Machine learning: lecture 13

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Topics

- Sequential prediction and description length
  - minimum description length principle (MDL), asymptotic expansion
- Probability models and structure
  - mixing, mixtures, and the EM-algorithm

Fair sequential prediction

- We wish to predict (generate) labels $y_1, \ldots, y_n$ associated with input examples $x_1, \ldots, x_n$.
- In a fair sequential prediction we predict each label based on the corresponding input and preceding labels and examples

  y_1 is predicted based on x_1 alone
  y_2 is predicted based on x_2 and $D_1 = \{(x_1, y_1)\}$
  y_3 is predicted based on x_3 and $D_2 = \{(x_1, y_1), (x_2, y_2)\}$
  $\ldots$

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y_1 is predicted based on x_1 alone

$$P(y_1|x_1) = \int P(y_1|x_1, \theta) P(\theta) d\theta$$

y_2 is predicted based on x_2 and $D_1 = \{(x_1, y_1)\}$

$$P(y_2|x_2, D_1) = \int P(y_2|x_2, \theta) P(\theta|D_1) d\theta$$

y_3 is predicted based on x_3 and $D_2 = \{(x_1, y_1), (x_2, y_2)\}$

$$P(y_3|x_3, D_2) = \int P(y_3|x_3, \theta) P(\theta|D_2) d\theta$$

Fair sequential prediction

- Our fair sequential prediction method defines a valid probability distribution over the training labels given the examples:

$$P(y_1|x_1)P(y_2|x_2, D_1)P(y_3|x_3, D_2)\cdots P(y_n|x_n, D_{n-1})$$

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This distribution does not depend on the order in which we processed the examples and, in fact, is equal to *Bayesian marginal likelihood:*

$$\int P(y_1|x_1, \theta)\cdots P(y_n|x_n, \theta)P(\theta)d\theta$$

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How well this distribution predicts the training labels depends on the "complexity" of the model $P(y|x, \theta)$, $\theta \in \Theta$ and how appropriate the prior $P(\theta)$ is.

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  - if the model is *too flexible:* the posterior $P(\theta|D_{i-1})$ requires many training examples before it focuses on useful parameter values

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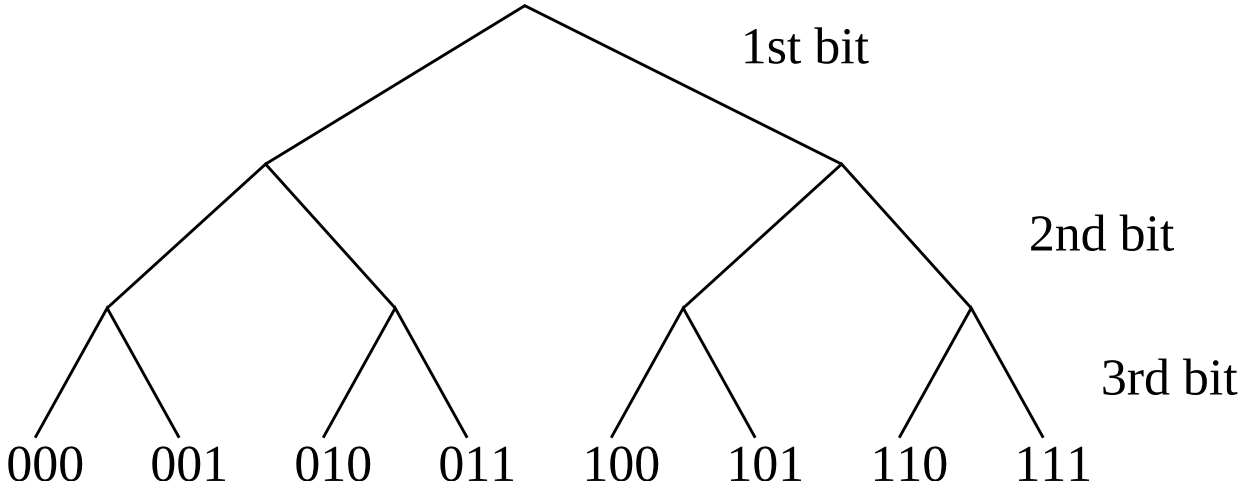
How well this distribution predicts the training labels depends on the "complexity" of the model $P(y|x, \theta)$, $\theta \in \Theta$ and how appropriate the prior $P(\theta)$ is.

