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Machine Learning – Lecture 4

Mixture Models and EM

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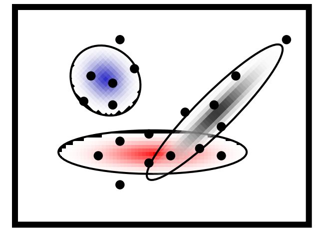
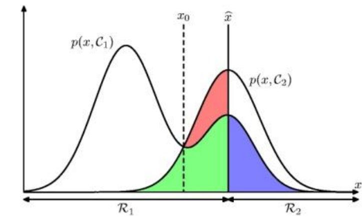
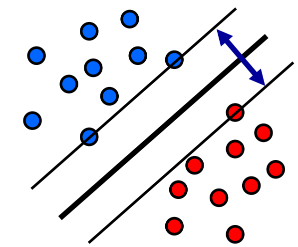
Many slides adapted from B. Schiele

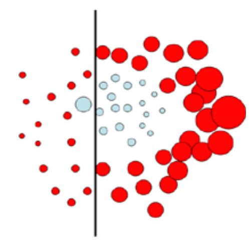
Course Outline

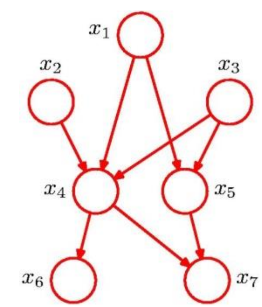
- Fundamentals (2 weeks)
  - Bayes Decision Theory
  - Probability Density Estimation
- Discriminative Approaches (5 weeks)
  - Linear Discriminant Functions
  - Support Vector Machines
  - Ensemble Methods & Boosting
  - Randomized Trees, Forests & Ferns
- Generative Models (4 weeks)
  - Bayesian Networks
  - Markov Random Fields

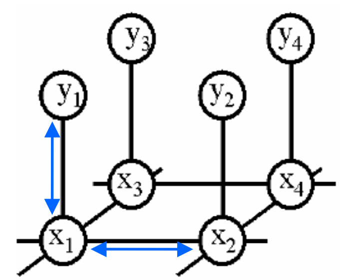












Recap: Bayesian Learning Approach

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

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

Assumption: given θ, 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 θ (i.e. by the parametric form of the pdf).

Recap: Bayesian Learning Approach

- Discussion

Likelihood of the parametric form θ given the data set X.

Estimate for x based on parametric form θ

Prior for the parameters θ

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

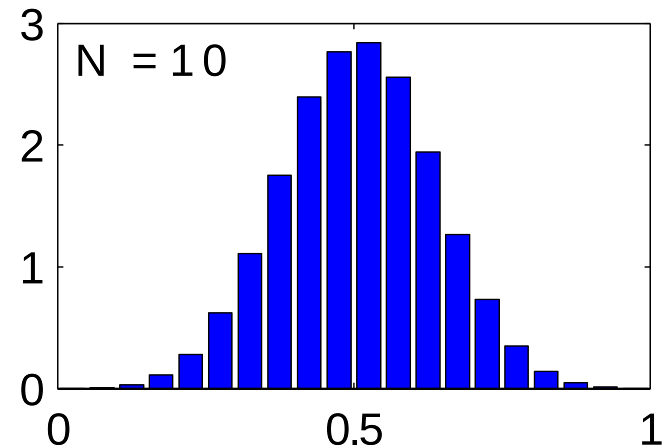
Normalization: integrate over all possible values of θ

- The more uncertain we are about θ, the more we average over all possible parameter values.

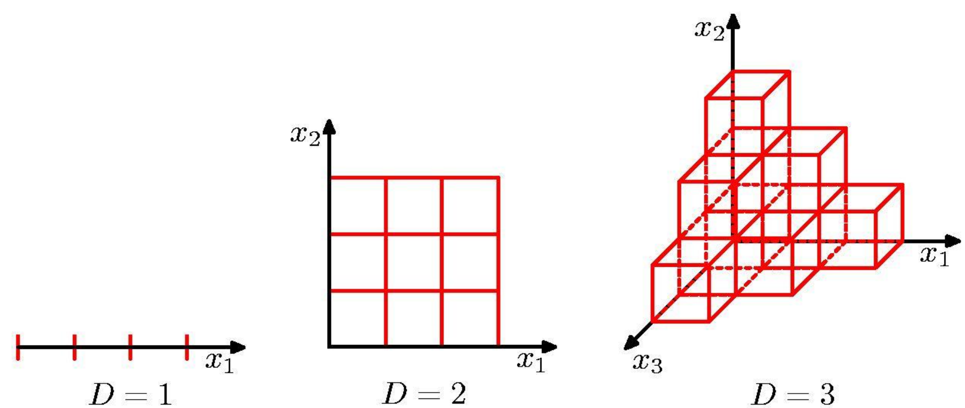
Recap: Histograms

- **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!

Image source: C.M. Bishop, 2006

Recap: Kernel Density Estimation

see Exercise 1.4

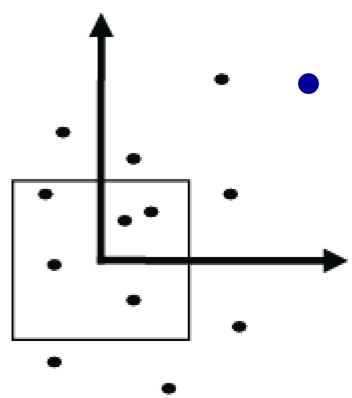
- **Approximation formula:**

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

fixed V
determine K
→ **Kernel Methods**

fixed K
determine V
→ **K-Nearest Neighbor**

- **Kernel methods**
  - Place a *kernel window* k at location $\mathbf{x}$ and count how many data points fall inside it.



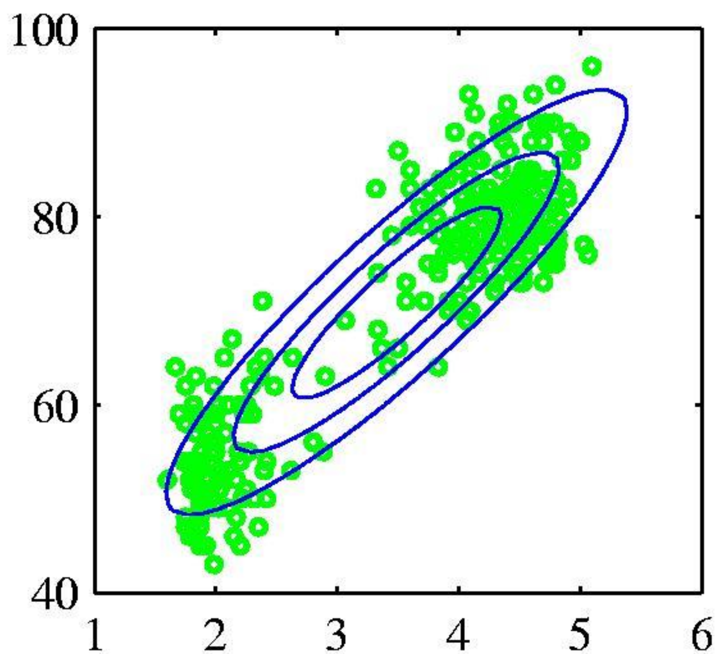
- **K-Nearest Neighbor**
  - Increase the volume V until the K next data points are found.

Topics of This Lecture

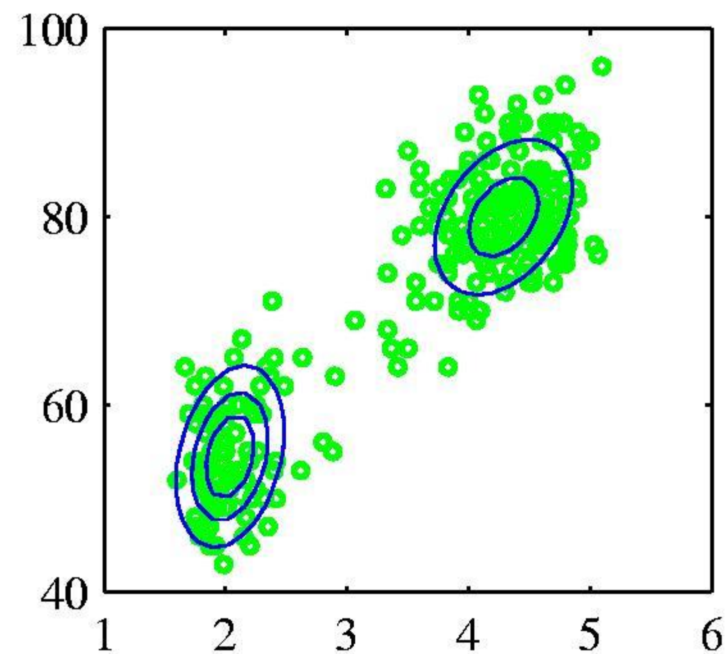
- Mixture distributions
  - Mixture of Gaussians (MoG)
  - Maximum Likelihood estimation attempt
- K-Means Clustering
  - Algorithm
  - Applications
- EM Algorithm
  - Credit assignment problem
  - MoG estimation
  - EM Algorithm
  - Interpretation of K-Means
  - Technical advice
- Applications

