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Statistical Machine Learning

Lecture 2: Bayesian Decision Theory

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Today's Objectives

- Make you understand how to make an optimal decision!
- Covered Topics:
  - Classification from a Bayesian point of view
  - Bayesian Optimal Decisions
  - Risk-based Classification
  - Probability Density Estimation (First Part)

Outline

Outline

Statistical Methods

- All statistical methods in machine learning share the fundamental assumption that the data generation process is governed by the rules of probability
- The data is understood to be a set of random samples from some underlying probability distribution
- Keep in mind for future lectures: Even if we do not explicitly mention the existence of an underlying probability distribution the basic assumption about how the data is generated is always there!

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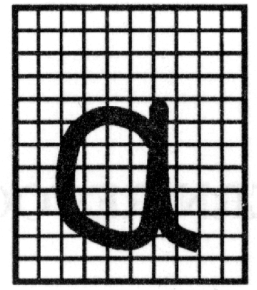
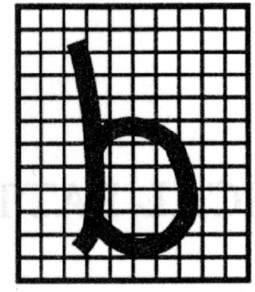
Example: Handwritten Character Recognition





- *How to model this? Regression or Classification.*
  A: **Classification**
- **Goal**: classify a new letter such that the probability of misclassification is minimized

First concept: Class Priors

- The *a priori* probability of a data point belonging to a particular class is called the class prior
- What we can tell about the probability *before* seeing new data
- Example:
  - abaaa babaa aabba aaaaa
- *What are $p(a)$ and $p(b)$?*
  A:

$$\mathcal{C}_1 = a \quad p(\mathcal{C}_1) = 0.75$$
$$\mathcal{C}_2 = b \quad p(\mathcal{C}_2) = 0.25$$
$$\sum_k p(\mathcal{C}_k) = 1$$

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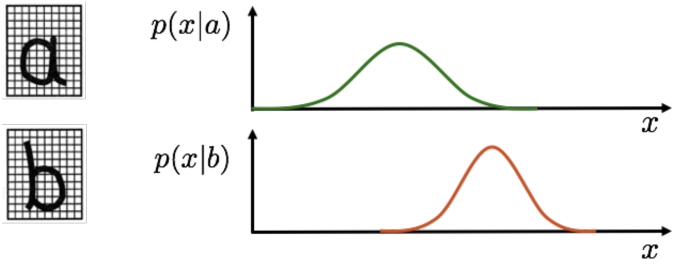
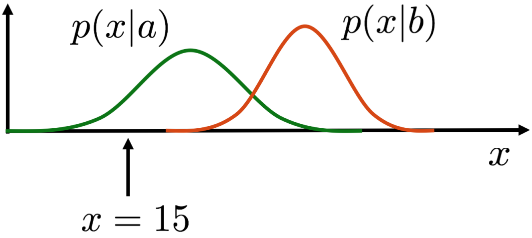
Second concept: Class conditional probabilities

- Probability (Likelihood) of making an observation x given that it comes from some class $\mathcal{C}_k$
- Here, x is often a feature vector, which measures/describes certain properties of the input data, e.g. number of black pixels, aspect ratio, ...

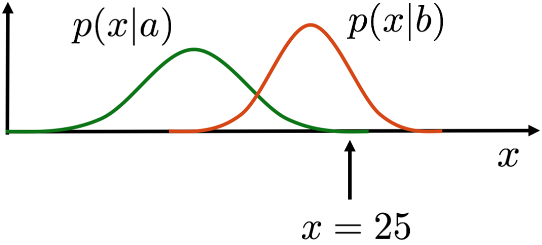


Example: Class conditional probabilities



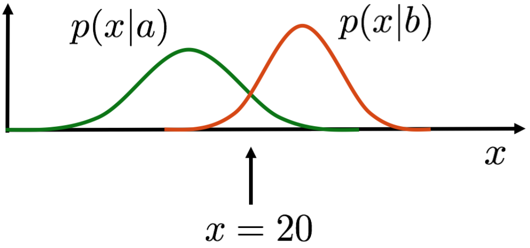
- How do we decide which class the data point belongs to?
- Since $p(x|b)$ is much smaller than $p(x|a)$, we should decide for class a.

Example: Class conditional probabilities



- How do we decide which class the data point belongs to?
- Since $p(x|a)$ is much smaller than $p(x|b)$, we should now decide for class b.

