k-NN

  ⇒ *Submit your results to Ishrat/Michael until evening of 29.04.*

- Work in teams (of up to 3 people) is encouraged
  - Who is not part of an exercise team yet?

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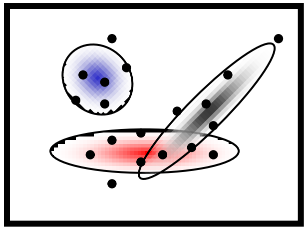
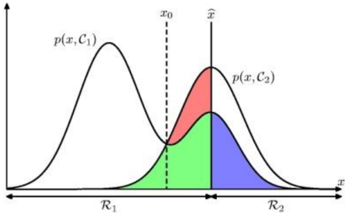
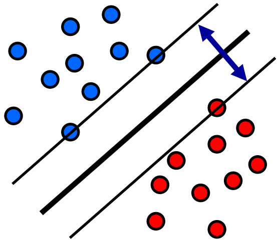
# Course Outline

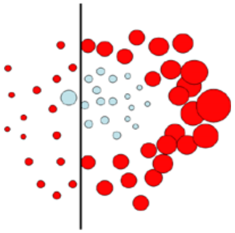
- Fundamentals (2 weeks)
  - Bayes Decision Theory
  - Probability Density Estimation

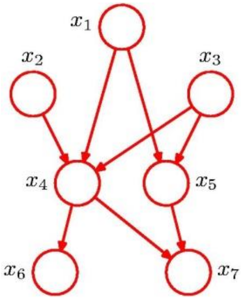




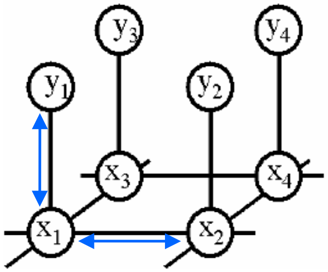

- Discriminative Approaches (5 weeks)
  - Linear Discriminant Functions
  - Support Vector Machines
  - Ensemble Methods & Boosting
  - Randomized Trees, Forests & Ferns








- Generative Models (4 weeks)
  - Bayesian Networks
  - Markov Random Fields

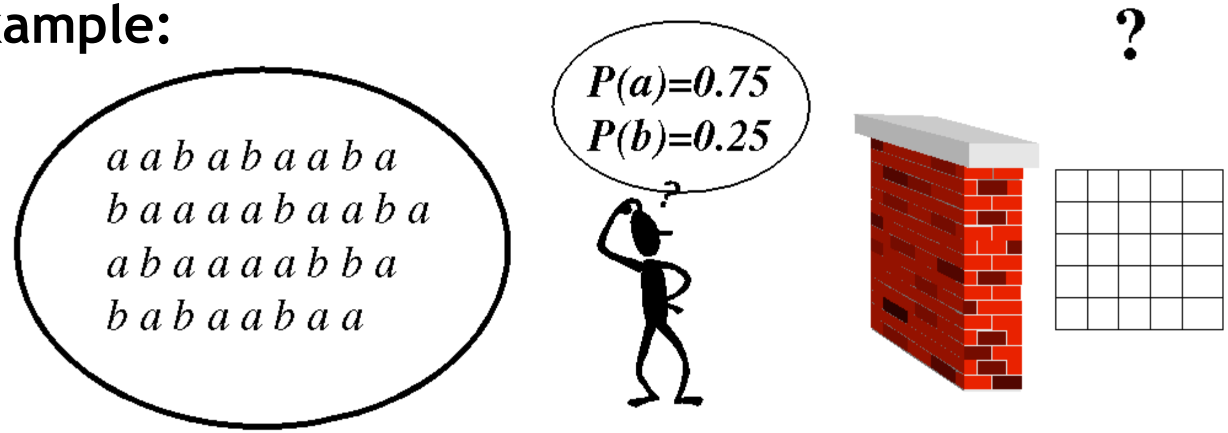


# Topics of This Lecture

- 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

# Recap: Bayes Decision Theory Concepts

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



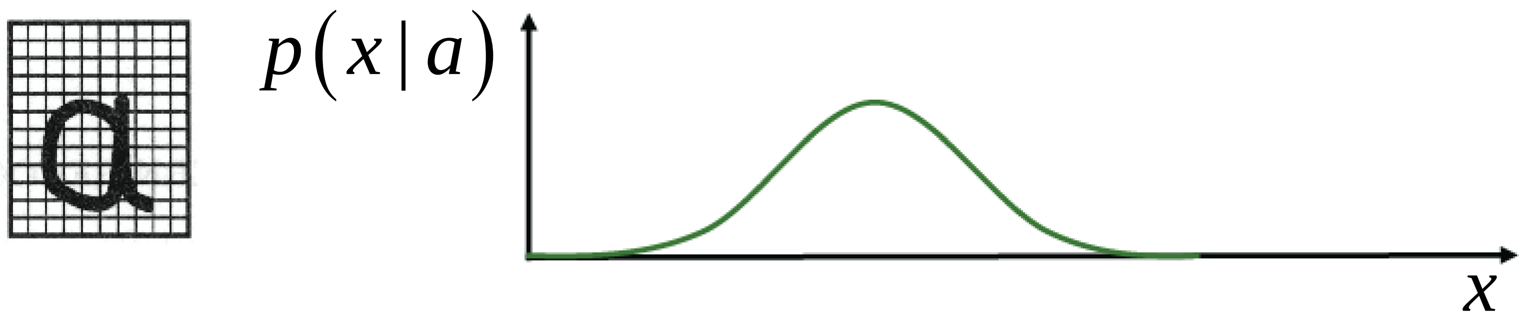

$$C_1 = a \qquad p(C_1) = 0.75$$

$$C_2 = b \qquad p(C_2) = 0.25$$

- **In general:** $\sum_k p(C_k) = 1$

# Recap: Bayes Decision Theory Concepts

- **Concept 2: Conditional probabilities** $\boxed{p(x|C_k)}$
  - 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 $C_k$.