- if the model is *too flexible:* the posterior $P(\theta|D_{i-1})$ requires many training examples before it focuses on useful parameter values
- if the model is *too simple:* the posterior concentrates quickly but the predictions remain poor

Description length and probabilities

- If we can predict the training labels with high probability, then we can communicate them effectively (with few bits)
- It takes $-\log_2 P(y_1, \ldots, y_n)$ bits to communicate $y_1, \ldots, y_n$ according to distribution P.

  Example: suppose each configuration (y_1, y_2, y_3) is equally likely according to P



  We need $-\log_2 P(y_1, y_2, y_3) = -\log_2(1/8) = 3$ bits to describe each y.

Description length and model selection

- We need

$$-\log_2 \int P(y_1|x_1,\theta)\cdots P(y_n|x_n,\theta)P(\theta)d\theta$$

  bits to communicate labels $y_1,\ldots,y_n$ given examples $x_1,\ldots,x_n$ with a model $P(y|x,\theta), \theta \in \Theta$ and prior $P(\theta)$.

- **Minimum description length (MDL) principle:**
  We select the model+prior combination that requires the fewest number of bits (maximizes the Bayesian marginal likelihood)

Asymptotic approximation

- For large n we can use the following asymptotic expansion:

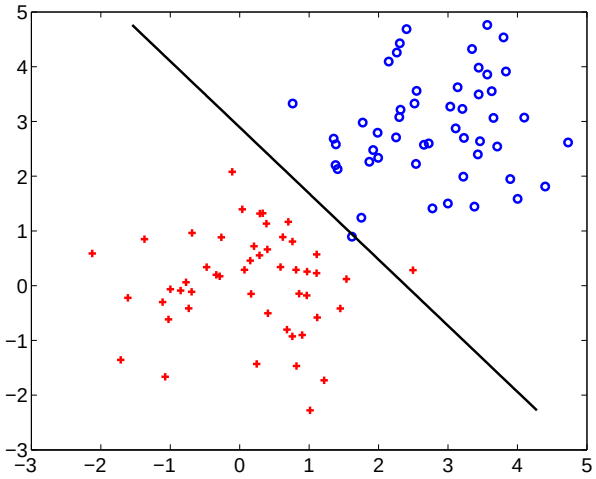
$$\overbrace{\sum_{i=1}^{n}\left(-\log_2 P(y_i|\mathbf{x}_i,\hat{\theta})\right)}^{\approx \text{ DL of data}} + \overbrace{\frac{d}{2}\log_2(n)}^{\approx \text{ DL of model}}$$

  where $\hat{\theta}$ is the maximum likelihood setting of the parameters and d is the effective number of parameters in the model.

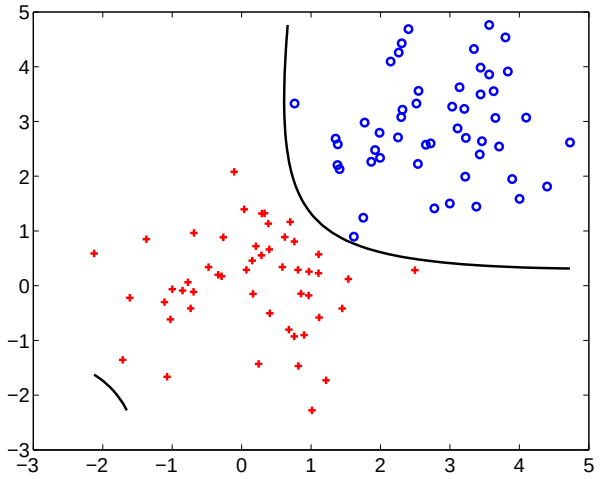
- The negative of this is also known as the *Bayesian information criterion* or BIC for short.

Description length: example

- Example: polynomial logistic regression, $n = 100$



linear



quadratic

$$\sum_{i=1}^{n} \left(-\log_2 P(y_i | \mathbf{x}_i, \hat{\theta}) \right) + \frac{d}{2} \log_2(n)$$