Mixture Distributions

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



Single Gaussian

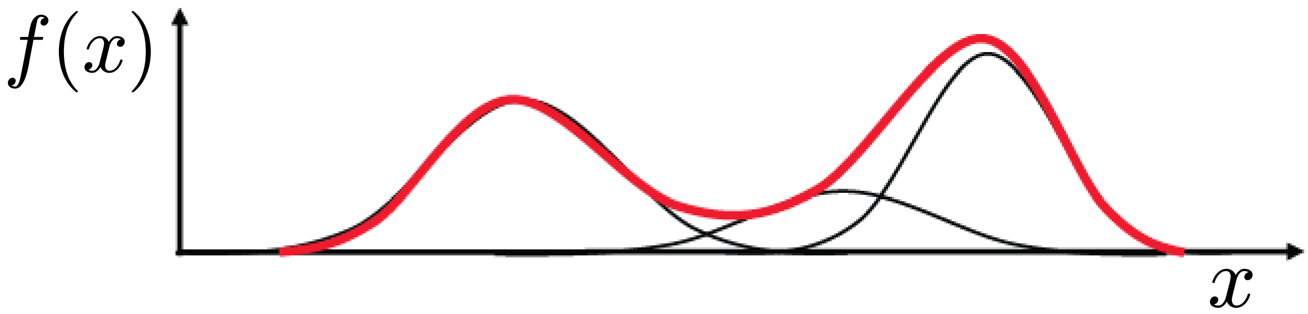


Mixture of two Gaussians

Image source: C.M. Bishop, 2006

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

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

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** $\sum_{j=1}^{M} \pi_j = 1.$

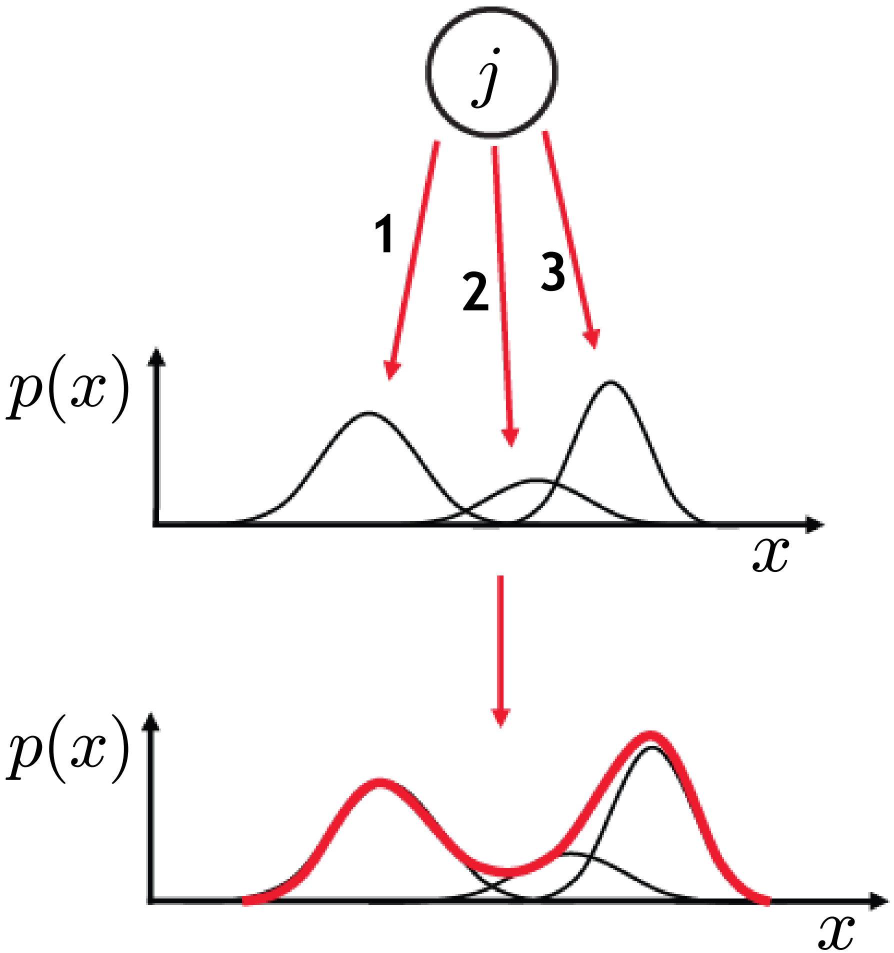
Prior of component j

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

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

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

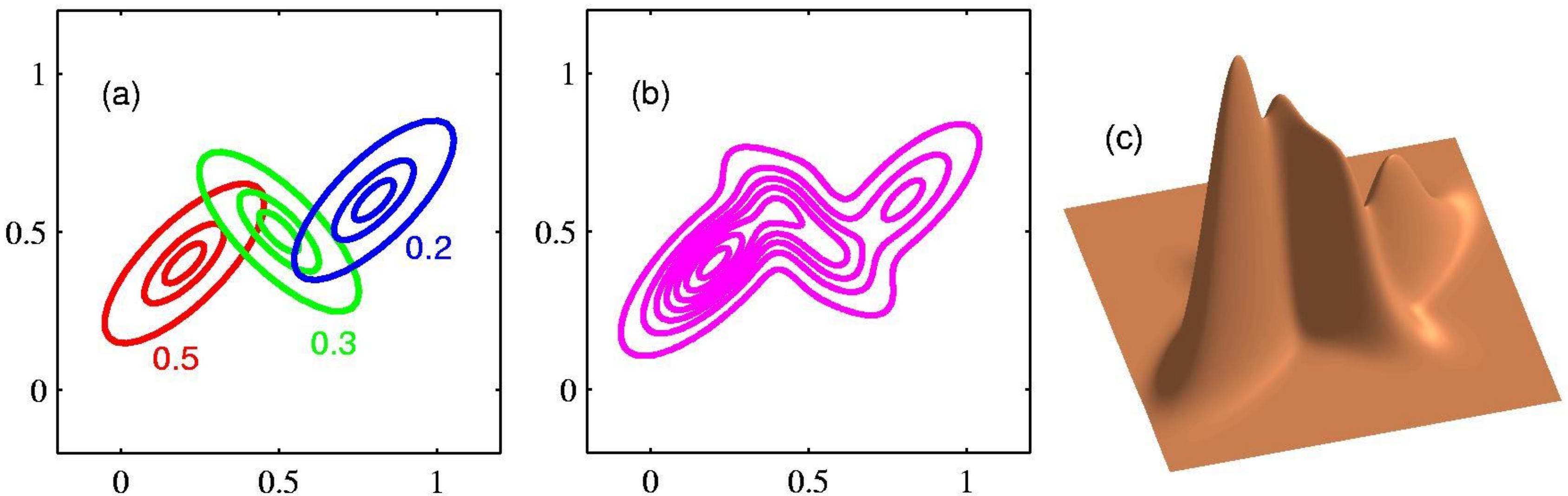


Image source: C.M. Bishop, 2006

Mixture of Multivariate Gaussians

- **Multivariate Gaussians**

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

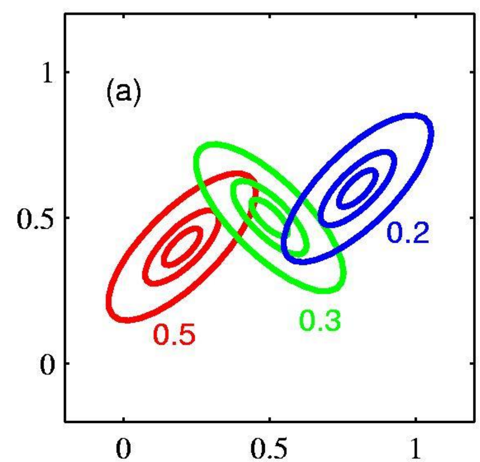
$$p(\mathbf{x}|\theta_j) = \frac{1}{(2\pi)^{D/2}|\boldsymbol{\Sigma}_j|^{1/2}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_j)^{\mathrm{T}}\boldsymbol{\Sigma}_j^{-1}(\mathbf{x}-\boldsymbol{\mu}_j)\right\}$$

