Machine Learning – Lecture 2

Probability Density Estimation

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Announcements

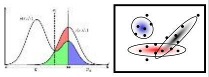
- Exceptional number of lecture participants this year
  - Current count: 449 participants
  - This is very nice, but it stretches our resources to their limits
- Monday lecture slot
  - Shifted to 8:30 – 10:00 in AH IV (276 seats)
  - We will monitor the situation and take further action if the space is not sufficient
- Thursday lecture slot
  - Will stay at 14:15 – 15:45 in H02 (C.A.R.L, 786 seats)
- Exercises (non-mandatory)
  - We will try to offer corrections, but we will have to see how to handle those numbers…

Announcements

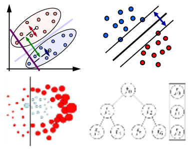
- L2P electronic repository
  - Slides, exercises, and supplementary material will be made available here
  - Lecture recordings will be uploaded 2-3 days after the lecture
- Course webpage
  - http://www.vision.rwth-aachen.de/courses/
  - Slides will also be made available on the webpage
- Please subscribe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

Course Outline

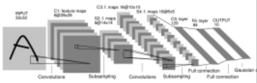
- Fundamentals
  - Bayes Decision Theory
  - Probability Density Estimation



- 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

Bayes Decision Theory

Thomas Bayes, 1701-1761

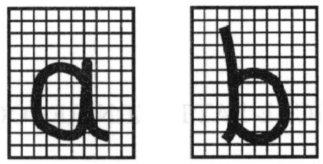
"The theory of inverse probability is founded upon an error, and must be wholly rejected."

R.A. Fisher, 1925

Image source: Wikipedia

Bayes Decision Theory

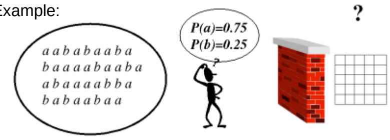
- Example: handwritten character recognition



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

Bayes Decision Theory

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

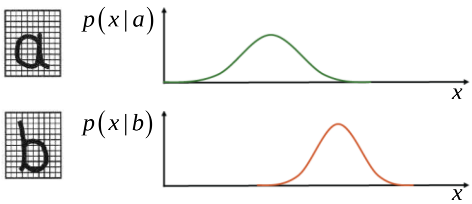


$$C_1 = a \qquad p(C_1) = 0.75$$
$$C_2 = b \qquad p(C_2) = 0.25$$

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

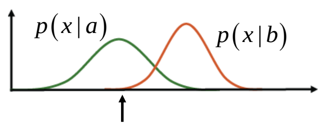
Bayes Decision Theory

- 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.



Bayes Decision Theory

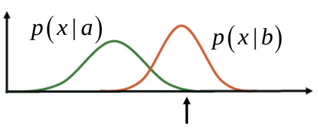
- Example:



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

Bayes Decision Theory

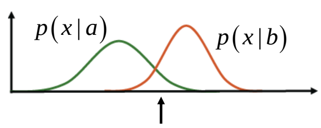
- Example:



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

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'.
  - $\Rightarrow$ How can we formalize this?

Bayes Decision Theory

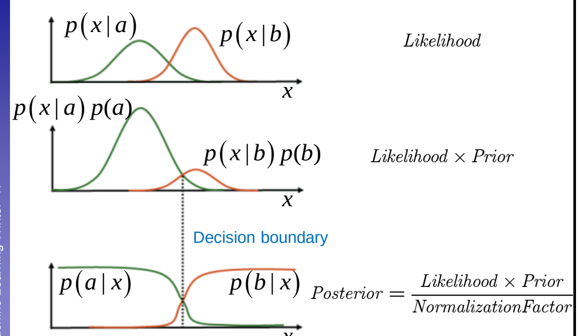
- Concept 3: Posterior probabilities $p(C_k \mid x)$
  - We are typically interested in the *a posteriori* probability, i.e. the probability of class C_k given the measurement vector x.
- Bayes' Theorem:

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

- Interpretation

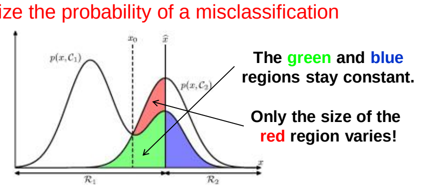
$$Posterior = \frac{Likelihood \times Prior}{Normalization\ Factor}$$

Bayes Decision Theory



Bayesian Decision Theory

- Goal: Minimize the probability of a misclassification



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

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)

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

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

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

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 L_{kj}

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

- Example: cancer diagnosis

Decision

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

Classifying with Loss Functions

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

"invest" "don't invest"

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

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

⇒ 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

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

- 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: α_1, α_2
  - Loss function: $L(\alpha_j|\mathcal{C}_k) = L_{kj}$
  - Expected loss (= risk R) for the two decisions:

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

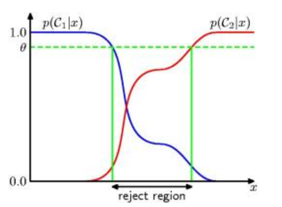
- Goal: Decide such that expected loss is minimized
  - I.e. decide α_1 if $R(\alpha_2|\mathbf{x}) > R(\alpha_1|\mathbf{x})$