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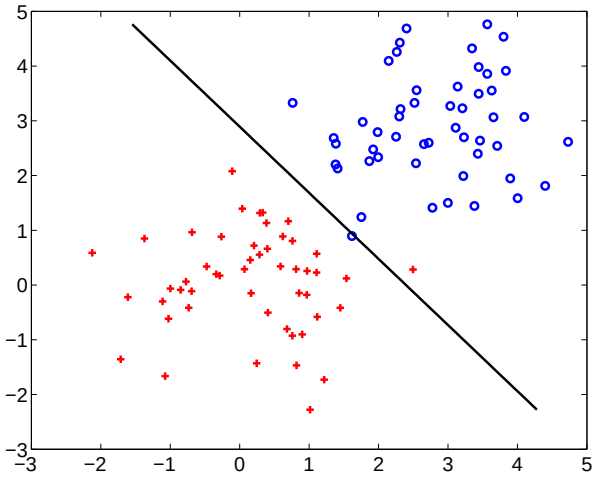
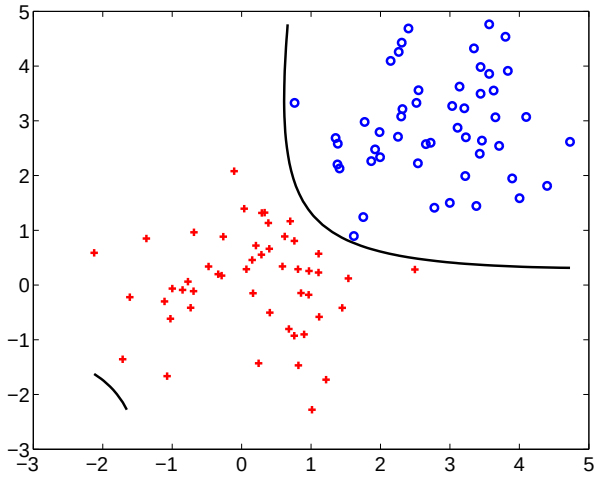


linear



quadratic

$$\sum_{i=1}^{n} \Big(-\log_2 P(y_i|\mathbf{x}_i, \hat{\theta}) \Big) + \frac{d}{2} \log_2(n)$$

degree	# param	DL(data)	DL(model)	MDL score
1	3	5.6 bits	9.9 bits	15.5 bits
2	6	2.4 bits	19.9 bits	22.3 bits

Topics

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- Probability models and structure
  - mixing, mixtures, and the EM-algorithm

What are we missing?

- So far we have solved simple binary classification problems, predicting y given $\mathbf{x}$, by estimating
  - discriminant functions (e.g., SVMs and boosting)
  - conditional probabilities (e.g., logistic regression)
- What about problems where
  - we have to predict multiple inter-connected labels for each input example (e.g., a set of topics for a document)
  - we have to switch between classifiers in the course of making predictions (e.g., changes in market conditions)
  - the inputs are incomplete in the sense that some of the components are missing (e.g., patient records)
  - the input examples come in different potentially unobserved types (e.g., mixed populations)

Structure and mixtures

- If we wish to take into account the fact that there are different underlying types of examples, we have to first identify them
- We can hypothesize that
  1. there are m underlying types $y = 1, \ldots, m$
  2. each type y occurs with frequency $P(y)$
  3. examples of type y are governed by distribution $p(\mathbf{x}|y)$
- According to this model each observed example $\mathbf{x}$ can be assumed to have come from a "mixture distribution":

$$p(\mathbf{x}) = \sum_{j=1}^{m} P(y = j) p(\mathbf{x}|y = j)$$

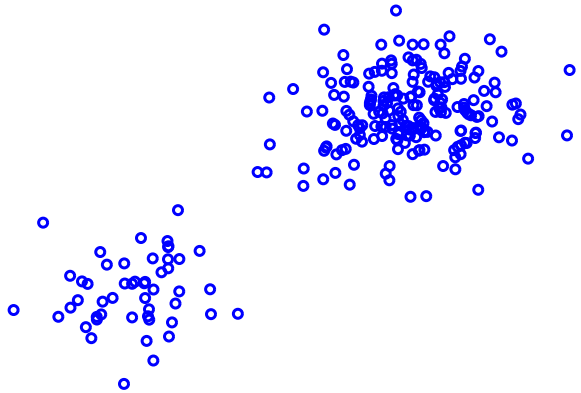
- We need to parameterize and estimate such models from samples $\mathbf{x}_1, \ldots, \mathbf{x}_n$

Mixture densities

- A mixture of Gaussians model

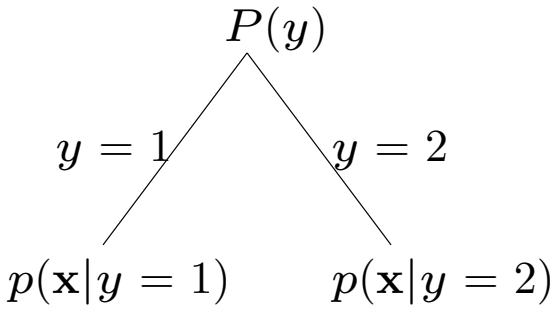
$$p(\mathbf{x}|\theta) = \sum_{i=1}^{m} p_j \, p(\mathbf{x}|\mu_j, \Sigma_j)$$