  - **Mixture weights / mixture coefficients:**

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

  - **Parameters:**

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



Mixture of Multivariate Gaussians

- "Generative model"

$$p(j) = \pi_j$$

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

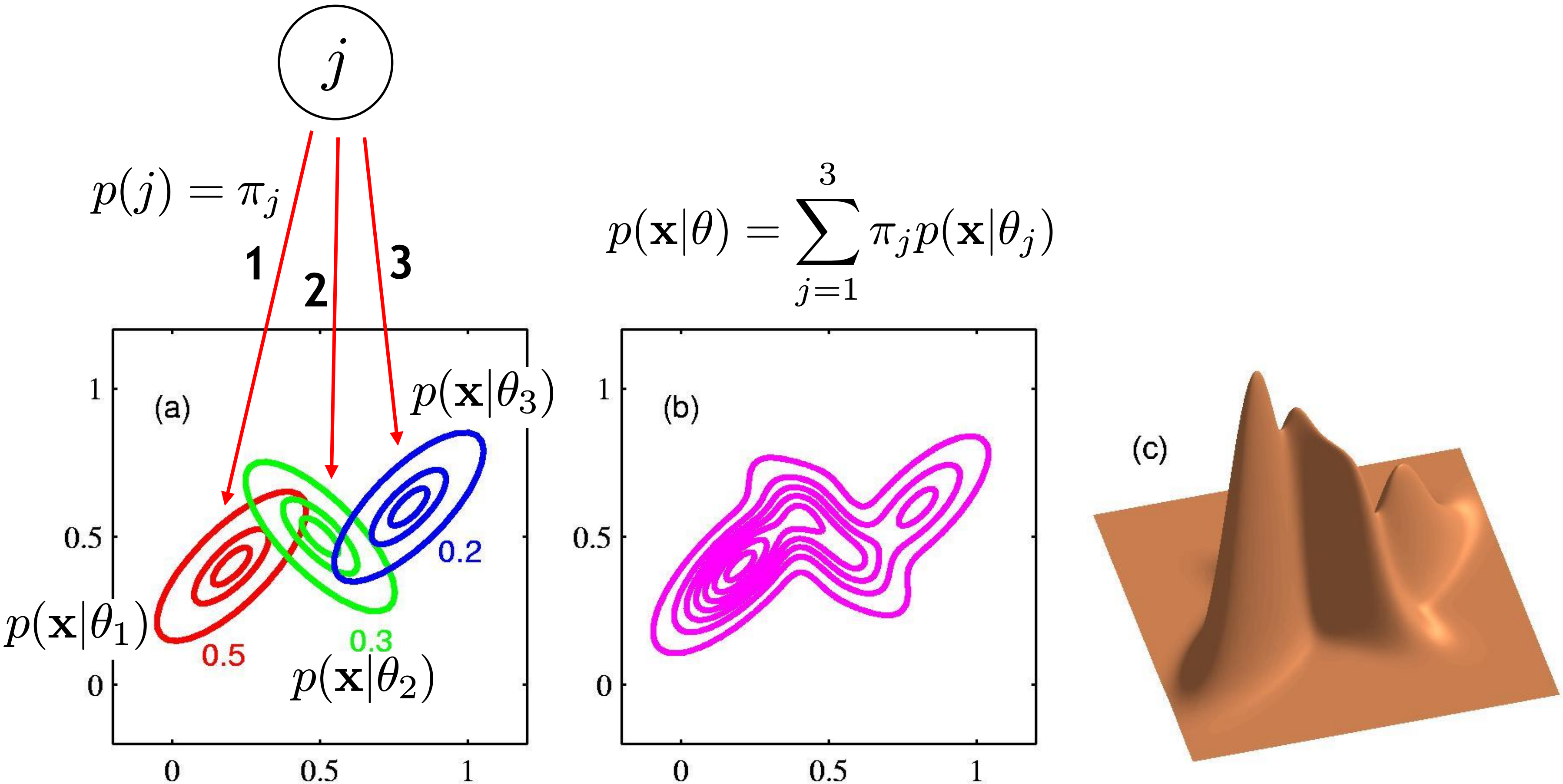
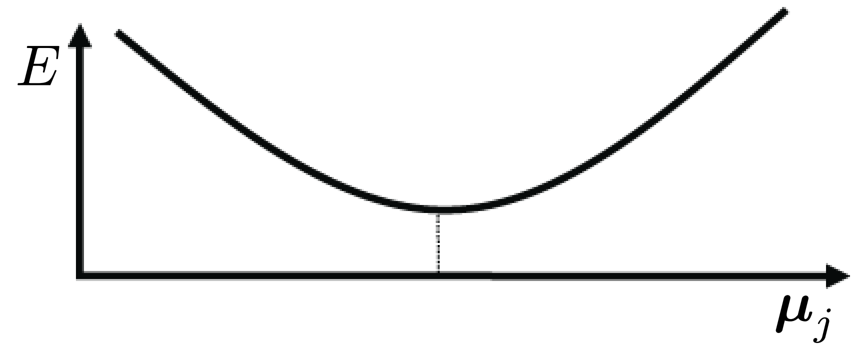


Image source: C.M. Bishop, 2006

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!

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Mixture of Gaussians – 1st Estimation Attempt

- **Minimization:**

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

$$\begin{aligned}\frac{\partial E}{\partial \boldsymbol{\mu}_j} &= -\sum_{n=1}^{N} \frac{\frac{\partial}{\partial \boldsymbol{\mu}_j} p(\mathbf{x}_n|\theta_j)}{\sum_{k=1}^{K} p(\mathbf{x}_n|\theta_k)} \\ &= -\sum_{n=1}^{N} \left(\boldsymbol{\Sigma}^{-1}(\mathbf{x}_n - \boldsymbol{\mu}_j) \frac{p(\mathbf{x}_n|\theta_j)}{\sum_{k=1}^{K} p(\mathbf{x}_n|\theta_k)} \right) \\ &= -\boldsymbol{\Sigma}^{-1} \sum_{n=1}^{N} (\mathbf{x}_n - \boldsymbol{\mu}_j) \frac{\pi_j \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}{\sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)} \stackrel{!}{=} 0\end{aligned}$$

$$= \gamma_j(\mathbf{x}_n)$$

"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…

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

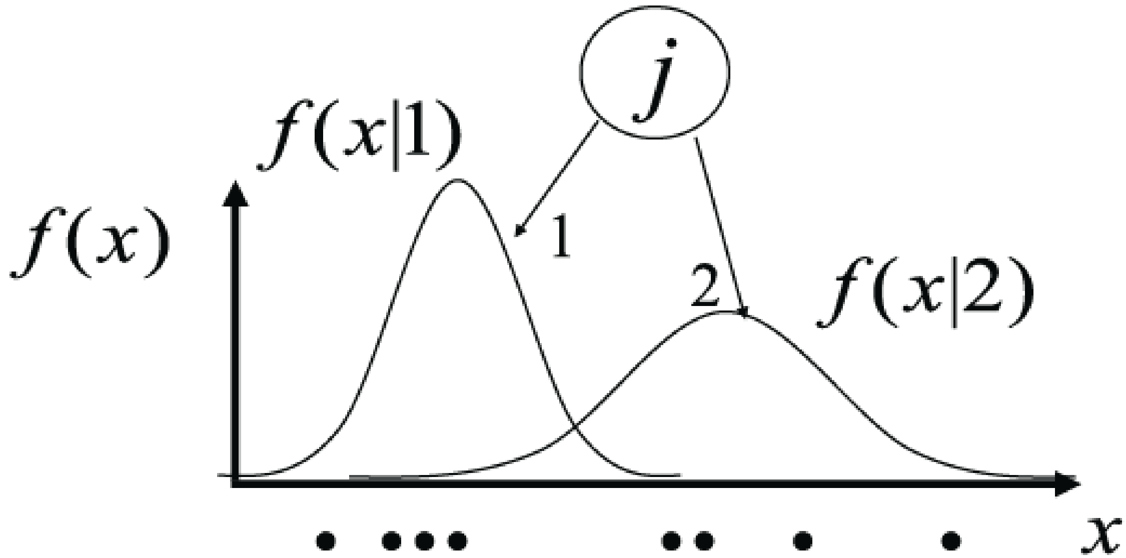
- I.e. there is no direct analytical solution!

$$\frac{\partial E}{\partial \boldsymbol{\mu}_j} = f\left(\pi_1, \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1, \ldots, \pi_M, \boldsymbol{\mu}_M, \boldsymbol{\Sigma}_M\right)$$

  - 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:**



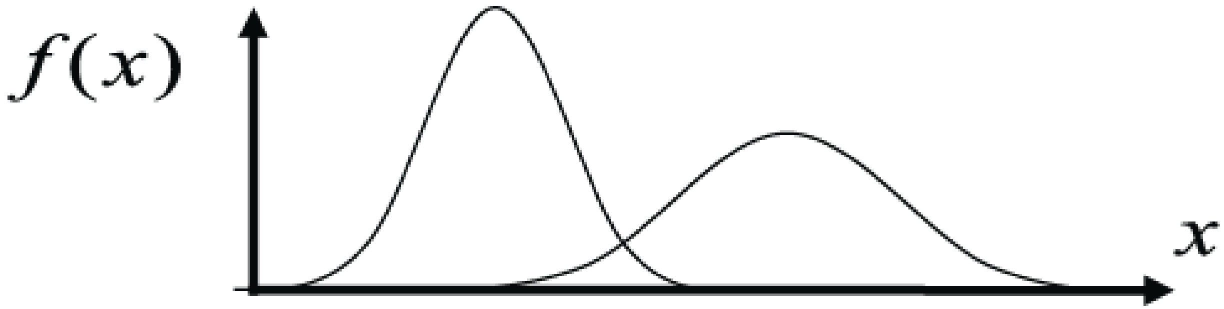
  - **Observed data:**
  - **Unobserved data:** 1 111 22 2 2
    - Unobserved = "hidden variable": j|x

