Machine Learning – Lecture 3

Probability Density Estimation II

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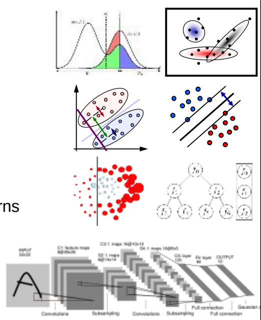
Announcements

- Exam dates
  - We're in the process of fixing the first exam date
- Exercises
  - The first exercise sheet is available on L2P now
  - First exercise lecture on 30.10.2017
  - ⇒ *Please submit your results by evening of 29.10. via L2P (detailed instructions can be found on the exercise sheet)*

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



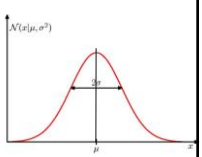
Topics of This Lecture

- Recap: Parametric Methods
  - Gaussian distribution
  - Maximum Likelihood approach
- Non-Parametric Methods
  - Histograms
  - Kernel density estimation
  - K-Nearest Neighbors
  - k-NN for Classification
- Mixture distributions
  - Mixture of Gaussians (MoG)
  - Maximum Likelihood estimation attempt

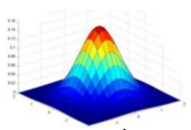
Recap: Gaussian (or Normal) Distribution

- 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



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

Image source: C.M. Bishop, 2006

Recap: Maximum Likelihood Approach

- Computation of the likelihood
  - Single data point: $p(x_n|\theta)$
  - Assumption: all data points $X = \{x_1,\ldots,x_n\}$ 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)
  - ⇒ Take the derivative and set it to zero.

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

Slide credit: Bernt Schiele

Maximum Likelihood Approach

- When applying ML to the Gaussian distribution, we 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

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

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

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

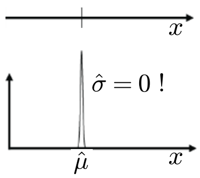
- Corrected estimate:

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

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:

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

  - 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

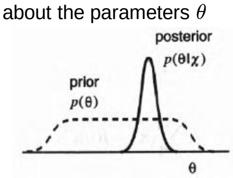
- To see the difference…
  - Suppose we want to estimate the uncertainty whether the Arctic ice cap will have disappeared by the end of the century.
  - This question makes no sense in a Frequentist view, since the event cannot be repeated numerous times.
  - In the Bayesian view, we generally have a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

$$\textit{Posterior} \propto \textit{Likelihood} \times \textit{Prior}$$

  - 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.
  - ⇒ I will introduce it in more detail in the Advanced ML lecture.

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  - Gaussian distribution
  - Maximum Likelihood approach
- Non-Parametric Methods
  - Histograms
  - Kernel density estimation
  - K-Nearest Neighbors
  - k-NN for Classification
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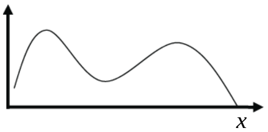
Non-Parametric Methods

- Non-parametric representations
  - Often the functional form of the distribution is unknown

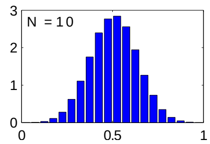


- Estimate probability density from data
  - Histograms
  - Kernel density estimation (Parzen window / Gaussian kernels)
  - k-Nearest-Neighbor

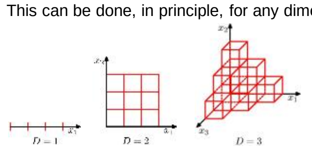
Histograms

- Basic idea:
  - Partition the data space into distinct bins with widths Δ_i and count the number of observations, n_i, in each bin.

$$p_i = \frac{n_i}{N\Delta_i}$$



  - Often, the same width is used for all bins, $\Delta_i = \Delta$.
  - This can be done, in principle, for any dimensionality D…



…but the required number of bins grows exponentially with D!