Example: Class conditional probabilities



- How do we decide which class the data point belongs to?
- Assuming the previous priors $p(a) = 0.75$ and $p(b) = 0.25$, we should decide for class a
- How can we formalize this?

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Third Concept: Class posterior probabilities

- We want to find the *a posteriori* probability (posterior), i.e. the probability of class $\mathcal{C}_k$ given the observation x
- Bayes' Theorem

$$p\left(\mathcal{C}_k|x\right) = \frac{p\left(x|\mathcal{C}_k\right)p\left(\mathcal{C}_k\right)}{p\left(x\right)} = \frac{p\left(x|\mathcal{C}_k\right)p\left(\mathcal{C}_k\right)}{\sum_j p\left(x|\mathcal{C}_j\right)p\left(\mathcal{C}_j\right)}$$

- Interpretation

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

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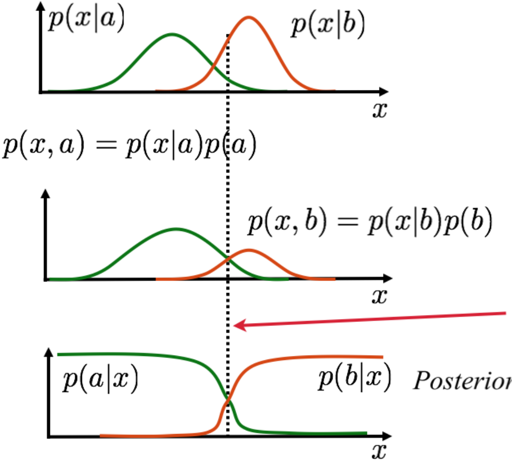
Bayesian Decision Theory



Likelihood

Likelihood × Prior

$$\textit{Posterior} = \frac{\textit{Likelihood} \times \textit{Prior}}{\textit{Normalization factor}}$$

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Bayesian Decision Theory

- Why is it called this way?
  - To some extent, because it involves applying Bayes' rule
  - But this is not the whole story...
  - The real reason is that it is built on so-called Bayesian probabilities

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Bayesian Probabilities

- Probability is not just interpreted as a frequency of a certain event happening
- Rather, it is seen as a degree of belief in an outcome
- Only this allows us to assert a prior belief in a data point coming from a certain class
- Even though this might seem easy to accept to you now, this interpretation was quite contentious in statistics for a long time

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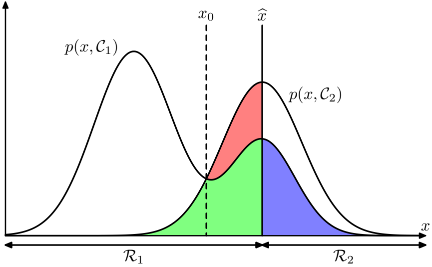
Bayesian Decision Theory

- Goal: Minimize the probability of misclassification



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

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Bayesian Decision Theory

- Optimal Decision rule
  - Decide for $\mathcal{C}_1$ if

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

  - This is equivalent to

$$\begin{aligned} \frac{p(x|\mathcal{C}_1)\,p(\mathcal{C}_1)}{p(x)} &> \frac{p(x|\mathcal{C}_2)\,p(\mathcal{C}_2)}{p(x)} \\ p(x|\mathcal{C}_1)\,p(\mathcal{C}_1) &> p(x|\mathcal{C}_2)\,p(\mathcal{C}_2) \end{aligned}$$

  - Which results in the Likelihood-Ratio Test:

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

  - A classifier obeying this rule is called a Bayes Optimal Classifier

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Generalization to more than two classes

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

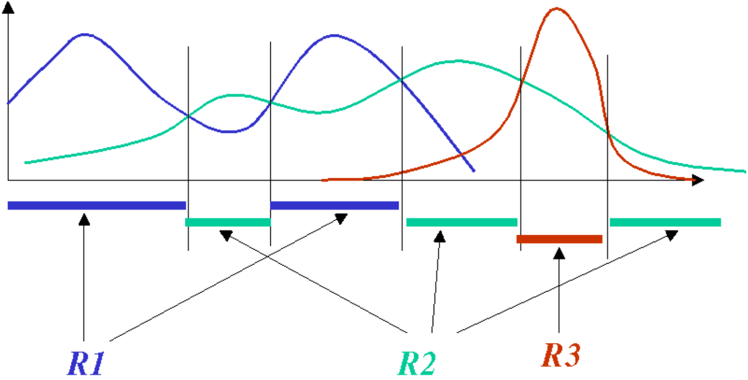
$$p\left(\mathcal{C}_k|x\right) > p\left(\mathcal{C}_j|x\right) \quad \forall j \neq k$$