$$h(j=1|x_n) = \quad 1 \;\; 111 \qquad 00 \;\; 0 \;\; 0$$

$$h(j=2|x_n) = \quad 0 \;\; 000 \qquad 11 \;\; 1 \;\; 1$$

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

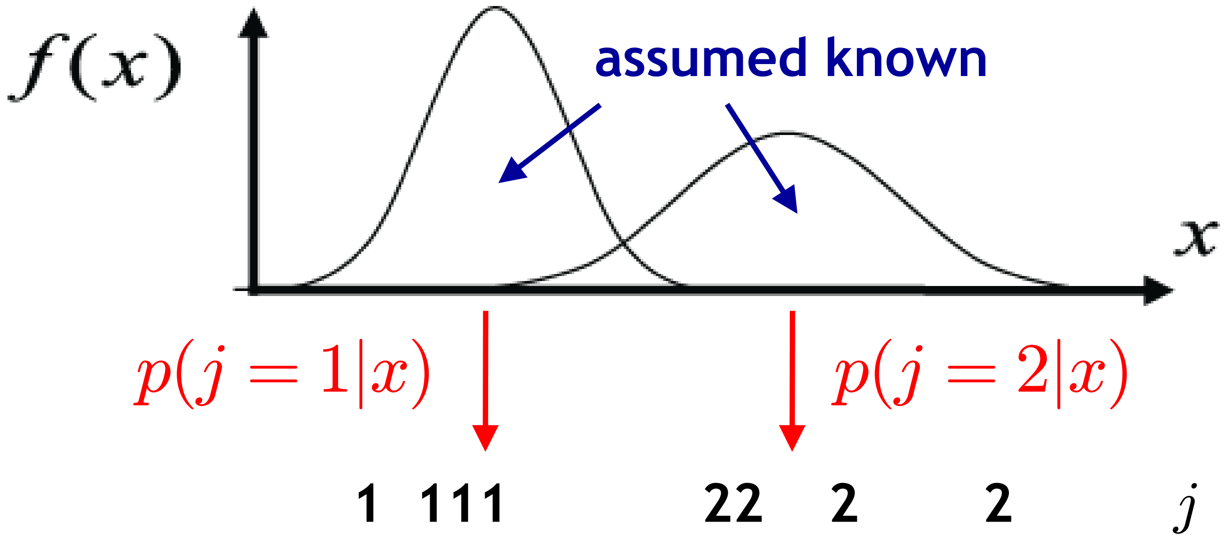
$$h(j=1|x_n) = \quad 1 \;\; 111 \qquad 00 \;\; 0 \;\; 0$$

$$h(j=2|x_n) = \quad 0 \;\; 000 \qquad 11 \;\; 1 \;\; 1$$

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

Mixture of Gaussians – Other Strategy

- **Assuming we knew the mixture components…**

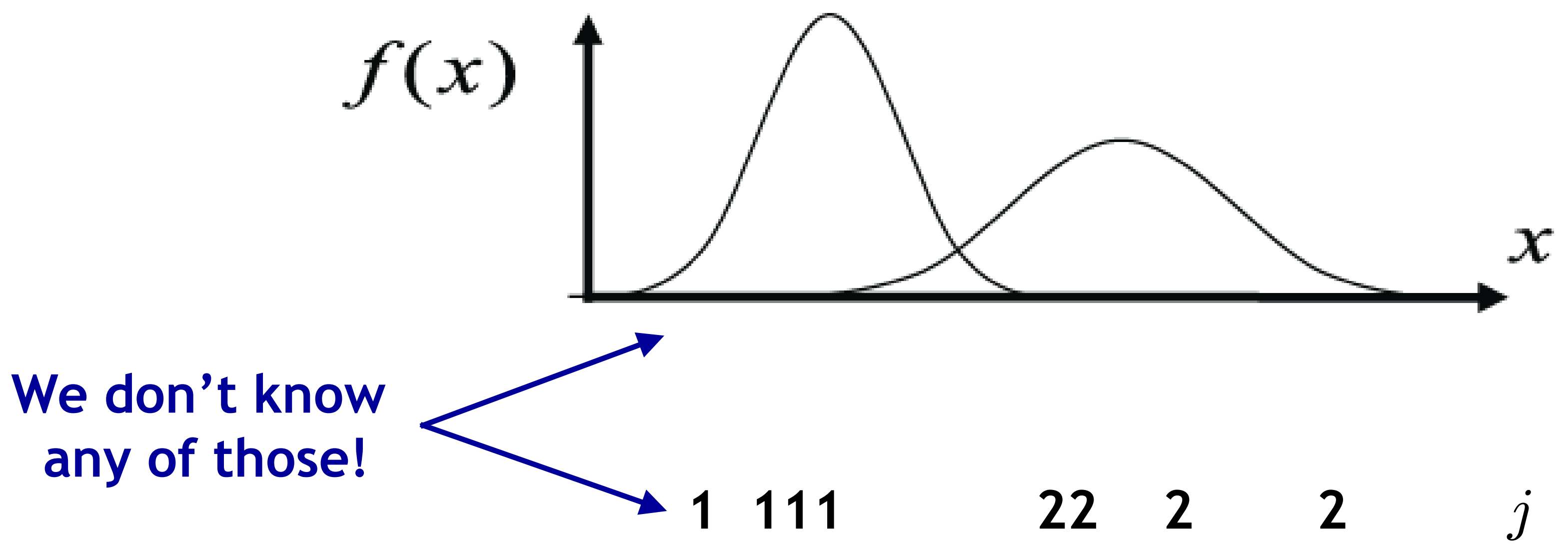


- **Bayes decision rule: Decide $j = 1$ if**

$$p(j=1|x_n) > p(j=2|x_n)$$

Mixture of Gaussians – Other Strategy

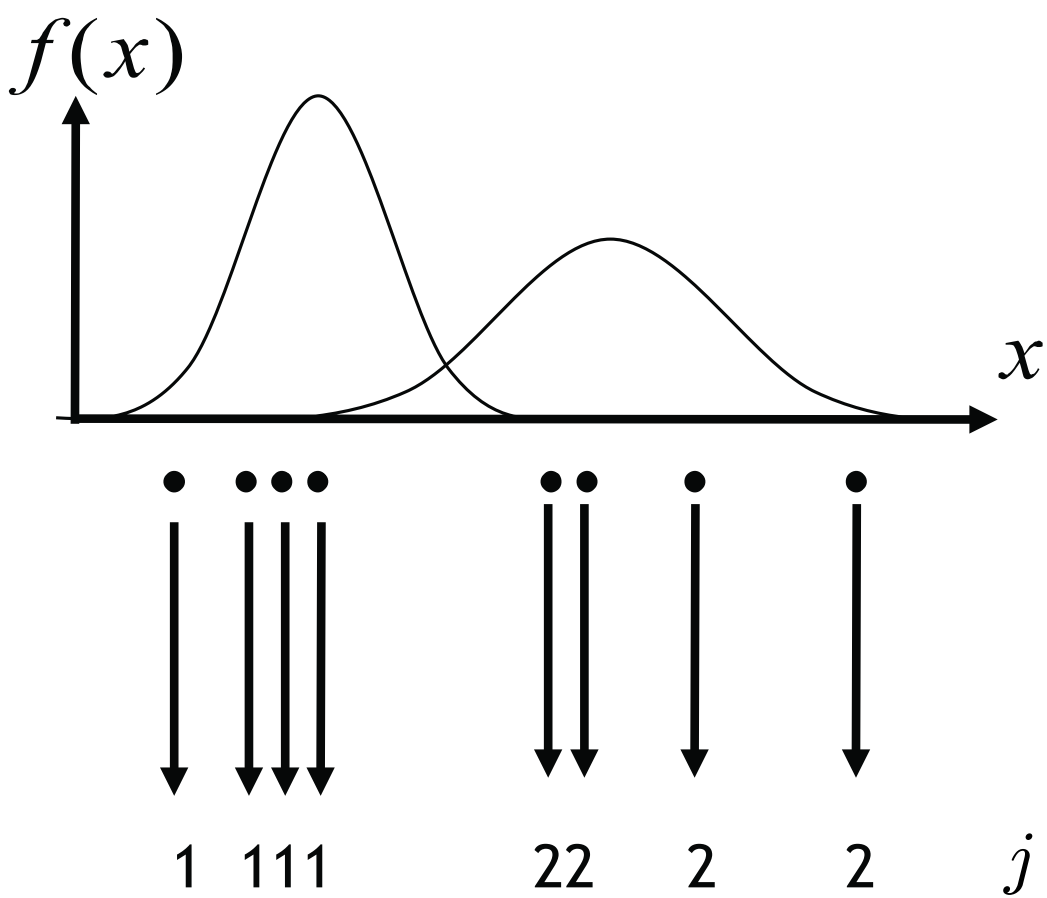
- Chicken and egg problem – what comes first?