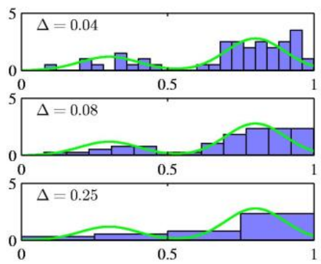
Histograms

- The bin width Δ acts as a smoothing factor.

not smooth enough

about OK

too smooth



Summary: Histograms

- Properties
  - Very general. In the limit ($N \to \infty$), every probability density can be represented.
  - No need to store the data points once histogram is computed.
  - Rather brute-force
- Problems
  - High-dimensional feature spaces
    - D-dimensional space with M bins/dimension will require M^D bins!
    - ⇒ Requires an exponentially growing number of data points
    - ⇒"Curse of dimensionality"
  - Discontinuities at bin edges
  - Bin size?
    - too large: too much smoothing
    - too small: too much noise

Statistically Better-Founded Approach

- Data point $\mathbf{x}$ comes from pdf $p(\mathbf{x})$
  - Probability that x falls into small region $\mathcal{R}$

$$P = \int_{\mathcal{R}} p(y)dy$$

- If $\mathcal{R}$ is sufficiently small, $p(\mathbf{x})$ is roughly constant
  - Let V be the volume of $\mathcal{R}$

$$P = \int_{\mathcal{R}} p(y)dy \approx p(\mathbf{x})V$$

- If the number N of samples is sufficiently large, we can estimate P as

$$P = \frac{K}{N} \qquad \Rightarrow p(\mathbf{x}) \approx \frac{K}{NV}$$

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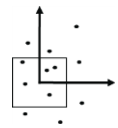
Statistically Better-Founded Approach

$$p(\mathbf{x}) \approx \frac{K}{NV}$$

fixed V determine K → Kernel Methods

fixed K determine V → K-Nearest Neighbor

- Kernel methods
  - Example: Determine the number K of data points inside a fixed hypercube…



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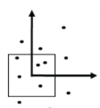
Kernel Methods

- Parzen Window
  - Hypercube of dimension D with edge length h:



$$k(\mathbf{u}) = \begin{cases} 1, & |u_i| \leq \frac{1}{2}h, \quad i = 1, \dots, D \\ 0, & else \end{cases}$$

"Kernel function"

$$K = \sum_{n=1}^{N} k(\mathbf{x} - \mathbf{x}_n) \qquad V = \int k(\mathbf{u})d\mathbf{u} = h^D$$

  - Probability density estimate:

$$p(\mathbf{x}) \approx \frac{K}{NV} = \frac{1}{Nh^D} \sum_{n=1}^{N} k(\mathbf{x} - \mathbf{x}_n)$$

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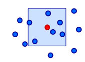
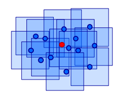
Kernel Methods: Parzen Window

- Interpretations
  1. We place a *kernel window k at location $\mathbf{x}$* and count how many data points fall inside it.



  2. We place a *kernel window k around each data point $\mathbf{x}_n$* and sum up their influences at location $\mathbf{x}$.



  ⇒ Direct visualization of the density.

- Still, we have artificial discontinuities at the cube boundaries…
  - We can obtain a smoother density model if we choose a smoother kernel function, e.g. a Gaussian

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Kernel Methods: Gaussian Kernel

- Gaussian kernel
  - Kernel function

$$k(\mathbf{u}) = \frac{1}{(2\pi h^2)^{1/2}} \exp\left\{-\frac{\mathbf{u}^2}{2h^2}\right\}$$

$$K = \sum_{n=1}^{N} k(\mathbf{x} - \mathbf{x}_n) \qquad V = \int k(\mathbf{u})d\mathbf{u} = 1$$

  - Probability density estimate

$$p(\mathbf{x}) \approx \frac{K}{NV} = \frac{1}{N} \sum_{n=1}^{N} \frac{1}{(2\pi)^{D/2}h} \exp\left\{-\frac{||\mathbf{x} - \mathbf{x}_n||^2}{2h^2}\right\}$$

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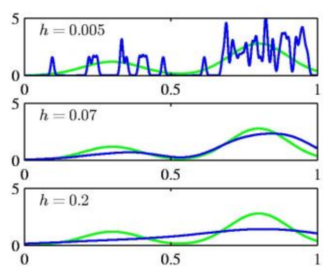
Gauss Kernel: Examples

not smooth enough

about OK

too smooth



h acts as a smoother.