- which again results in the Likelihood-Ratio Test:

$$\begin{aligned} p\left(x|\mathcal{C}_k\right) p\left(\mathcal{C}_k\right) &> p\left(x|\mathcal{C}_j\right) p\left(\mathcal{C}_j\right) \quad \forall j \neq k \\ \frac{p\left(x|\mathcal{C}_k\right)}{p\left(x|\mathcal{C}_j\right)} &> \frac{p\left(\mathcal{C}_j\right)}{p\left(\mathcal{C}_k\right)} \quad \forall j \neq k \end{aligned}$$

Visualization of the general case

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



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High Dimensional Features

- So far we have only considered one-dimensional features, i.e., $x \in \mathbb{R}$
- We can use more features and generalize to an arbitrary D-dimensional feature space, i.e., $\boldsymbol{x} \in \mathbb{R}^D$
  - For example, in the salmon vs. sea-bass classification task

$$\boldsymbol{x} = \begin{bmatrix} x_1 & x_2 \end{bmatrix}^\intercal \in \mathbb{R}^2$$

  - Where x_1 is the width, and x_2 is the lightness
- The decision boundary we devised still applies to $\boldsymbol{x} \in \mathbb{R}^D$. We just need to use multivariate class-conditional densities $p\left(\boldsymbol{x}|\mathcal{C}_k\right)$

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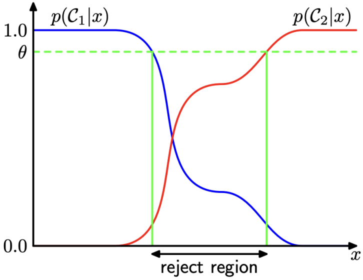
Reject Option



- Classification errors arise from decision regions where the largest posterior probability $p(\mathcal{C}_k|x)$ is significantly less than 1
  - Relatively high uncertainty about class memberships
  - For some applications, it may be better to reject an automatic decision entirely by introducing a decision threshold θ
  - Or use a dummy class "don't know" to which the system assigns all ambiguous cases

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Reject Option

What are further reasons why we might want the machine learning model to abstain from making predictions?

A:

- **Insufficient training data**
- **Out-of-distribution test data**
- **Adversarial attacks**
- **Biased outputs**
- **Output not aligned with certain values**
- **High risk**
- **And many more ...**

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Outline

2. Risk Minimization

- So far, we have tried to minimize the misclassification rate
- There are many cases when not every misclassification is equally bad
- Smoke detector
  - If there is a fire, we need to be very sure that we classify it as such
  - If there is no fire, it is ok to occasionally have a false alarm
- Medical diagnosis
  - If the patient is sick, we need to be very sure that we report them as sick
  - If they are healthy, it is ok to classify them as sick and order further testing that may help clarifying this up

Decisions with Loss Functions

- Differentiate between the possible decisions α_i and the possible true classes $\mathcal{C}_j$
- The loss may be asymmetric as in the medical diagnosis example

$$\text{loss}\left(\text{decision} = \text{healthy} \middle| \text{patient} = \text{sick}\right) >>$$
$$\text{loss}\left(\text{decision} = \text{sick} \middle| \text{patient} = \text{healthy}\right)$$

- Expected loss of making a decision α_i

$$R\left(\alpha_i|x\right) = \mathbb{E}_{\mathcal{C}_k \sim p(\mathcal{C}_k|x)}\left[\lambda\left(\alpha_i|\mathcal{C}_k\right)\right] = \sum_j \lambda\left(\alpha_i|\mathcal{C}_j\right) p\left(\mathcal{C}_j|x\right)$$

with loss function: $\lambda\left(\alpha_i|\mathcal{C}_j\right)$

Minimize the overall risk

- The expected loss of a decision is also called the risk of making a decision
- So, instead of minimizing the misclassification rate (recap)

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

- We minimize the overall risk

$$
R(\alpha_i|x) = \mathbb{E}_{\mathcal{C}_k \sim p(\mathcal{C}_k|x)}\left[\lambda(\alpha_i|\mathcal{C}_k)\right] = \sum_j \lambda(\alpha_i|\mathcal{C}_j)\,p(\mathcal{C}_j|x)
$$