# Bayes Decision Theory Concepts

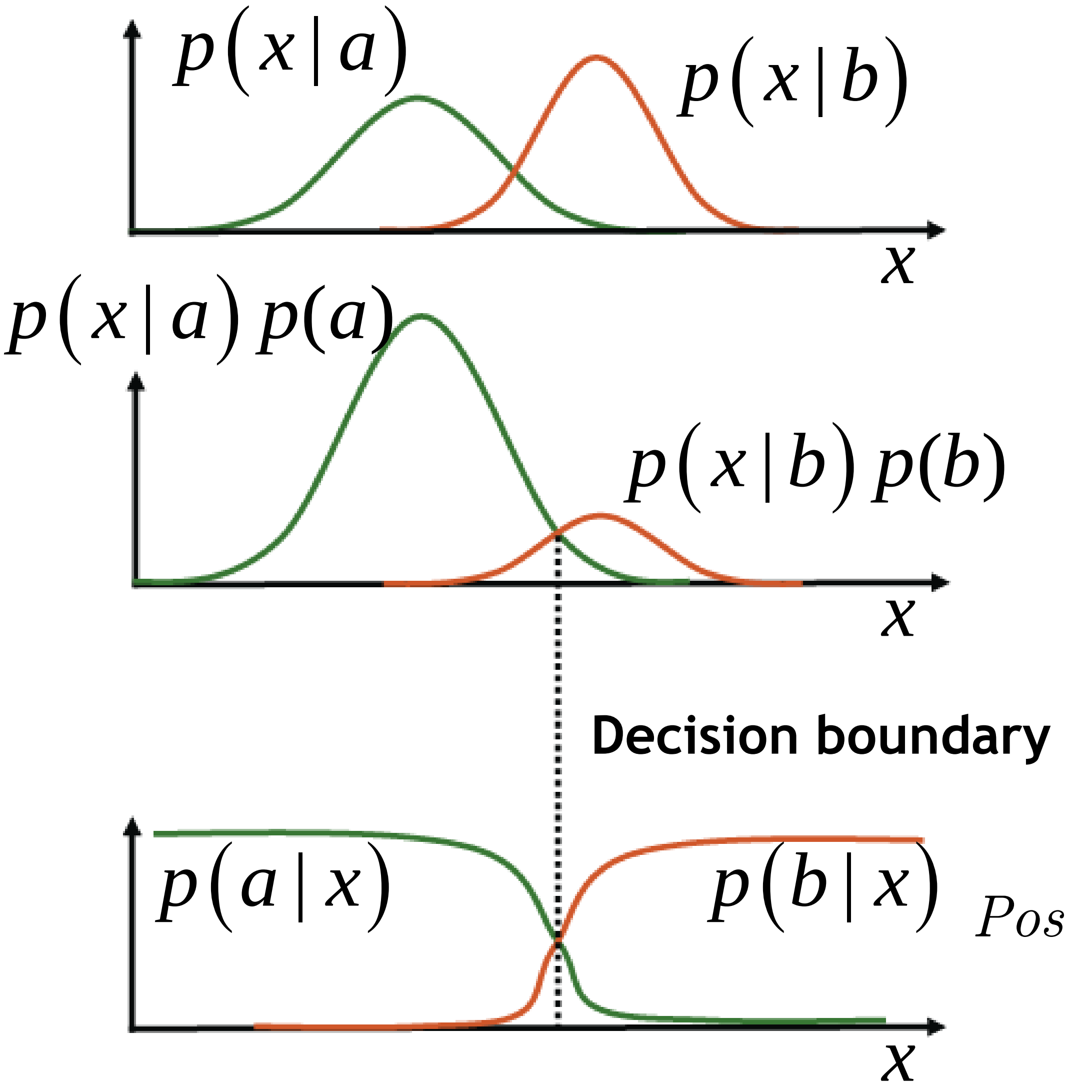
- Concept 3: Posterior probabilities $\boxed{p(C_k \mid x)}$
  - We are typically interested in the *a posteriori* probability, i.e. the probability of class $C_k$ given the measurement vector $x$.
- Bayes' Theorem:

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

- Interpretation

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

# Bayes Decision Theory



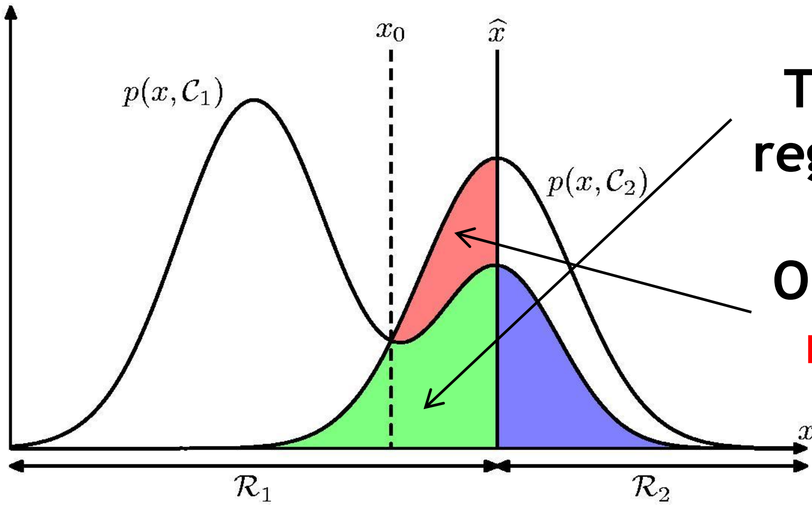

$$\mathit{Likelihood}$$

$$\mathit{Likelihood} \times \mathit{Prior}$$

$$\mathit{Posterior} = \frac{\mathit{Likelihood} \times \mathit{Prior}}{\mathit{NormalizationFactor}}$$

# 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!**

$$
\begin{aligned}
p(\text{mistake}) &= p(\mathbf{x} \in \mathcal{R}_1, \mathcal{C}_2) + p(\mathbf{x} \in \mathcal{R}_2, \mathcal{C}_1) \\
&= \int_{\mathcal{R}_1} p(\mathbf{x}, \mathcal{C}_2)\, \mathrm{d}\mathbf{x} + \int_{\mathcal{R}_2} p(\mathbf{x}, \mathcal{C}_1)\, \mathrm{d}\mathbf{x}. \\
&= \int_{\mathcal{R}_1} p(\mathcal{C}_2|\mathbf{x}) p(\mathbf{x}) d\mathbf{x} + \int_{\mathcal{R}_2} p(\mathcal{C}_1|\mathbf{x}) p(\mathbf{x}) d\mathbf{x}
\end{aligned}
$$



Image source: C.M. Bishop, 2006

# Bayes Decision Theory

- **Optimal decision rule**
  - **Decide for $C_1$ 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)**

$$\frac{p(x|\mathcal{C}_1)}{p(x|\mathcal{C}_2)} > \underbrace{\frac{p(\mathcal{C}_2)}{p(\mathcal{C}_1)}}_{\textbf{Decision threshold } \theta}$$