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Image source: C.M. Bishop, 2006

Kernel Methods

- In general
  - Any kernel such that

$$k(\mathbf{u}) \geqslant 0, \qquad \int k(\mathbf{u})\,\mathrm{d}\mathbf{u} = 1$$

can be used. Then

$$K = \sum_{n=1}^{N} k(\mathbf{x} - \mathbf{x}_n)$$

  - And we get the probability density estimate

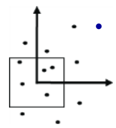
$$p(\mathbf{x}) \approx \frac{K}{NV} = \frac{1}{N}\sum_{n=1}^{N} k(\mathbf{x} - \mathbf{x}_n)$$

Statistically Better-Founded Approach

$$p(\mathbf{x}) \approx \frac{K}{NV}$$

fixed V determine K → Kernel Methods

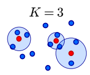
fixed K determine V → K-Nearest Neighbor



- K-Nearest Neighbor
  - Increase the volume V until the K next data points are found.

K-Nearest Neighbor

- Nearest-Neighbor density estimation
  - Fix K, estimate V from the data.
  - Consider a hypersphere centred on $\mathbf{x}$ and let it grow to a volume $V^\star$ that includes K of the given N data points.
  - Then



$$p(\mathbf{x}) \simeq \frac{K}{NV^\star}.$$

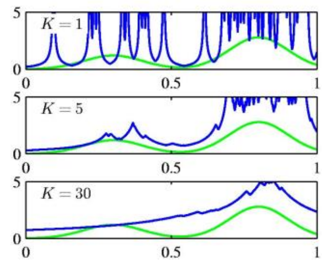
- Side note
  - Strictly speaking, the model produced by K-NN is not a true density model, because the integral over all space diverges.
  - E.g. consider $K = 1$ and a sample exactly on a data point $\mathbf{x} = x_j$.

k-Nearest Neighbor: Examples

not smooth enough

about OK

too smooth



K acts as a smoother.

Summary: Kernel and k-NN Density Estimation

- Properties
  - Very general. In the limit ($N\rightarrow\infty$), every probability density can be represented.
  - No computation involved in the training phase
  - ⇒ Simply storage of the training set
- Problems
  - Requires storing and computing with the entire dataset.
  - ⇒ Computational cost linear in the number of data points.
  - ⇒ This can be improved, at the expense of some computation during training, by constructing efficient tree-based search structures.
  - Kernel size / K in K-NN?
    - Too large: too much smoothing
    - Too small: too much noise

K-Nearest Neighbor Classification

- Bayesian Classification

$$p(\mathcal{C}_j|\mathbf{x}) = \frac{p(\mathbf{x}|\mathcal{C}_j)p(\mathcal{C}_j)}{p(\mathbf{x})}$$

- Here we have

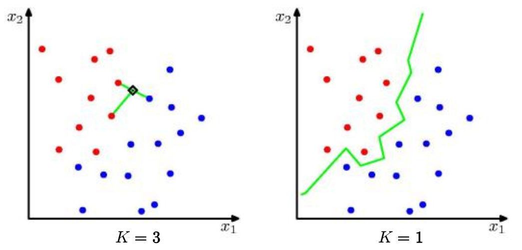
$$p(\mathbf{x}) \approx \frac{K}{NV}$$

$$p(\mathbf{x}|\mathcal{C}_j) \approx \frac{K_j}{N_j V} \longrightarrow p(\mathcal{C}_j|\mathbf{x}) \approx \frac{K_j}{N_j V}\frac{N_j}{N}\frac{NV}{K} = \frac{K_j}{K}$$

$$p(\mathcal{C}_j) \approx \frac{N_j}{N}$$

k-Nearest Neighbor classification

K-Nearest Neighbors for Classification



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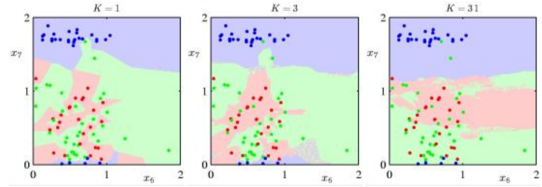
K-Nearest Neighbors for Classification