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

Clustering with Hard Assignments

- Let's first look at clustering with "hard assignments"

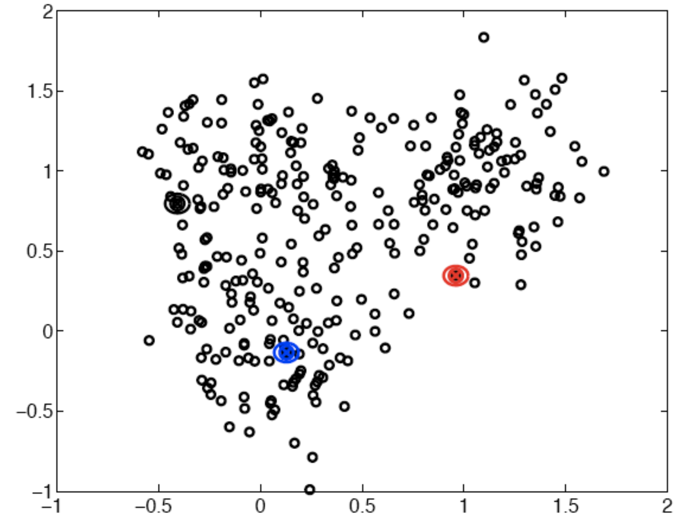


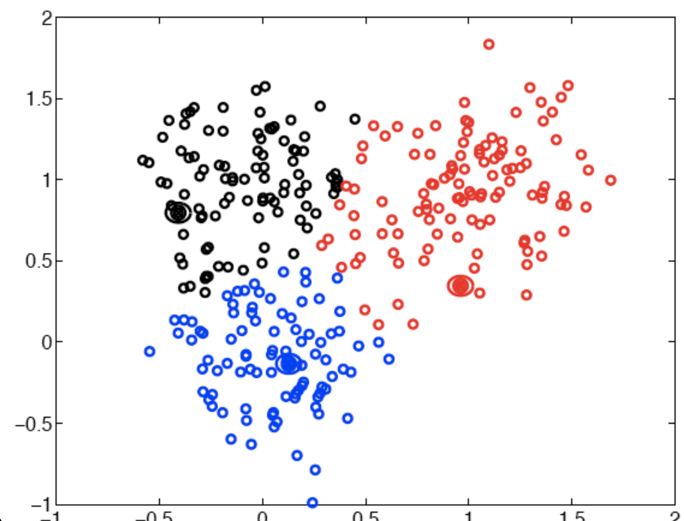
Topics of This Lecture

- Mixture distributions
  - Mixture of Gaussians (MoG)
  - Maximum Likelihood estimation attempt
- **K-Means Clustering**
  - Algorithm
  - Applications
- EM Algorithm
  - Credit assignment problem
  - MoG estimation
  - EM Algorithm
  - Interpretation of K-Means
  - Technical advice
- Applications

K-Means Clustering

- Iterative procedure
  1. Initialization: pick K arbitrary centroids (cluster means)
  2. Assign each sample to the closest centroid.
  3. Adjust the centroids to be the means of the samples assigned to them.
  4. Go to step 2 (until no change)





- Algorithm is guaranteed to converge after finite #iterations.
  - Local optimum
  - Final result depends on initialization.

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K-Means – Example with K=2

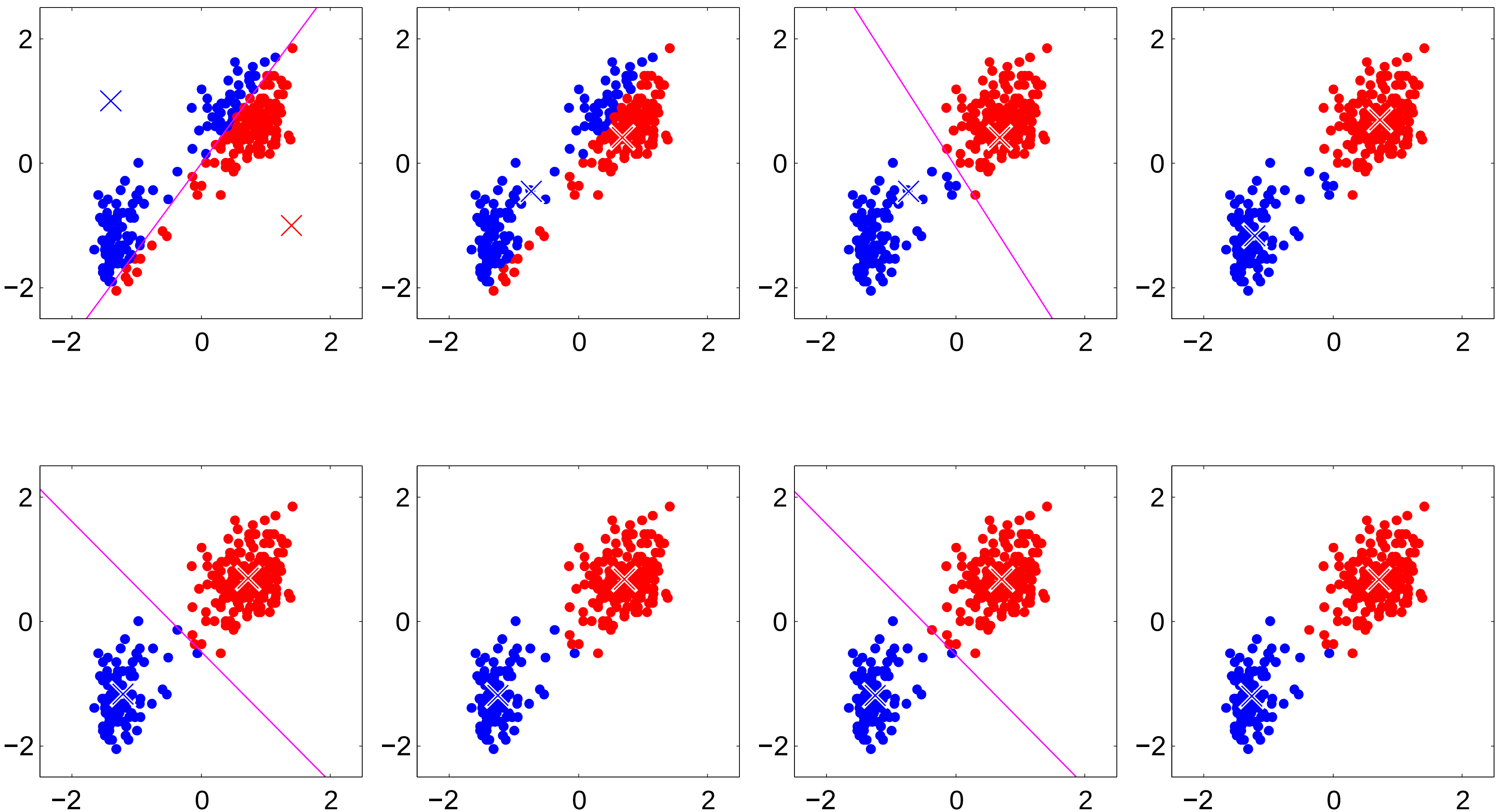
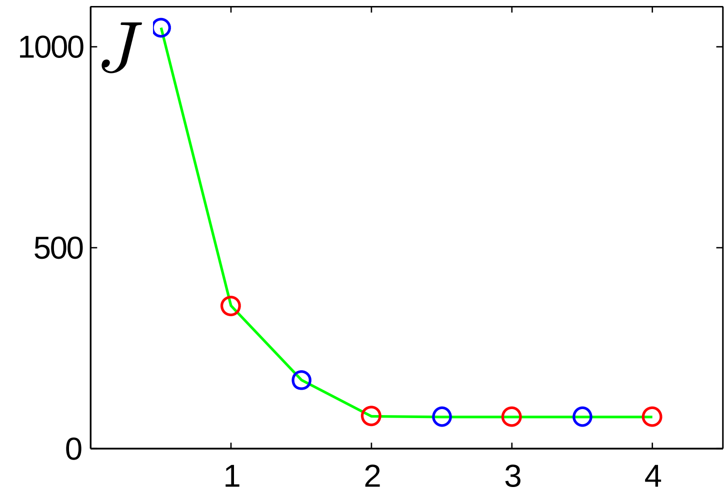


Image source: C.M. Bishop, 2006

K-Means Clustering

- **K-Means optimizes the following objective function:**

$$J = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} ||\mathbf{x}_n - \boldsymbol{\mu}_k||^2$$



  - **where**

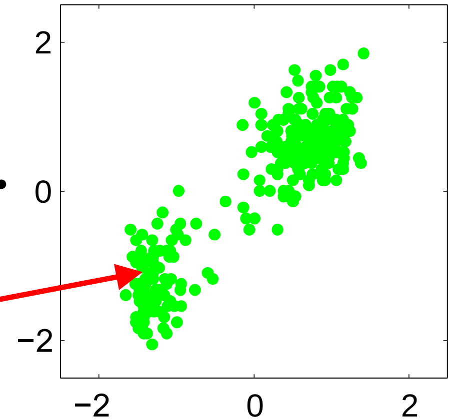
$$r_{nk} = \begin{cases} 1 & \text{if } k = \arg\min_j ||\mathbf{x}_n - \boldsymbol{\mu}_j||^2 \\ 0 & \text{otherwise.} \end{cases}$$

  - **In practice, this procedure usually converges quickly to a local optimum.**

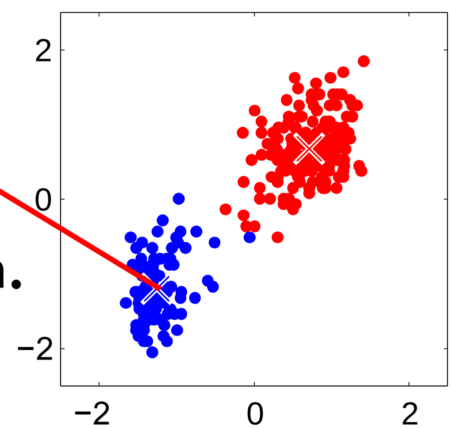
Image source: C.M. Bishop, 2006

Example Application: Image Compression

Take each pixel
as one data point.



K-Means
Clustering



Set the pixel color
to the cluster mean.