# Generalization to More Than 2 Classes



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

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

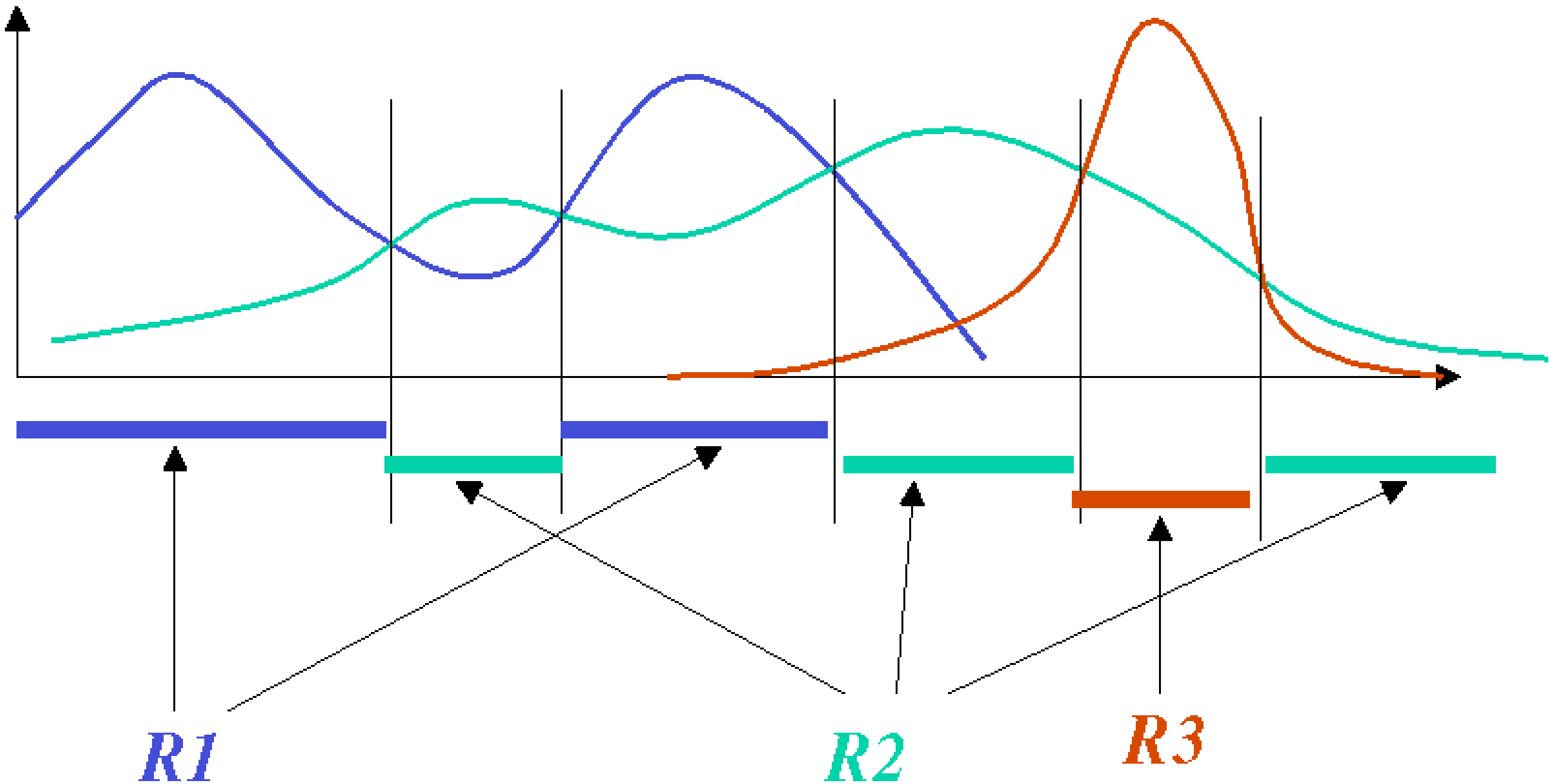
$$p(x|\mathcal{C}_k)p(\mathcal{C}_k) > p(x|\mathcal{C}_j)p(\mathcal{C}_j) \quad \forall j \neq k$$

- **Likelihood-ratio test**

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

# Bayes Decision Theory

- **Decision regions:** $\mathcal{R}_1, \mathcal{R}_2, \mathcal{R}_3, \ldots$



# 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:** **diagnosis is *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 $L_{kj}$

$$L_{kj} = loss\ for\ decision\ \mathcal{C}_j\ if\ truth\ is\ \mathcal{C}_k.$$

- Example: cancer diagnosis

$$L_{cancer\ diagnosis} = \begin{array}{cc} & \textbf{Decision} \\ & \begin{array}{cc} \text{cancer} & \text{normal} \end{array} \\ \textbf{Truth} \begin{array}{c} \text{cancer} \\ \text{normal} \end{array} & \begin{pmatrix} 0 & 1000 \\ 1 & 0 \end{pmatrix} \end{array}$$

# Classifying with Loss Functions

- **Loss functions may be different for different actors.**

  - **Example:**

$$
\begin{array}{cc}
 & \begin{array}{cc} \text{“invest”} & \text{“don't invest”} \end{array} \\
L_{stocktrader}(subprime) = & \begin{pmatrix} -\frac{1}{2}c_{gain} & 0 \\ 0 & 0 \end{pmatrix}
\end{array}
$$

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

$\Rightarrow$ **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

$$\mathbb{E}[L] = \sum_k \sum_j \int_{\mathcal{R}_j} L_{kj} p(\mathbf{x}, \mathcal{C}_k) \, \mathrm{d}\mathbf{x}$$

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

# Minimizing the Expected Loss

- **Example:**
  - **2 Classes:** $C_1, C_2$
  - **2 Decision:** $\alpha_1, \alpha_2$
  - **Loss function:** $L(\alpha_j|\mathcal{C}_k) = L_{kj}$
  - **Expected loss (= risk $R$) for the two decisions:**

$$\mathbb{E}_{\alpha_1}[L] = R(\alpha_1|\mathbf{x}) \;=\; L_{11}p(\mathcal{C}_1|\mathbf{x}) + L_{21}p(\mathcal{C}_2|\mathbf{x})$$
$$\mathbb{E}_{\alpha_2}[L] = R(\alpha_2|\mathbf{x}) \;=\; L_{12}p(\mathcal{C}_1|\mathbf{x}) + L_{22}p(\mathcal{C}_2|\mathbf{x})$$