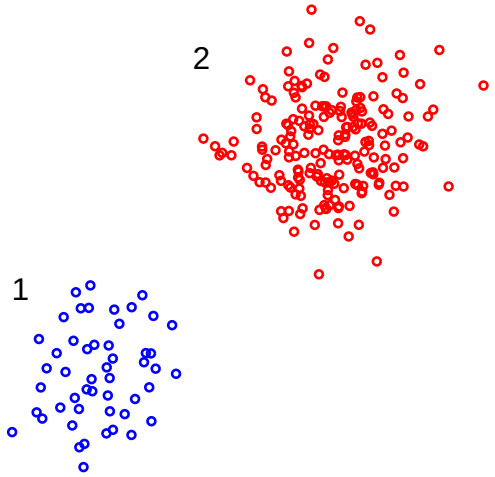
where $\theta = \{p_1, \ldots, p_m, \mu_1, \ldots, \mu_m, \Sigma_1, \ldots, \Sigma_m\}$ contains all the parameters of the mixture model. $\{p_j\}$ are known as *mixing proportions or coefficients*.



Mixture densities

- Data generation process:





$$p(\mathbf{x}|\theta) = \sum_{j=1,2} p_j \cdot p(\mathbf{x}|\mu_j, \Sigma_j) \quad \text{(mixture of Gaussians)}$$

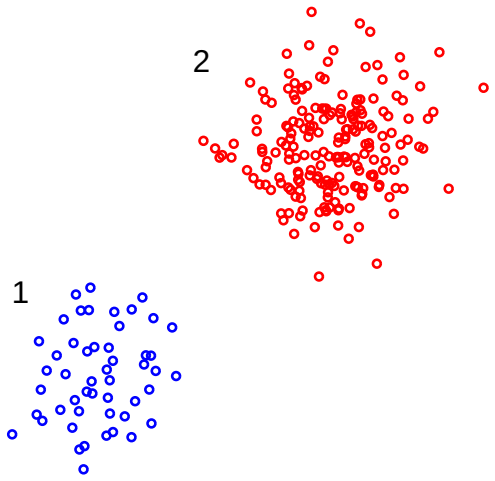
- Any data point $\mathbf{x}$ could have been generated in two ways; the component responsible for generating $\mathbf{x}$ needs to be *inferred*.

Mixture density estimation

- Suppose we want to estimate a two component mixture of Gaussians model.

$$p(\mathbf{x}|\theta) = p_1\, p(\mathbf{x}|\mu_1, \Sigma_1) + p_2\, p(\mathbf{x}|\mu_2, \Sigma_2)$$

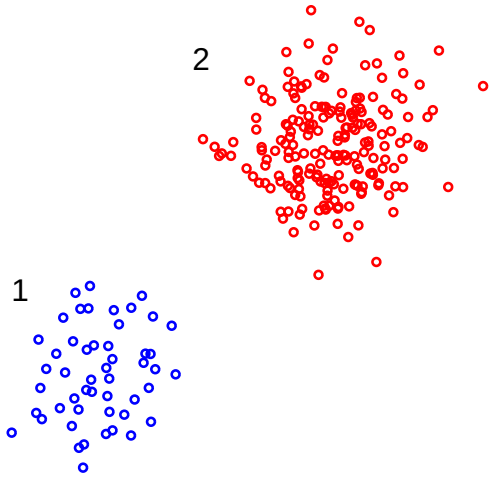
- If each example $\mathbf{x}_i$ in the training set were labeled $y_i = 1, 2$ according to which mixture component (1 or 2) had generated it, then the estimation would be easy.