Image source: C.M. Bishop, 2006

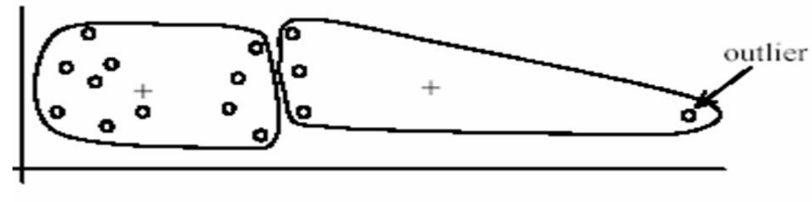
Example Application: Image Compression

K = 2 | K = 3 | K =10 | Original image

Image source: C.M. Bishop, 2006

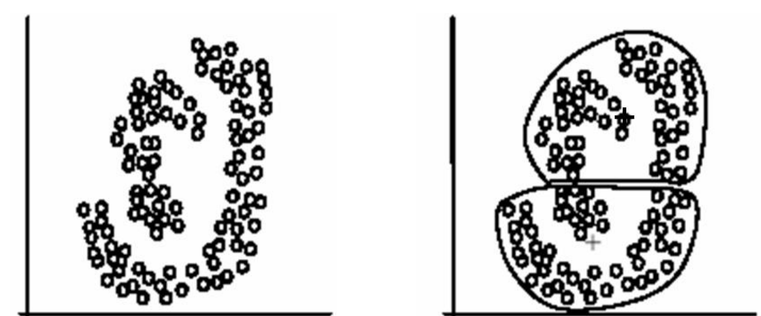
Summary K-Means

- **Pros**
  - Simple, fast to compute
  - Converges to local minimum of within-cluster squared error
- **Problem cases**
  - Setting k?
  - Sensitive to initial centers
  - Sensitive to outliers
  - Detects spherical clusters only
- **Extensions**
  - Speed-ups possible through efficient search structures
  - General distance measures: k-medoids



(A): Undesirable clusters

(B): Ideal clusters



(A): Two natural clusters

(B): *k*-means clusters

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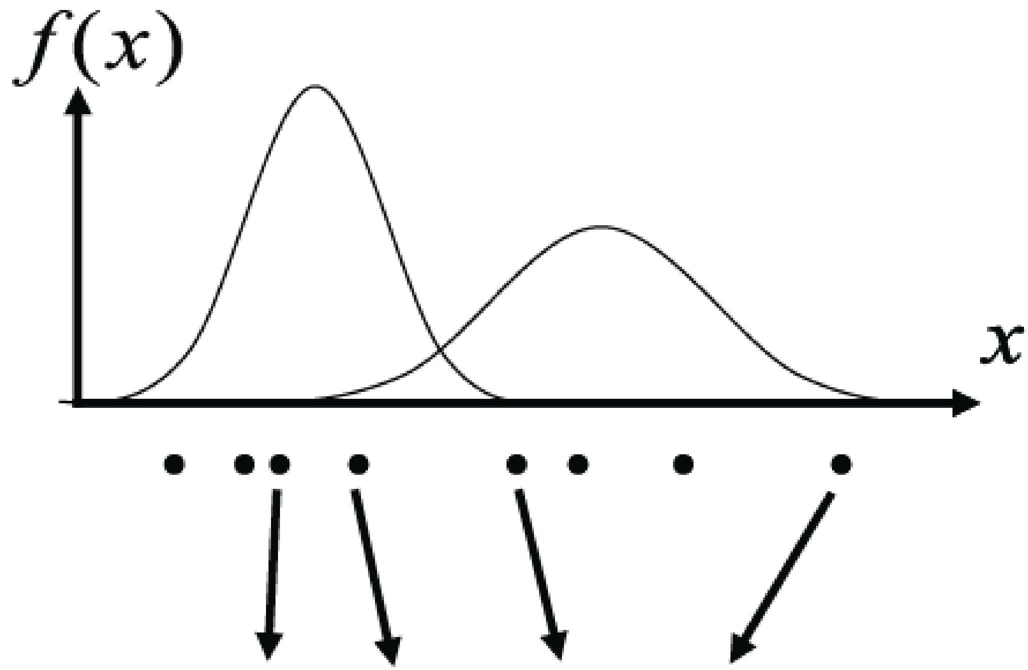
EM Clustering

- Clustering with "soft assignments"
  - Expectation step of the EM algorithm

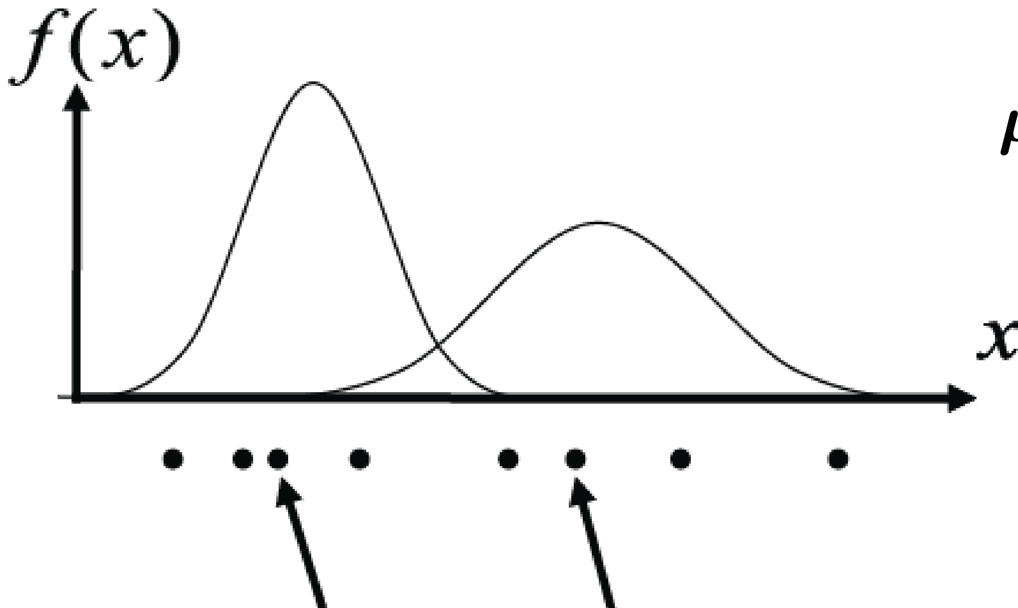


$p(j|x)$

$p(1\|x)$	0.99	0.8	0.2	0.01	j
$p(2\|x)$	0.01	0.2	0.8	0.99	

EM Clustering

- Clustering with "soft assignments"
  - Maximization step of the EM algorithm



$$\boldsymbol{\mu}_j = \frac{\sum_{n=1}^{N} p(j|\mathbf{x}_n)\mathbf{x}_n}{\sum_{n=1}^{N} p(j|\mathbf{x}_n)}$$

$p(1\|x)$	0.99	0.8	0.2	0.01
$p(2\|x)$	0.01	0.2	0.8	0.99

Maximum Likelihood estimate

EM Algorithm

- **Expectation-Maximization (EM) Algorithm**
  - **E-Step**: softly assign samples to mixture components

$$\gamma_j(\mathbf{x}_n) \leftarrow \frac{\pi_j \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}{\sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)} \qquad \forall j = 1,\ldots,K, \quad n = 1,\ldots,N$$

  - **M-Step**: re-estimate the parameters (separately for each mixture component) based on the soft assignments

$$\hat{N}_j \leftarrow \sum_{n=1}^{N} \gamma_j(\mathbf{x}_n)$$ = soft number of samples labeled j

$$\hat{\pi}_j^{\text{new}} \leftarrow \frac{\hat{N}_j}{N}$$

$$\hat{\boldsymbol{\mu}}_j^{\text{new}} \leftarrow \frac{1}{\hat{N}_j} \sum_{n=1}^{N} \gamma_j(\mathbf{x}_n)\mathbf{x}_n$$

$$\hat{\boldsymbol{\Sigma}}_j^{\text{new}} \leftarrow \frac{1}{\hat{N}_j} \sum_{n=1}^{N} \gamma_j(\mathbf{x}_n)(\mathbf{x}_n - \hat{\boldsymbol{\mu}}_j^{\text{new}})(\mathbf{x}_n - \hat{\boldsymbol{\mu}}_j^{\text{new}})^{\mathrm{T}}$$