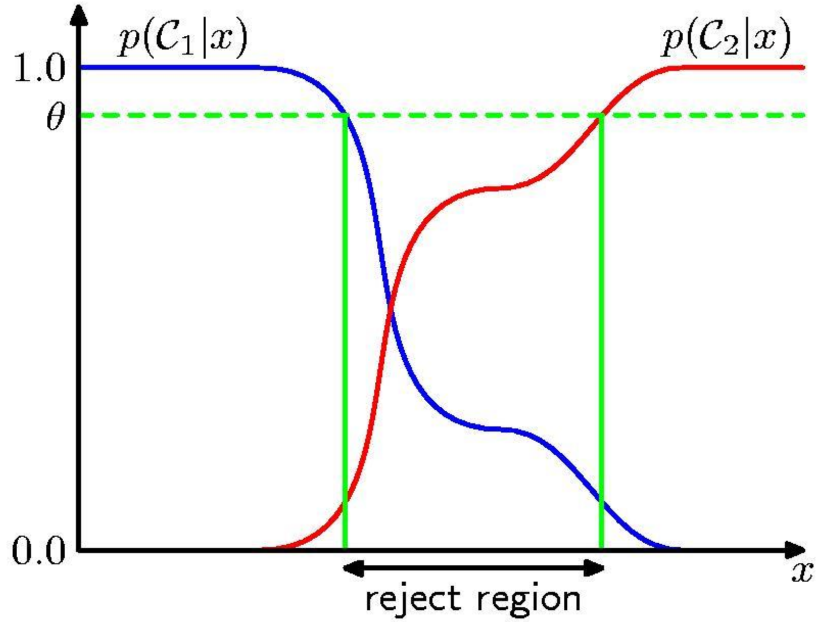
- **Goal: Decide such that expected loss is minimized**
  - **I.e. decide $\alpha_1$ if** $R(\alpha_2|\mathbf{x}) > R(\alpha_1|\mathbf{x})$

# Minimizing the Expected Loss

$$
\begin{aligned}
R(\alpha_2|\mathbf{x}) &> R(\alpha_1|\mathbf{x}) \\
L_{12}p(\mathcal{C}_1|\mathbf{x}) + L_{22}p(\mathcal{C}_2|\mathbf{x}) &> L_{11}p(\mathcal{C}_1|\mathbf{x}) + L_{21}p(\mathcal{C}_2|\mathbf{x}) \\
(L_{12} - L_{11})p(\mathcal{C}_1|\mathbf{x}) &> (L_{21} - L_{22})p(\mathcal{C}_2|\mathbf{x}) \\
\frac{(L_{12} - L_{11})}{(L_{21} - L_{22})} &> \frac{p(\mathcal{C}_2|\mathbf{x})}{p(\mathcal{C}_1|\mathbf{x})} = \frac{p(\mathbf{x}|\mathcal{C}_2)p(\mathcal{C}_2)}{p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1)} \\
\frac{p(\mathbf{x}|\mathcal{C}_1)}{p(\mathbf{x}|\mathcal{C}_2)} &> \frac{(L_{21} - L_{22})}{(L_{12} - L_{11})} \frac{p(\mathcal{C}_2)}{p(\mathcal{C}_1)}
\end{aligned}
$$

$\Rightarrow$ **Adapted decision rule taking into account the loss.**

# 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.**


Image source: C.M. Bishop, 2006

# Discriminant Functions

- **Formulate classification in terms of comparisons**
  - **Discriminant functions**

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

  - **Classify $x$ as class $C_k$ if**

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

- **Examples (Bayes Decision Theory)**

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

# 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.

# 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

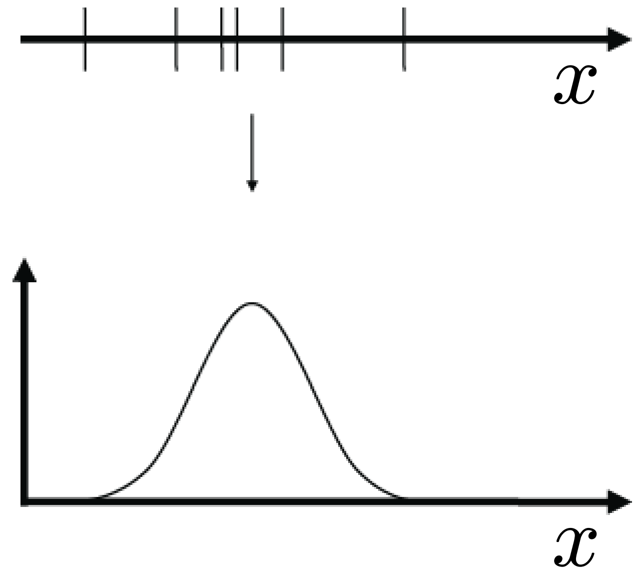
- Up to now
  - Bayes optimal classification
  - Based on the probabilities $p(\mathbf{x}|\mathcal{C}_k)p(\mathcal{C}_k)$
- How can we estimate (=learn) those probability densities?
  - Supervised training case: data and class labels are known.
  - Estimate the probability density for each class $\mathcal{C}_k$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

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

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

# Probability Density Estimation

- **Data:** $x_1, x_2, x_3, x_4, \ldots$



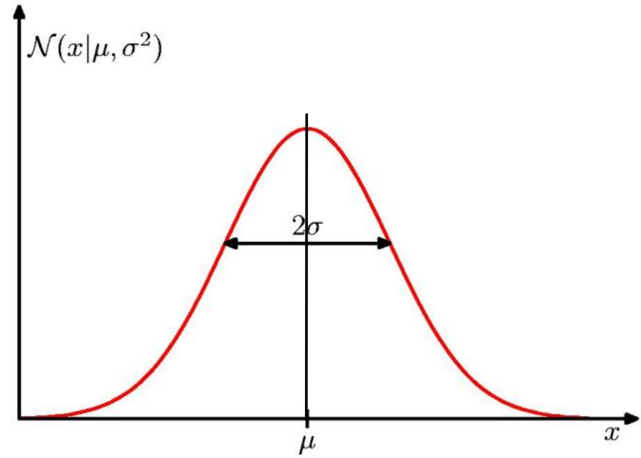

- **Estimate:** $p(x)$

- **Methods**
  - Parametric representations
  - Non-parametric representations
  - Mixture models (next lecture)

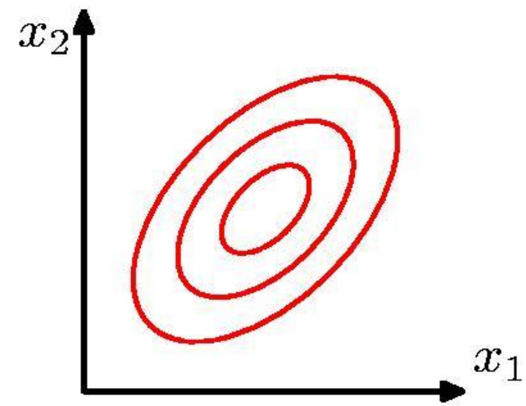
# The Gaussian (or Normal) Distribution

- **One-dimensional case**
  - Mean $\mu$
  - Variance $\sigma^2$

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




- **Multi-dimensional case**
  - Mean $\boldsymbol{\mu}$
  - Covariance $\Sigma$




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



Image source: C.M. Bishop, 2006

# Gaussian Distribution - Properties

- Central Limit Theorem
  - "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.