Minimizing the Expected Loss

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

⇒ 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.
  - ⇒ *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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- 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

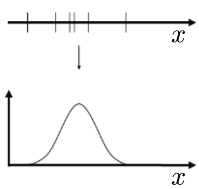
- Up to now
  - Bayes optimal classification
  - Based on the probabilities $p(\mathbf{x}|\mathcal{C}_k)p(\mathcal{C}_k)$
- How can we estimate (=learn) those probability densities?
  - Supervised training case: data and class labels are known.
  - Estimate the probability density for each class $\mathcal{C}_k$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

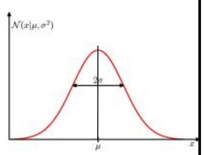


- Methods
  - Parametric representations (today)
  - Non-parametric representations (lecture 3)
  - Mixture models (lecture 4)

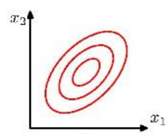
The Gaussian (or Normal) Distribution

- One-dimensional case
  - Mean μ
  - 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
  - Mean μ
  - Covariance Σ



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

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.

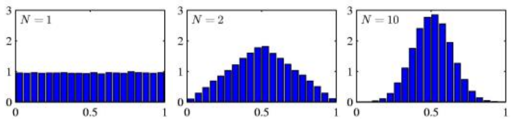


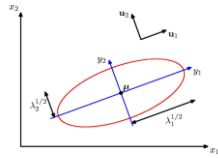
Image source: C.M. Bishop, 2006

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, Δ is often called the Mahalanobis distance from $\mathbf{x}$ to μ.



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

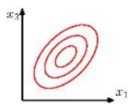
Image source: C.M. Bishop, 2006

Gaussian Distribution – Properties

- Special cases
  - Full covariance matrix

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

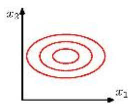
$\Rightarrow$ General ellipsoid shape



  - Diagonal covariance matrix

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

$\Rightarrow$ Axis-aligned ellipsoid



  - Uniform variance

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

$\Rightarrow$ Hypersphere

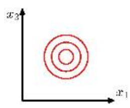
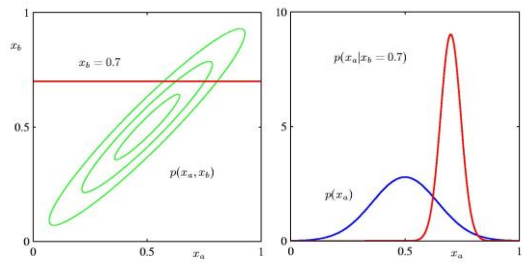


Image source: C.M. Bishop, 2006

Gaussian Distribution – Properties

- The marginals of a Gaussian are again Gaussians:



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  - Minimizing the expected loss
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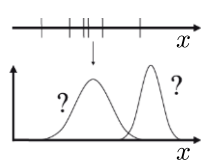
Parametric Methods

- Given
  - 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
  - Estimation of the parameters θ
- Likelihood of θ
  - Probability that the data X have indeed been generated from a probability density with parameters θ

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

Slide adapted from Bernt Schiele

Maximum Likelihood Approach

- 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

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

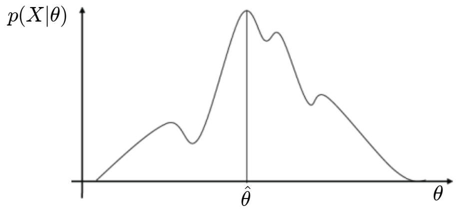
  - Log-likelihood

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

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

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

$$\hat{\mu} = \frac{1}{N}\sum_{n=1}^{N}x_n \qquad \text{"sample mean"}$$

- In a similar fashion, we get

$$\hat{\sigma}^2 = \frac{1}{N}\sum_{n=1}^{N}(x_n-\hat{\mu})^2 \qquad \text{"sample variance"}$$

- $\hat{\theta} = (\hat{\mu}, \hat{\sigma})$ 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 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

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

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

- Corrected estimate:

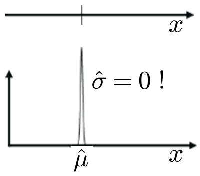
$$\tilde{\sigma}^2 = \frac{N}{N-1}\sigma^2_{\mathrm{ML}} = \frac{1}{N-1}\sum_{n=1}^{N}(x_n-\hat{\mu})^2$$

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

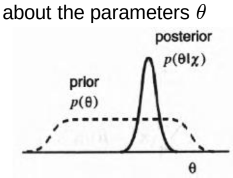
- To see the difference…
  - Suppose we want to estimate the uncertainty whether the Arctic ice cap will have disappeared by the end of the century.
  - This question makes no sense in a Frequentist view, since the event cannot be repeated numerous times.
  - In the Bayesian view, we generally have a 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 θ to be unknown, but fixed.
  - In Bayesian learning, we consider θ to be a random variable.
- This allows us to use knowledge about the parameters θ
  - i.e. to use a prior for θ
  - 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.

  $\Rightarrow$ 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
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