- Results on an example data set



- K acts as a smoothing parameter.
- Theoretical guarantee
  - For $N \to \infty$, the error rate of the 1-NN classifier is never more than twice the optimal error (obtained from the true conditional class distributions).

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Bias-Variance Tradeoff

- Probability density estimation
  - Histograms: bin size?
    - Δ too large: too smooth
    - Δ too small: not smooth enough
  - Kernel methods: kernel size?
    - h too large: too smooth
    - h too small: not smooth enough
  - K-Nearest Neighbor: K?
    - K too large: too smooth
    - K too small: not smooth enough

Too much bias
Too much variance

- This is a general problem of many probability density estimation methods
  - Including parametric methods and mixture models

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Discussion

- The methods discussed so far are all simple and easy to apply. They are used in many practical applications.
- However…
  - Histograms scale poorly with increasing dimensionality.
  - $\Rightarrow$ Only suitable for relatively low-dimensional data.
  - Both k-NN and kernel density estimation require the entire data set to be stored.
  - $\Rightarrow$ Too expensive if the data set is large.
  - Simple parametric models are very restricted in what forms of distributions they can represent.
  - $\Rightarrow$ Only suitable if the data has the same general form.
- We need density models that are efficient and flexible!
  - $\Rightarrow$ Next topic…

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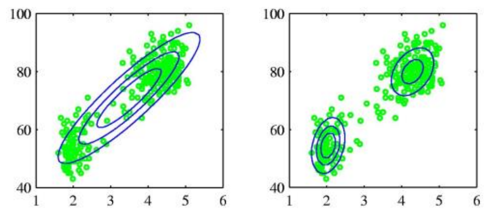
Mixture Distributions

- A single parametric distribution is often not sufficient
  - E.g. for multimodal data



Single Gaussian

Mixture of two Gaussians

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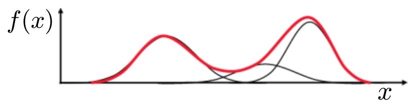
Mixture of Gaussians (MoG)

- Sum of M individual Normal distributions



  - In the limit, every smooth distribution can be approximated this way (if M is large enough)

$$p(x|\theta) = \sum_{j=1}^{M} p(x|\theta_j)p(j)$$

Mixture of Gaussians

$$p(x|\theta) = \sum_{j=1}^{M} \boxed{p(x|\theta_j)}\boxed{p(j)}$$

Likelihood of measurement x given mixture component j

$$p(x|\theta_j) = \mathcal{N}(x|\mu_j, \sigma_j^2) = \frac{1}{\sqrt{2\pi}\sigma_j} \exp\left\{-\frac{(x-\mu_j)^2}{2\sigma_j^2}\right\}$$

$p(j) = \pi_j$ with $0 \cdot \pi_j \cdot 1$ and $\sum_{j=1}^{M} \pi_j = 1$

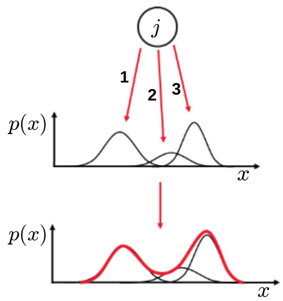
Prior of component j

- Notes
  - The mixture density integrates to 1: $\int p(x)dx = 1$
  - The mixture parameters are

$$\theta = (\pi_1, \mu_1, \sigma_1, \dots, , \pi_M, \mu_M, \sigma_M)$$

Mixture of Gaussians (MoG)

- "Generative model"