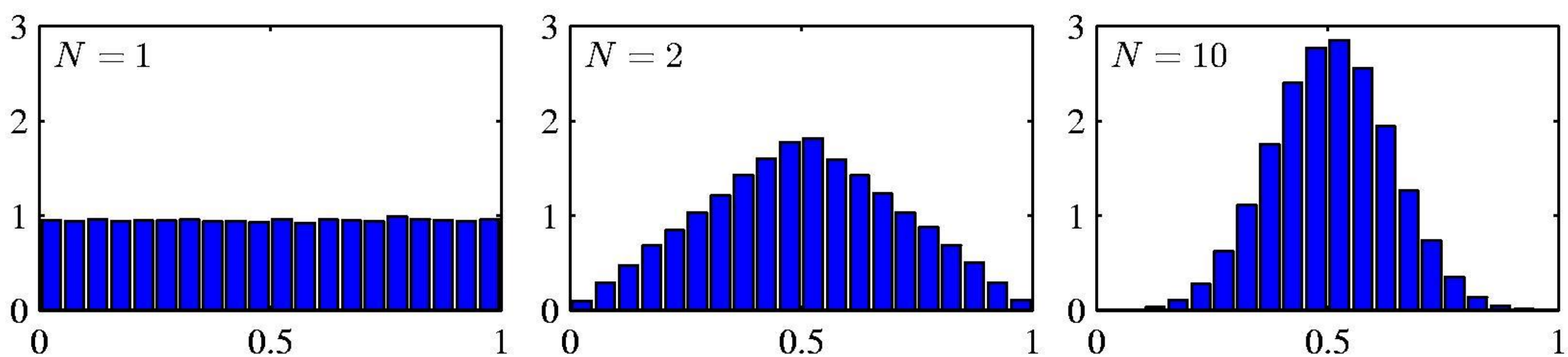




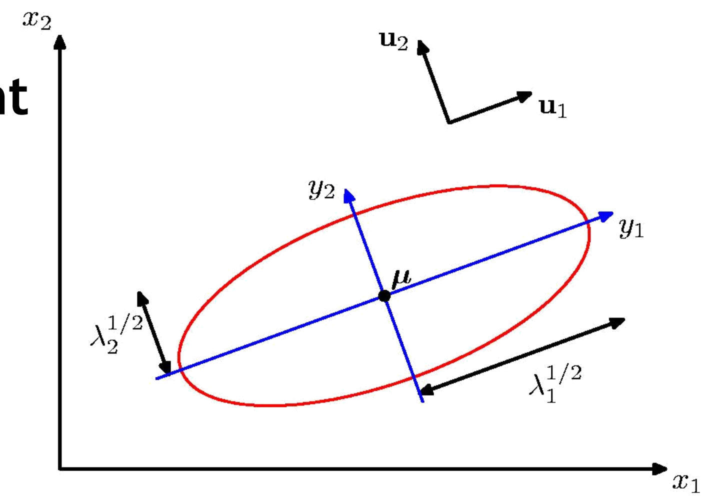
Image source: C.M. Bishop, 2006

# Gaussian Distribution - Properties

- Quadratic Form
  - $\mathcal{N}$ depends on $\mathbf{x}$ through the exponent

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

  - Here, $\Delta$ is often called the Mahalanobis distance from $\mu$ to $\mathbf{x}$.




- Shape of the Gaussian
  - $\Sigma$ 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 $\sqrt{\lambda_i}$.