Labeled examples $\Rightarrow$ no credit assignment problem

Mixture density estimation

- When examples are labeled, we can estimate each Gaussian independently



- Let $\delta(j|i)$ be an indicator function of whether example i is labeled j. Then for each $j = 1, 2$

$$\hat{p}_j \leftarrow \frac{\hat{n}_j}{n}, \quad \text{where } \hat{n}_j = \sum_{i=1}^{n} \delta(j|i)$$

$$\hat{\mu}_j \leftarrow \frac{1}{\hat{n}_j} \sum_{i=1}^{n} \delta(j|i)\, \mathbf{x}_i$$

$$\hat{\Sigma}_j \leftarrow \frac{1}{\hat{n}_j} \sum_{i=1}^{n} \delta(j|i)\, (\mathbf{x}_i - \hat{\mu}_j)(\mathbf{x}_i - \hat{\mu}_j)^T$$

Mixture density estimation: credit assignment

- Of course we don't have such labels ... but we can guess what the labels might be based on our current mixture distribution
- We can, for example, evaluate the posterior probability that an observed $\mathbf{x}$ was generated from the first mixture component

$$
\begin{aligned}
P(y=1|\mathbf{x},\theta) &= \frac{P(y=1)\cdot p(\mathbf{x}|y=1)}{\sum_{j=1,2} P(y=j)\cdot p(\mathbf{x}|y=j)} \\
&= \frac{p_1\, p(\mathbf{x}|\mu_1,\Sigma_1)}{\sum_{j=1,2} p_j\, p(\mathbf{x}|\mu_j,\Sigma_j)}
\end{aligned}
$$

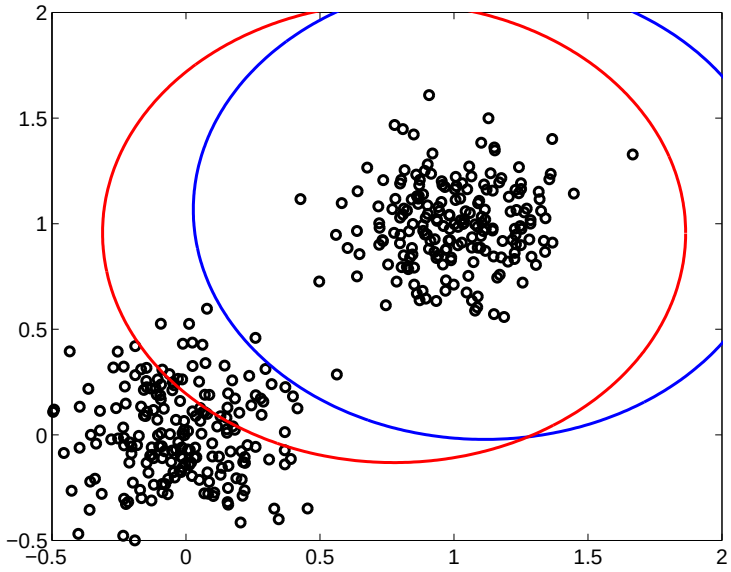
This solves the *credit assignment* problem

Mixture density estimation: credit assignment

- We get soft labels or posterior probabilities of which Gaussian generated which example:

$$\hat{p}(j|i) \leftarrow P(y_i = j|\mathbf{x}_i, \theta)$$

where $\sum_{j=1,2} \hat{p}(j|i) = 1$ for all $i = 1, \ldots, n$.



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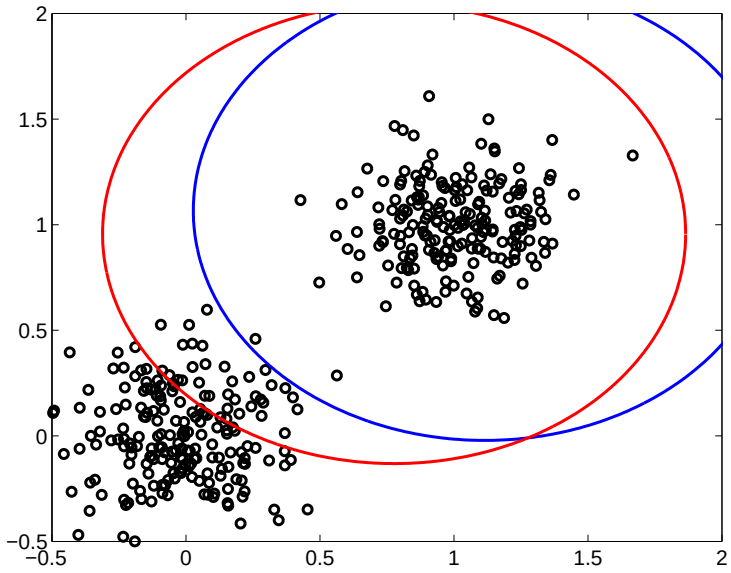


- When the Gaussians are almost identical (as in the figure), $\hat{p}(1|i) \approx \hat{p}(2|i)$ for almost any available point $\mathbf{x}_i$.

  Even slight differences can help us determine how we should modify the Gaussians.