Slide adapted from Bernt Schiele

EM Algorithm – An Example

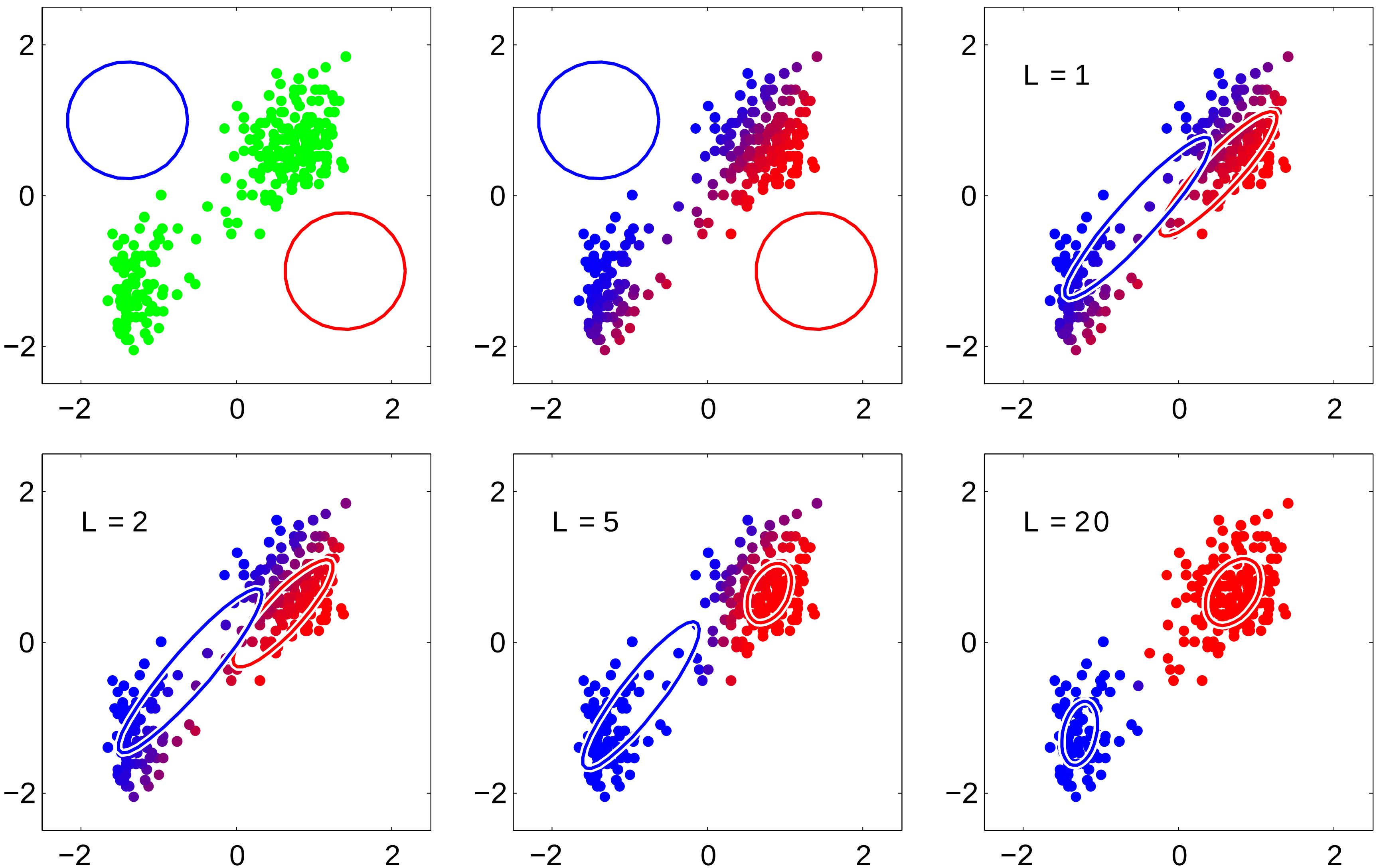
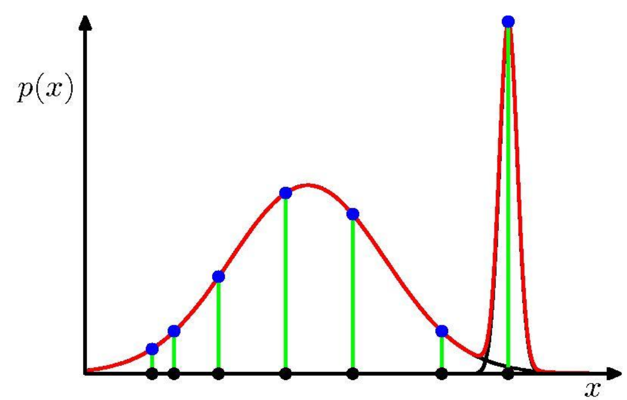


Image source: C.M. Bishop, 2006

EM – Technical Advice

- **When implementing EM, we need to take care to avoid singularities in the estimation!**
  - Mixture components may collapse on single data points.
  - E.g. consider the case $\Sigma_k = \sigma_k^2 \mathbf{I}$ (this also holds in general)
  - Assume component j is exactly centered on data point $\mathbf{x}_n$. This data point will then contribute a term in the likelihood function

$$\mathcal{N}(\mathbf{x}_n | \mathbf{x}_n, \sigma_j^2 \mathbf{I}) = \frac{1}{\sqrt{2\pi}\sigma_j}$$



  - For $\sigma_j \to 0$, this term goes to infinity!

$\Rightarrow$ **Need to introduce regularization**

  - Enforce minimum width for the Gaussians
  - E.g., instead of $\mathbf{\Sigma}^{-1}$, use $(\mathbf{\Sigma} + \sigma_{\min}\mathbf{I})^{-1}$

Image source: C.M. Bishop, 2006

EM – Technical Advice (2)

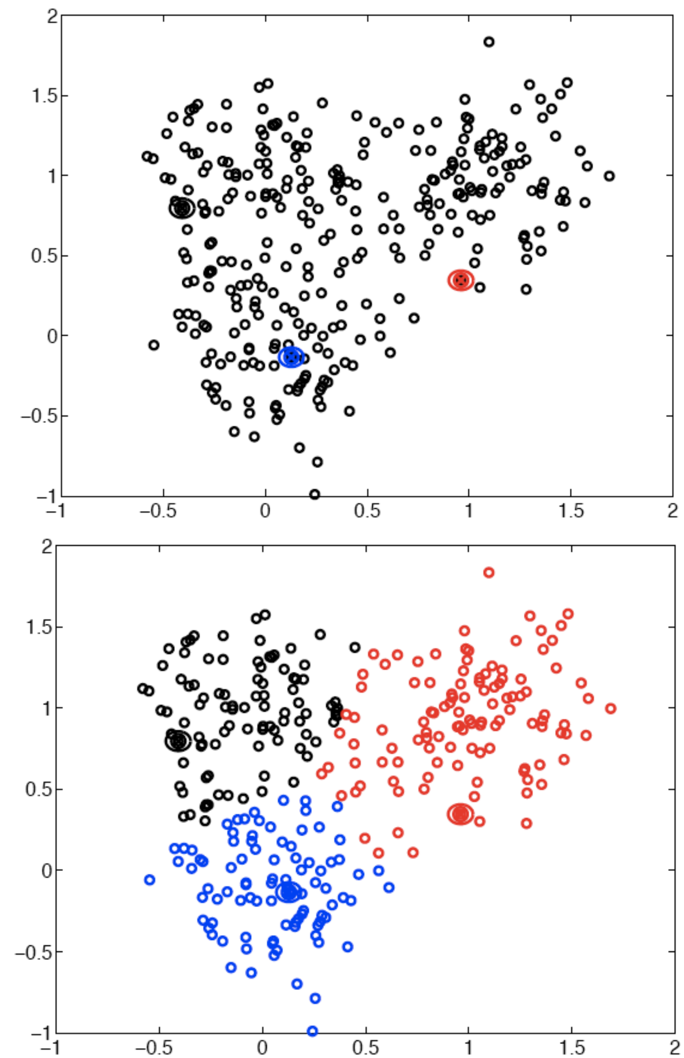
- EM is very sensitive to the initialization
  - Will converge to a local optimum of E.
  - Convergence is relatively slow.

$\Rightarrow$ Initialize with k-Means to get better results!
  - k-Means is itself initialized randomly, will also only find a local optimum.
  - But convergence is much faster.

- Typical procedure
  - Run k-Means M times (e.g. $M = 10\text{-}100$).
  - Pick the best result (lowest error J).
  - Use this result to initialize EM
    - Set μ_j to the corresponding cluster mean from k-Means.
    - Initialize Σ_j to the sample covariance of the associated data points.

K-Means Clustering Revisited

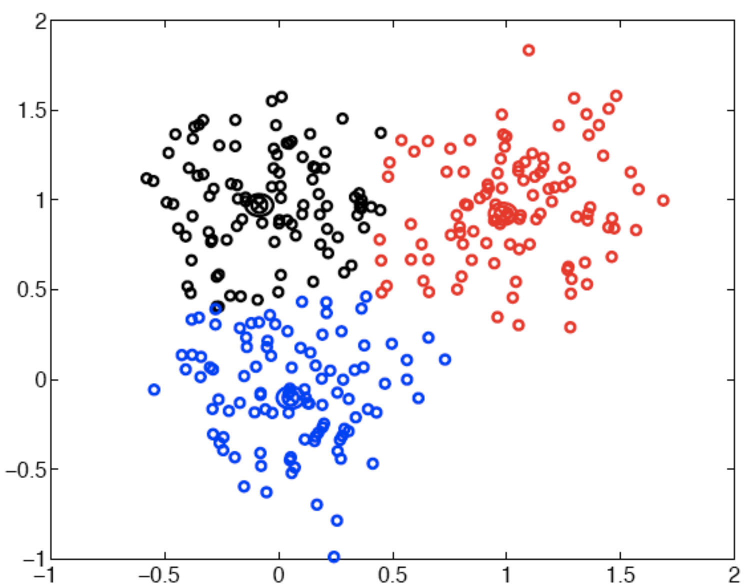
- **Interpreting the procedure**
  1. **Initialization: pick K arbitrary centroids (cluster means)**
  2. **Assign each sample to the closest centroid. (E-Step)**
  3. **Adjust the centroids to be the means of the samples assigned to them. (M-Step)**
  4. **Go to step 2 (until no change)**