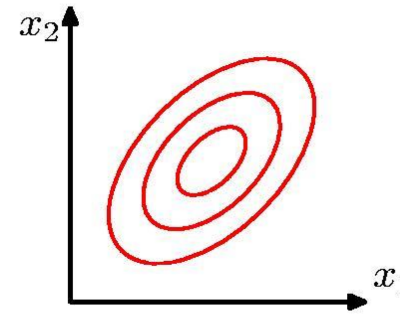

Image source: C.M. Bishop, 2006

# Gaussian Distribution - Properties

- Special cases
  - Full covariance matrix

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

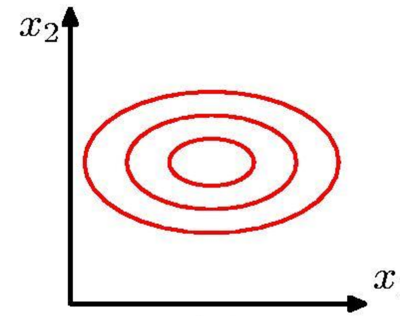
$\Rightarrow$ General ellipsoid shape




  - Diagonal covariance matrix

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

$\Rightarrow$ Axis-aligned ellipsoid




  - Uniform variance

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

$\Rightarrow$ Hypersphere

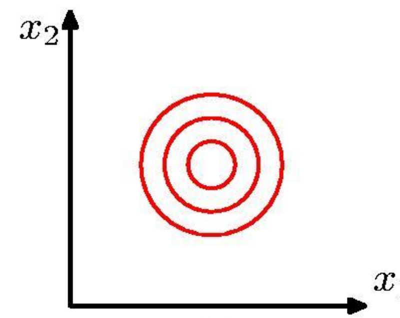



Image source: C.M. Bishop, 2006

# Gaussian Distribution – Properties

- **The marginals of a Gaussian are again Gaussians:**

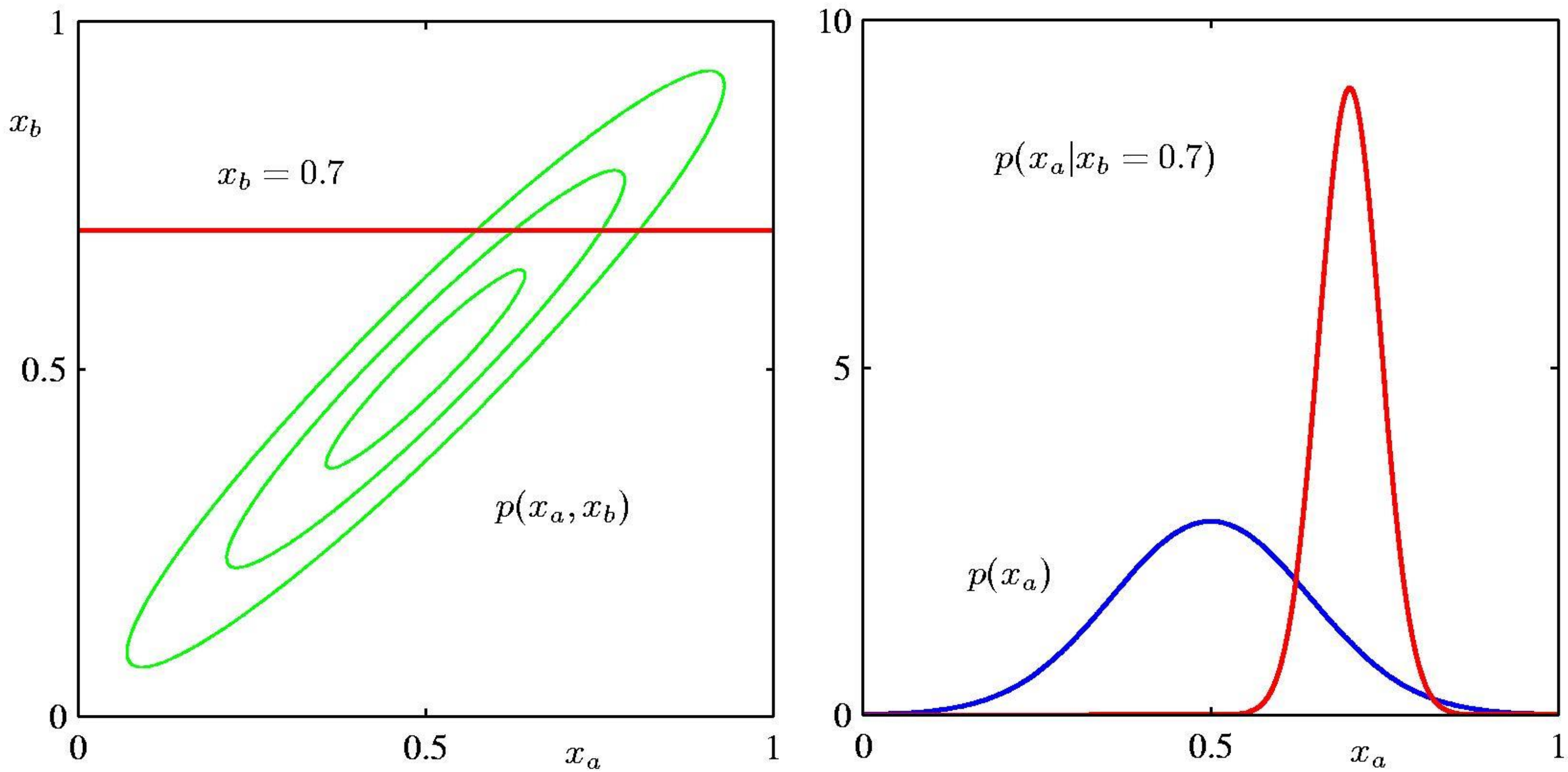




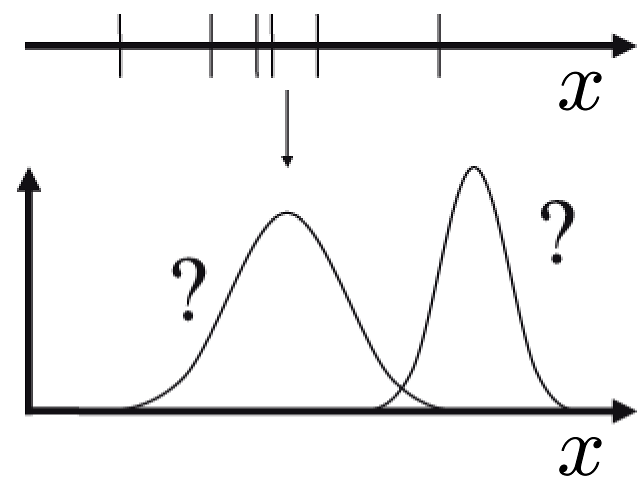

Image source: C.M. Bishop, 2006

# 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

# Parametric Methods

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




- **Learning**
  - Estimation of the parameters $\theta$

- **Likelihood of $\theta$**
  - Probability that the data $X$ have indeed been generated from a probability density with parameters $\theta$

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

# Maximum Likelihood Approach

- **Computation of the likelihood**
  - **Single data point:** $p(x_n|\theta)$
  - **Assumption: all data points are independent**

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

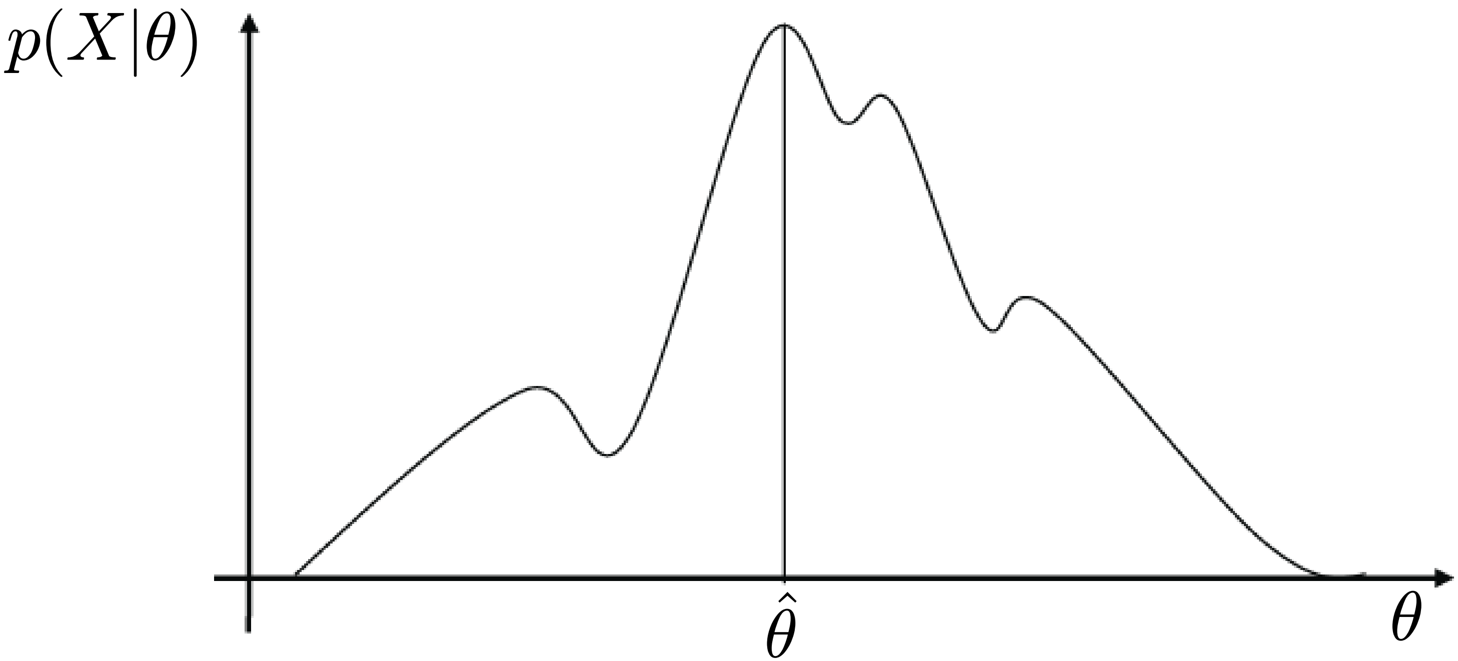
  - **Log-likelihood**

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

  - **Estimation of the parameters $\theta$ (Learning)**
    - **Maximize the likelihood**
    - **Minimize the negative log-likelihood**

# Maximum Likelihood Approach

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



# Maximum Likelihood Approach

- **Minimizing the log-likelihood**
  - How do we minimize a function?