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Simple example

- 2 classes: $\mathcal{C}_1, \mathcal{C}_2$
- 2 decisions: α_1, α_2
- Loss function: $\lambda\left(\alpha_i|\mathcal{C}_j\right) = \lambda_{ij}$
- Expected loss (= risk R) of both decisions

$$
\begin{aligned}
R\left(\alpha_1|x\right) &= \lambda_{11} p\left(\mathcal{C}_1|x\right) + \lambda_{12} p\left(\mathcal{C}_2|x\right) \\
R\left(\alpha_2|x\right) &= \lambda_{21} p\left(\mathcal{C}_1|x\right) + \lambda_{22} p\left(\mathcal{C}_2|x\right)
\end{aligned}
$$

- Goal: Create a decision rule such that overall risk is minimized
  - *When to decide α_1?*
    A: **if** $R\left(\alpha_2|x\right) > R\left(\alpha_1|x\right)$

Risk-aware decision rule

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

- It is reasonable to assume that the loss of a correct decision is smaller than that of a wrong decision: $\lambda_{ij} > \lambda_{ii} \quad \forall j \neq i$

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Risk Minimization with 0-1 Loss

- Risk-aware decision rule

$$\frac{p(x|C_1)}{p(x|C_2)} > \frac{\lambda_{12} - \lambda_{22}}{\lambda_{21} - \lambda_{11}} \frac{p(C_2)}{p(C_1)}$$

- 0-1 loss function:

$$\lambda(\alpha_i|\mathcal{C}_j) = \begin{cases} 0 & i = j \\ 1 & i \neq j \end{cases}$$

- Decide for α_1 if

$$\frac{p(x|C_1)}{p(x|C_2)} > \frac{p(C_2)}{p(C_1)}$$

- The 0-1 loss leads to the same decision rule that minimized the misclassification rate

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Outline

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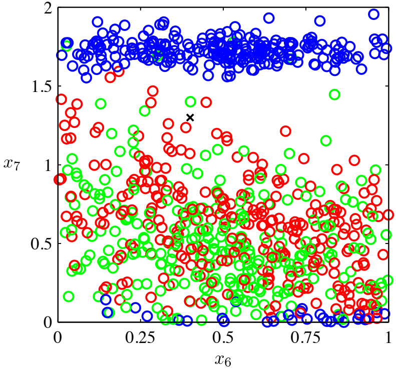
Training Data



- How do we get the probability distributions from this so that we can classify with them?

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Probability Density Estimation

- So far we have seen:
  - **Optimal Bayes Classification**, based on probability distributions $p(x|C_k)p(C_k)$
- The prior $p(C_k)$ is easy to deal with. We can "just count" the number of occurrences of each class in the training data
- We need to estimate/learn the **class-conditional probability density** $p(x|C_k)$
  - **Supervised training**: we know the input data points and their true labels (classes)
  - Estimate the density separately for each class C_k

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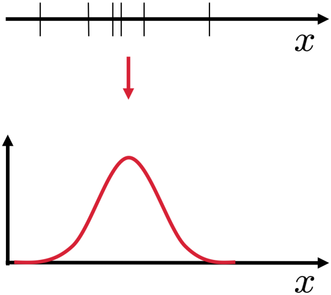
Probability Density Estimation

- **Remember:** The relationship between the outcomes of a random variable x and its probability $Pr(X = x)$ is referred to as the probability density, or simply the "density."

- Training data

$$x_1, x_2, x_3, \ldots$$

- Estimation $p(x)$



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Types of Probability Density Estimation models

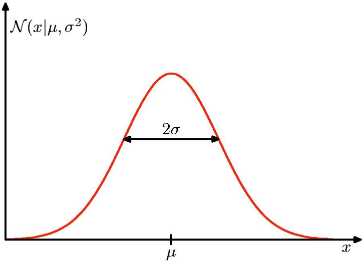
- **Parametric probability density estimation** involves selecting a common distribution and estimating the distribution parameters from data samples.
- **Non-parametric probability density estimation** involves fitting a model to the arbitrary distribution of the data, e.g., kernel density estimation – every known data point in the dataset is used as a parameter.
- **Mixture density models** are flexible models that combine parametric and non-parametric estimations.