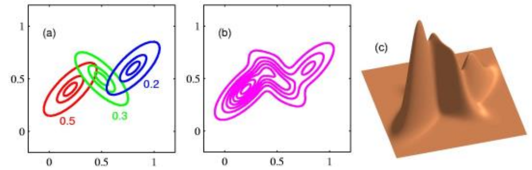
$p(j) = \pi_j$ "Weight" of mixture component

$p(x|\theta_j)$ Mixture component

Mixture density

$$p(x|\theta) = \sum_{j=1}^{M} p(x|\theta_j)p(j)$$

Mixture of Multivariate Gaussians



Mixture of Multivariate Gaussians

- Multivariate Gaussians

$$p(\mathbf{x}|\theta) = \sum_{j=1}^{M} p(\mathbf{x}|\theta_j)p(j)$$

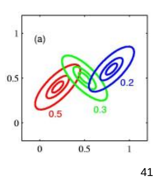
$$p(\mathbf{x}|\theta_j) = \frac{1}{(2\pi)^{D/2}|\boldsymbol{\Sigma}_j|^{1/2}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_j)^{\mathrm{T}}\boldsymbol{\Sigma}_j^{-1}(\mathbf{x}-\boldsymbol{\mu}_j)\right\}$$

  - Mixture weights / mixture coefficients:

$p(j) = \pi_j$ with $0 \cdot \pi_j \cdot 1$ and $\sum_{j=1}^{M} \pi_j = 1$

  - Parameters:

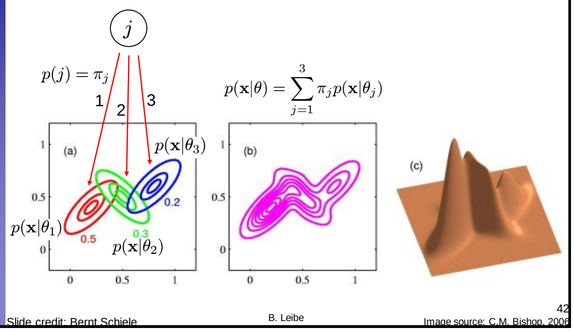
$$\theta = (\pi_1, \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1, \dots, \pi_M, \boldsymbol{\mu}_M, \boldsymbol{\Sigma}_M)$$



Mixture of Multivariate Gaussians

- "Generative model"

$$p(\mathbf{x}|\theta) = \sum_{j=1}^{3} \pi_j p(\mathbf{x}|\theta_j)$$



Mixture of Gaussians – 1st Estimation Attempt

- Maximum Likelihood
  - Minimize $E = -\ln L(\theta) = -\sum_{n=1}^{N} \ln p(\mathbf{x}_n|\theta)$
  - Let's first look at μ_j:
    $$\frac{\partial E}{\partial \boldsymbol{\mu}_j} = 0$$

  - We can already see that this will be difficult, since
    $$\ln p(\mathbf{X}|\boldsymbol{\pi},\boldsymbol{\mu},\boldsymbol{\Sigma}) = \sum_{n=1}^{N} \ln \left\{ \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k) \right\}$$
    This will cause problems!

Mixture of Gaussians – 1st Estimation Attempt

- Minimization:

$$\frac{\partial}{\partial \boldsymbol{\mu}_j}\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k) = \boldsymbol{\Sigma}^{-1}(\mathbf{x}_n-\boldsymbol{\mu}_j)\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k)$$

$$\frac{\partial E}{\partial \boldsymbol{\mu}_j} = -\sum_{n=1}^{N} \frac{\frac{\partial}{\partial \boldsymbol{\mu}_j} p(\mathbf{x}_n|\theta_j)}{\sum_{k=1}^{K} p(\mathbf{x}_n|\theta_k)}$$
$$= -\sum_{n=1}^{N} \left(\boldsymbol{\Sigma}^{-1}(\mathbf{x}_n-\boldsymbol{\mu}_j) \frac{p(\mathbf{x}_n|\theta_j)}{\sum_{k=1}^{K} p(\mathbf{x}_n|\theta_k)} \right)$$
$$= -\cancel{\boldsymbol{\Sigma}}^{-1} \sum_{n=1}^{N} (\mathbf{x}_n-\boldsymbol{\mu}_j) \underbrace{\frac{\pi_j \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j,\boldsymbol{\Sigma}_j)}{\sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k)}}_{= \gamma_j(\mathbf{x}_n)} \overset{!}{=} 0$$