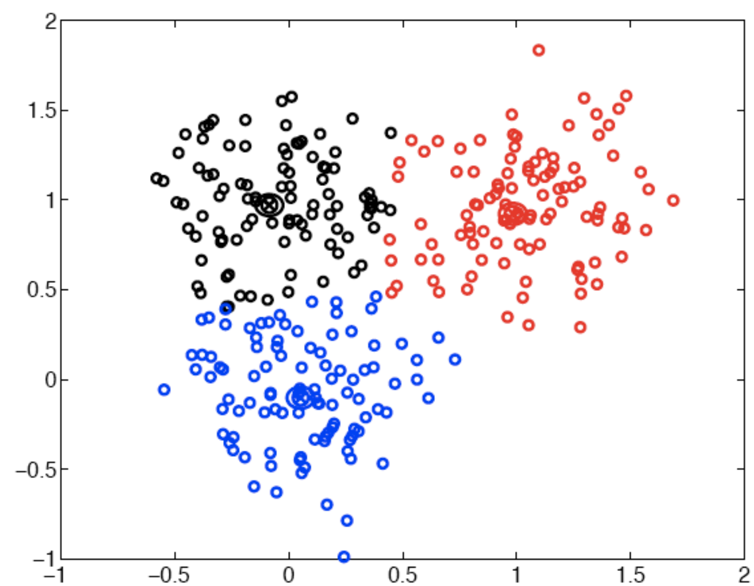
K-Means Clustering Revisited

- K-Means clustering essentially corresponds to a Gaussian Mixture Model (MoG or GMM) estimation with EM whenever
  - The covariances are of the K Gaussians are set to $\Sigma_j = \sigma^2 I$
  - For some small, fixed σ^2

k-Means



MoG



Summary: Gaussian Mixture Models

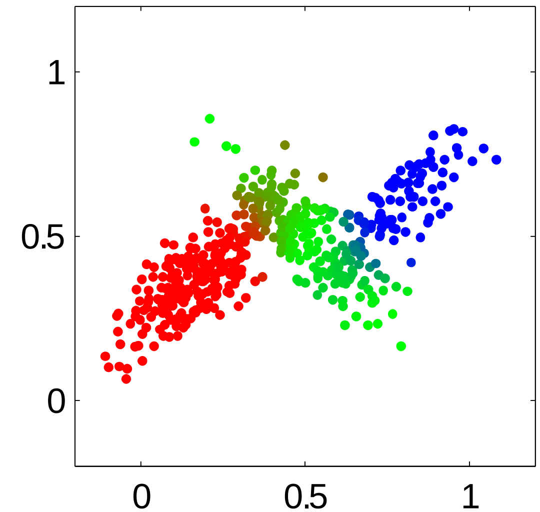
- Properties
  - Very general, can represent any (continuous) distribution.
  - Once trained, very fast to evaluate.
  - Can be updated online.
- Problems / Caveats
  - Some numerical issues in the implementation
    $\Rightarrow$ Need to apply regularization in order to avoid singularities.
  - EM for MoG is computationally expensive
    - Especially for high-dimensional problems!
    - More computational overhead and slower convergence than k-Means
    - Results very sensitive to initialization

    $\Rightarrow$ Run k-Means for some iterations as initialization!
  - Need to select the number of mixture components K.
    $\Rightarrow$ Model selection problem (see Lecture 16)

Topics of This Lecture

- Mixture distributions
  - Mixture of Gaussians (MoG)
  - Maximum Likelihood estimation attempt
- K-Means Clustering
  - Algorithm
  - Applications
- EM Algorithm
  - Credit assignment problem
  - MoG estimation
  - EM Algorithm
  - Interpretation of K-Means
  - Technical advice
- **Applications**

Applications



- Mixture models are used in many practical applications.
  - Wherever distributions with complex or unknown shapes need to be represented…

- Popular application in Computer Vision
  - Model distributions of pixel colors.
  - Each pixel is one data point in, e.g., RGB space.

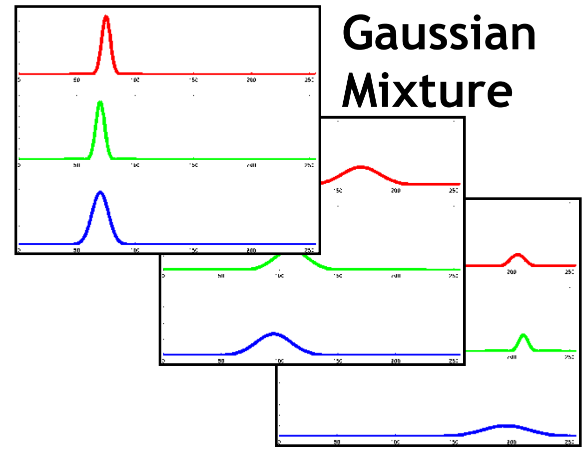
  ⇒ Learn a MoG to represent the class-conditional densities.

  ⇒ Use the learned models to classify other pixels.

Image source: C.M. Bishop, 2006

Application: Background Model for Tracking

- Train background MoG for each pixel
  - Model "common" appearance variation for each background pixel.
  - Initialization with an empty scene.
  - Update the mixtures over time
    - Adapt to lighting changes, etc.



- Used in many vision-based tracking applications
  - Anything that cannot be explained by the background model is labeled as foreground (=object).
  - Easy segmentation if camera is fixed.

C. Stauffer, E. Grimson, Learning Patterns of Activity Using Real-Time Tracking, *IEEE Trans. PAMI*, 22(8):747-757, 2000.

Image Source: Daniel Roth, Tobias Jäggli

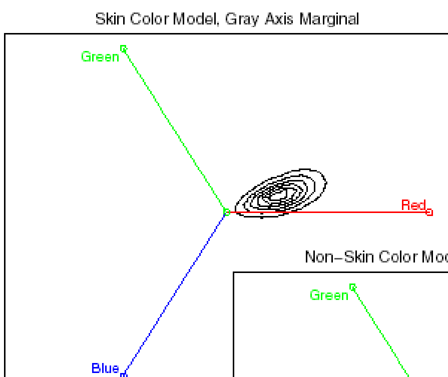
Application: Image Segmentation

(a) input image (b) user input (c) inferred segmentation

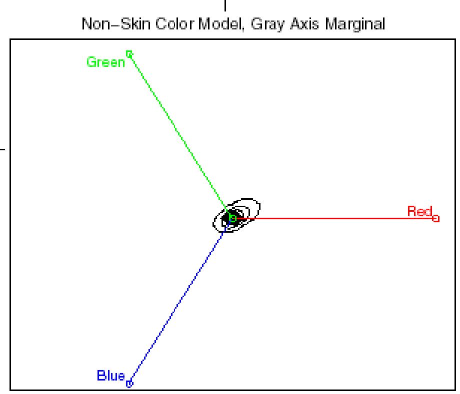
- User assisted image segmentation
  - User marks two regions for foreground and background.
  - Learn a MoG model for the color values in each region.
  - Use those models to classify all other pixels.
  - ⇒ Simple segmentation procedure
    (building block for more complex applications)

Application: Color-Based Skin Detection

- Collect training samples for skin/non-skin pixels.
- Estimate MoG to represent the skin/ non-skin densities



skin



non-skin

Classify skin color pixels in novel images

M. Jones and J. Rehg, Statistical Color Models with Application to Skin Detection, IJCV 2002.

Interested to Try It?

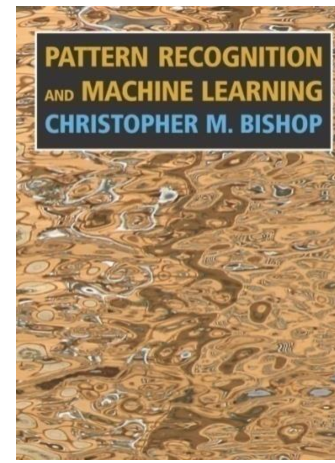
- Here's how you can access a webcam in Matlab:

```
function out = webcam
% uses "Image Acquisition Toolbox„
adaptorName = 'winvideo';
vidFormat = 'I420_320x240';
vidObj1= videoinput(adaptorName, 1, vidFormat);
set(vidObj1, 'ReturnedColorSpace', 'rgb');
set(vidObj1, 'FramesPerTrigger', 1);
out = vidObj1 ;


cam = webcam();
img=getsnapshot(cam);
```

References and Further Reading

- More information about EM and MoG estimation is available in Chapter 2.3.9 and the entire Chapter 9 of Bishop’s book (recommendable to read).



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

- Additional information
  - Original EM paper:
    - A.P. Dempster, N.M. Laird, D.B. Rubin, „Maximum-Likelihood from incomplete data via EM algorithm”, In Journal Royal Statistical Society, Series B. Vol 39, 1977
  - EM tutorial:
    - J.A. Bilmes, “A Gentle Tutorial of the EM Algorithm and its Application to Parameter Estimation for Gaussian Mixture and Hidden Markov Models“, TR-97-021, ICSI, U.C. Berkeley, CA,USA