Outline

Parametric Density Models

- Simple case: **Gaussian Distribution**

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



- Is governed by two parameters: mean and variance. If we know these parameters, we can fully describe $p(x)$

Parametric Density Models

- Notation for **parametric density models**

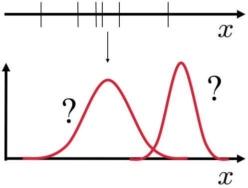
$$x \sim p(x|\theta)$$

- For the Gaussian distribution

$$\theta = (\mu, \sigma)$$
$$x \sim p(x|\mu, \sigma)$$

Parametric Density Models

- **Learning** means to estimate the parameters θ given the training data $\mathcal{D} = \{x_1, x_2, \ldots\}$



- **Likelihood** of θ is defined as the probability that the data $\mathcal{D}$ was generated from the probability density function with parameters θ

$$L(\theta) = p(\mathcal{D}|\theta)$$

Maximum Likelihood Method

- Consider a set of points $\mathcal{D} = \{x_1, \ldots, x_N\}$, we are interested in the likelihood of all data $p(\mathcal{D}|\theta)$.
- **Assumption**: the **data is i.i.d.** (independent and identically distributed)
  - The random variables x_1 and x_2 are independent if

$$P\left(x_1 \leq \alpha, x_2 \leq \beta\right) = P\left(x_1 \leq \alpha\right) P\left(x_2 \leq \beta\right) \quad \forall \alpha, \beta \in \mathbb{R}$$

  - The random variables x_1 and x_2 are identically distributed if

$$P\left(x_1 \leq \alpha\right) = P\left(x_2 \leq \alpha\right) \quad \forall \alpha \in \mathbb{R}$$

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Maximum Likelihood Method

- Likelihood

$$L(\theta) = p(\mathcal{D}|\theta) = p(x_1, \ldots, x_N|\theta)$$

(using the i.i.d. assumption)

$$= p(x_1|\theta) \cdot \ldots \cdot p(x_n|\theta)$$

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

- **Maximum Likelihood Estimation**: $\hat{\theta}_{\mathrm{ML}} = \arg\max_{\theta} p(\mathcal{D}|\theta)$ seeks for the parameter $\hat{\theta}_{\mathrm{ML}}$, which best explains the data $\mathcal{D}$

- $\hat{\theta}_{\mathrm{ML}}$ is a **random variable** – it is an estimate based on the available dataset. Consequently, we are interested in its **mean value** (the **most probable value**) and its **variance**.

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Maximum log-Likelihood Method

- It is more convenient and numerical stable to maximize the log-likelihood w.r.t. θ

$$LL(\theta) = \log L(\theta) = \log p(\mathcal{D}|\theta) = \log \prod_{n=1}^{N} p(x_n|\theta) = \sum_{n=1}^{N} \log p(x_n|\theta)$$

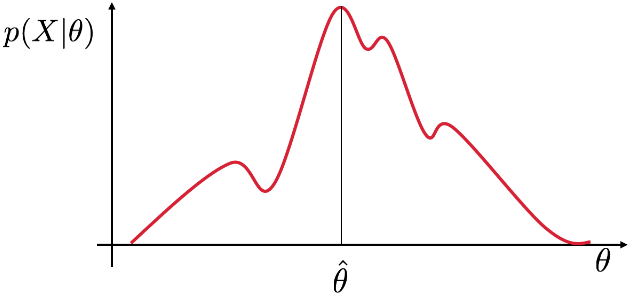
- Because the logarithm is monotonically increasing, it holds

$$\hat{\theta}_{\mathrm{ML}} = \arg\max_{\theta} \sum_{n=1}^{N} \log p(x_n|\theta) = \arg\max_{\theta} L(\theta)$$

- Maximizing a sum of terms is always easier than maximizing a product; cf., the difficulty of expressing the derivative of a long product of terms.

Likelihood Estimation

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



Outline

5. Wrap-Up

Now, you know:

- The definition of class priors, class conditional probabilities and class posteriors
- How to use Bayes Theorem for classification
- How to calculate the probability of misclassification
- How to obtain optimal decisions using Bayes optimal classifier
- How to generalize decision making using multi-dimensional features and more than 2 classes
- The value of risk minimization and how it relates to misclassification
- Maximum Likelihood Method

Self-Test Questions

- How do we incorporate prior knowledge on the class distribution?
- How can we decide on classifying a query based on simple and general loss functions?
- What does “Bayes optimal” mean?
- How can we deal with 2 or more classes?
- How can we deal with high dimensional feature vectors?
- What are the equations for misclassification rate and risk?

Reading Assignments

To get a deeper understanding of today's topics:

- Bayesian Decision Theory: Bishop 2006, Chapter 1.5 or Murphy 2023, Chapter 5.1.1, 5.1.2
- The Bayesian idea: Lindholm 2022, Chapter 9.1

Next week:

- Probability Distributions: Bishop, Chapter 2
- Mixtures Models and EM: Bishop, Chapter 9