"responsibility" of component j for $\mathbf{x}_n$

- We thus obtain
$$\Rightarrow \boldsymbol{\mu}_j = \frac{\sum_{n=1}^{N} \gamma_j(\mathbf{x}_n)\mathbf{x}_n}{\sum_{n=1}^{N} \gamma_j(\mathbf{x}_n)}$$

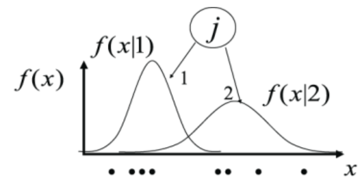
Mixture of Gaussians – 1st Estimation Attempt

- But…
$$\boldsymbol{\mu}_j = \frac{\sum_{n=1}^{N} \gamma_j(\mathbf{x}_n)\mathbf{x}_n}{\sum_{n=1}^{N} \gamma_j(\mathbf{x}_n)} \qquad \gamma_j(\mathbf{x}_n) = \frac{\pi_j \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j,\boldsymbol{\Sigma}_j)}{\sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k)}$$

- I.e. there is no direct analytical solution!
$$\frac{\partial E}{\partial \boldsymbol{\mu}_j} = f(\pi_1, \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1, \ldots, \pi_M, \boldsymbol{\mu}_M, \boldsymbol{\Sigma}_M)$$
  - Complex gradient function (non-linear mutual dependencies)
  - Optimization of one Gaussian depends on all other Gaussians!
  - It is possible to apply iterative numerical optimization here, but in the following, we will see a simpler method.

Mixture of Gaussians – Other Strategy

- Other strategy:



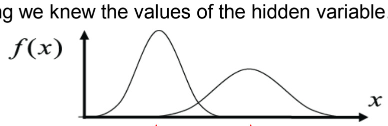
  - Observed data: • ••• •• • •
  - Unobserved data: 1 111 22 2 2
    - Unobserved = "hidden variable": j|x

$h(j=1|x_n) =$ 1 111 00 0 0

$h(j=2|x_n) =$ 0 000 11 1 1

Mixture of Gaussians – Other Strategy

- Assuming we knew the values of the hidden variable…



ML for Gaussian #1 ML for Gaussian #2

assumed known → 1 111 22 2 2 j

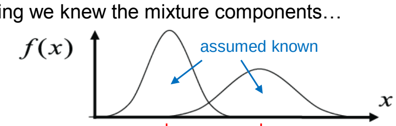
$h(j=1|x_n) =$ 1 111 00 0 0

$h(j=2|x_n) =$ 0 000 11 1 1

$$\mu_1 = \frac{\sum_{n=1}^{N} h(j=1|x_n)x_n}{\sum_{i=1}^{N} h(j=1|x_n)} \qquad \mu_2 = \frac{\sum_{n=1}^{N} h(j=2|x_n)x_n}{\sum_{i=1}^{N} h(j=2|x_n)}$$

Mixture of Gaussians – Other Strategy

- Assuming we knew the mixture components…



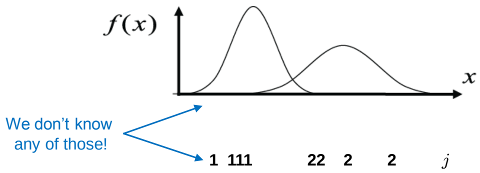
$p(j=1|x)$ $p(j=2|x)$

1 111 22 2 2 j

- Bayes decision rule: Decide $j = 1$ if
$$p(j=1|x_n) > p(j=2|x_n)$$

Mixture of Gaussians – Other Strategy

- Chicken and egg problem – what comes first?



- In order to break the loop, we need an estimate for j.
  - E.g. by clustering…
  - ⇒ Next lecture…

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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