  $\Rightarrow$ 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)**

$$\begin{aligned} E(\theta) &= -\sum_{n=1}^{N} \ln p(x_n|\mu,\sigma) \\ &= -\sum_{n=1}^{N} \ln \left( \frac{1}{\sqrt{2\pi}\sigma} \exp\left\{ -\frac{||x_n - \mu||^2}{2\sigma^2} \right\} \right) \end{aligned}$$

# Maximum Likelihood Approach

- **Minimizing the log-likelihood**

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

$$\begin{aligned}
\frac{\partial}{\partial\mu}E(\mu,\sigma) &= -\sum_{n=1}^{N} \frac{\frac{\partial}{\partial\mu}p(x_n|\mu,\sigma)}{p(x_n|\mu,\sigma)} \\
&= -\sum_{n=1}^{N} -\frac{2(x_n-\mu)}{2\sigma^2} \\
&= \frac{1}{\sigma^2}\sum_{n=1}^{N}(x_n-\mu) \\
&= \frac{1}{\sigma^2}\left(\sum_{n=1}^{N} x_n - N\mu\right)
\end{aligned}$$

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

# Maximum Likelihood Approach

- 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…

# Maximum Likelihood Approach

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

$$\begin{aligned}\mathbb{E}(\mu_{\mathrm{ML}}) &= \mu \\ \mathbb{E}(\sigma^2_{\mathrm{ML}}) &= \left(\frac{N-1}{N}\right)\sigma^2\end{aligned}$$

$\Rightarrow$ The ML estimate will underestimate the true variance.

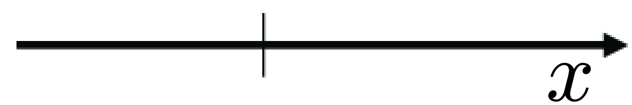
- Corrected estimate:

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

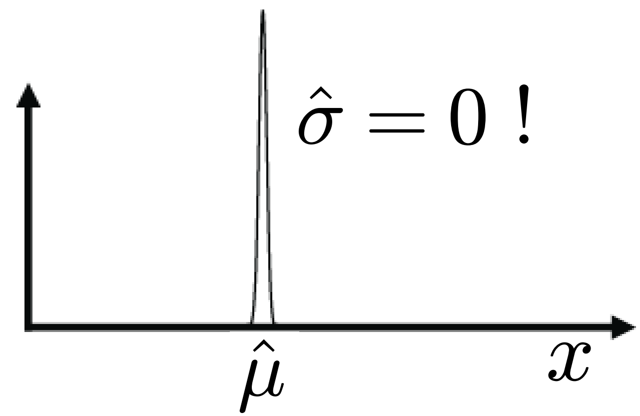
# Maximum Likelihood - Limitations

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

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



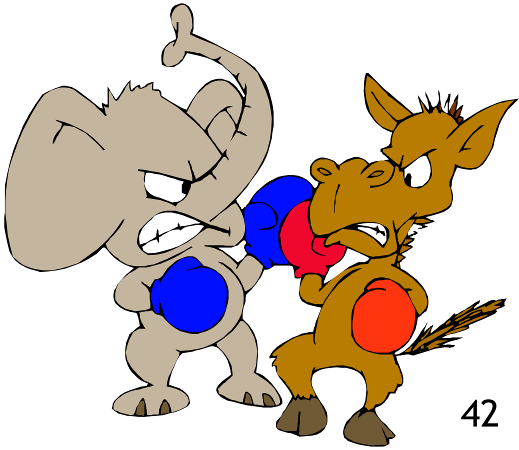

**$\Rightarrow$ Maximum-likelihood estimate:**




  - **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

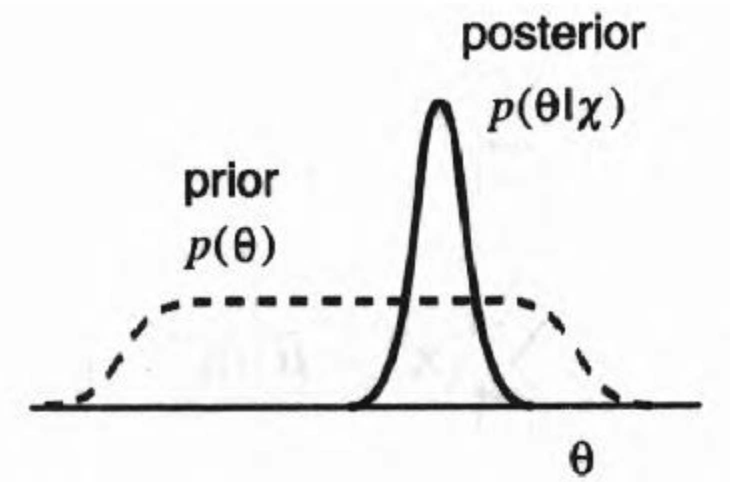
- To see the difference…
  - Suppose we want to estimate the uncertainty whether the Arctic ice cap will have disappeared by the end of the century.
  - This question makes no sense in a Frequentist view, since the event cannot be repeated numerous times.
  - In the Bayesian view, we generally have a 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.

# Bayesian Approach to Parameter Learning

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




  - The prior thus encodes knowledge we have about the type of distribution we expect to see for $\theta$.

# Bayesian Learning Approach

- **Bayesian view:**
  - Consider the parameter vector $\theta$ as a random variable.
  - When estimating the parameters, what we compute is

$$p(x|X) = \int p(x, \theta|X) d\theta$$

**Assumption: given $\theta$, this doesn't depend on X anymore**

$$p(x, \theta|X) = p(x|\theta, \cancel{X})p(\theta|X)$$

$$p(x|X) = \int \underbrace{p(x|\theta)}p(\theta|X) d\theta$$

**This is entirely determined by the parameter $\theta$ (i.e. by the parametric form of the pdf).**

# Bayesian Learning Approach

$$p(x|X) = \int p(x|\theta)\underbrace{p(\theta|X)}d\theta$$

$$p(\theta|X) = \frac{p(X|\theta)p(\theta)}{p(X)} = \frac{p(\theta)}{\underbrace{p(X)}}L(\theta)$$

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

- **Inserting this above, we obtain**

$$p(x|X) = \int \frac{p(x|\theta)L(\theta)p(\theta)}{p(X)}d\theta = \int \frac{p(x|\theta)L(\theta)p(\theta)}{\int L(\theta)p(\theta)d\theta}d\theta$$

# Bayesian Learning Approach

- Discussion

Likelihood of the parametric form $\theta$ given the data set $X$.

Estimate for $x$ based on parametric form $\theta$

Prior for the parameters $\theta$

$$p(x|X) = \int \frac{p(x|\theta)L(\theta)p(\theta)}{\underbrace{\int L(\theta)p(\theta)d\theta}}d\theta$$

Normalization: integrate over all possible values of $\theta$

  - If we now plug in a (suitable) prior $p(\theta)$, we can estimate $p(x|X)$ from the data set $X$.

# Bayesian Density Estimation

- Discussion

$$p(x|X) = \int p(x|\theta)p(\theta|X)d\theta = \int \frac{p(x|\theta)L(\theta)p(\theta)}{\int L(\theta)p(\theta)d\theta}d\theta$$

  - The probability $p(\theta|X)$ makes the dependency of the estimate on the data explicit.
  - If $p(\theta|X)$ is very small everywhere, but is large for one $\hat{\theta}$, then

$$p(x|X) \approx p(x|\hat{\theta})$$

$\Rightarrow$ The more uncertain we are about $\theta$, the more we average over all parameter values.

# Bayesian Density Estimation

- **Problem**
  - In the general case, the integration over $\theta$ is not possible (or only possible stochastically).

- **Example where an analytical solution is possible**
  - Normal distribution for the data, $\sigma^2$ assumed known and fixed.
  - Estimate the distribution of the mean:

$$p(\mu|X) = \frac{p(X|\mu)p(\mu)}{p(X)}$$

  - Prior: We assume a Gaussian prior over $\mu$,

$$p(\mu) = \mathcal{N}\left(\mu|\mu_0, \sigma_0^2\right).$$

# Bayesian Learning Approach

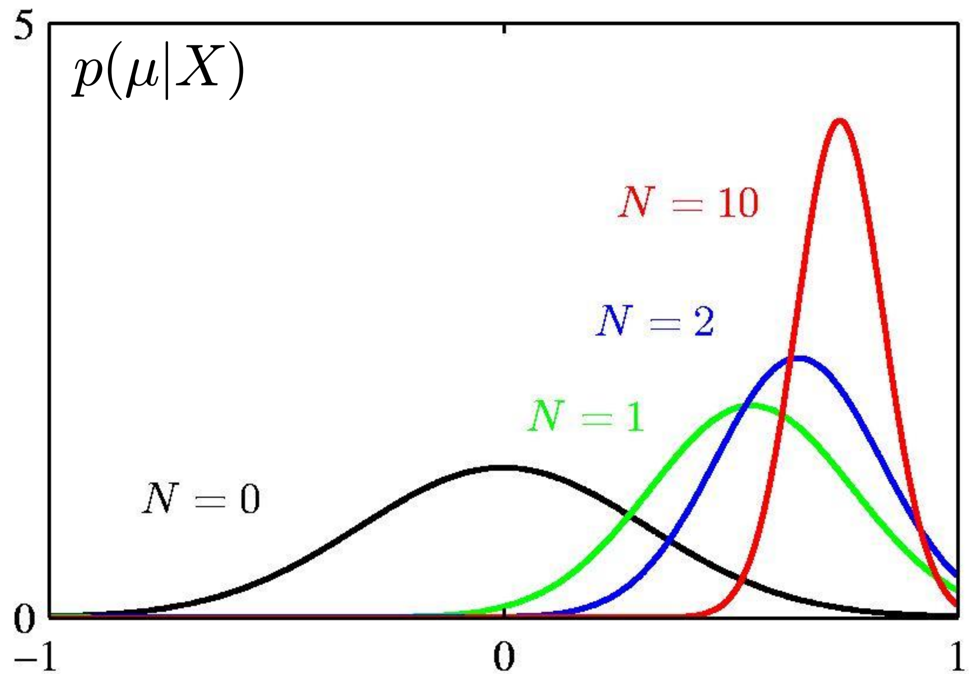
- **Sample mean:** $$\bar{x} = \frac{1}{N}\sum_{n=1}^{N} x_n$$
- **Bayes estimate:**

$$\mu_N = \frac{\sigma^2\mu_0 + N\sigma_0^2\bar{x}}{\sigma^2 + N\sigma_0^2}$$

$$\frac{1}{\sigma_N^2} = \frac{1}{\sigma_0^2} + \frac{N}{\sigma^2}$$

- **Note:**

| | $N = 0$ | $N \rightarrow \infty$ |
|---|---|---|
| $\mu_N$ | $\mu_0$ | $\mu_{\mathrm{ML}}$ |
| $\sigma_N^2$ | $\sigma_0^2$ | $0$ |




$\mu_0 = 0$


Image source: C.M. Bishop, 2006

# Summary: ML vs. Bayesian Learning

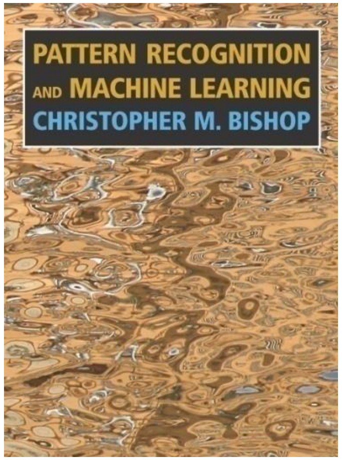
- **Maximum Likelihood**
  - Simple approach, often analytically possible.
  - Problem: estimation is biased, tends to overfit to the data.
    
    $\Rightarrow$ Often needs some correction or regularization.
  - But:
    - Approximation gets accurate for $N \to \infty$.

- **Bayesian Learning**
  - General approach, avoids the estimation bias through a prior.
  - Problems:
    - Need to choose a suitable prior (not always obvious).
    - Integral over $\theta$ often not analytically feasible anymore.
  - But:
    - Efficient stochastic sampling techniques available (see Lecture 15).

*(In this lecture, we'll use both concepts wherever appropriate)*

# 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.
- Additional information can be found in Duda & Hart
  - ML estimation: Ch. 3.2
  - Bayesian Learning: Ch. 3.3-3.5
  - Nonparametric methods: Ch. 4.1-4.5

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