The EM algorithm: iteration k

E-step: softly assign examples to mixture components

$$\hat{p}(j|i) \leftarrow P(y_i = j|\mathbf{x}_i, \theta^{(k)}), \quad \text{for all } j = 1, 2 \text{ and } i = 1, \ldots, n$$

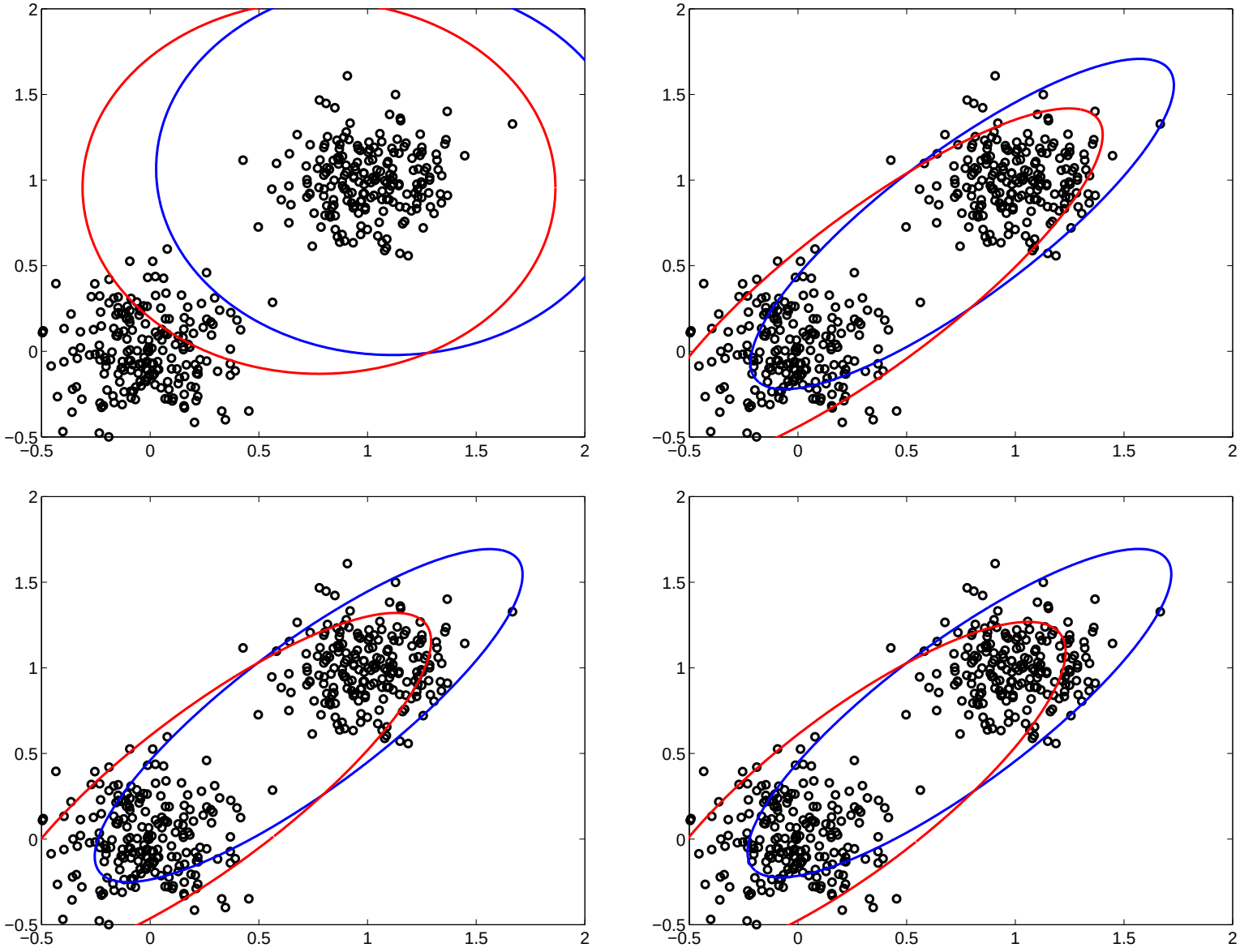
M-step: estimate new mixture parameters $\theta^{(k+1)}$ based on the soft assignments (can be done separately for the two Gaussians)

$$\hat{p}_j \leftarrow \frac{\hat{n}_j}{n}, \quad \text{where } \hat{n}_j = \sum_{i=1}^{n} \hat{p}(j|i)$$

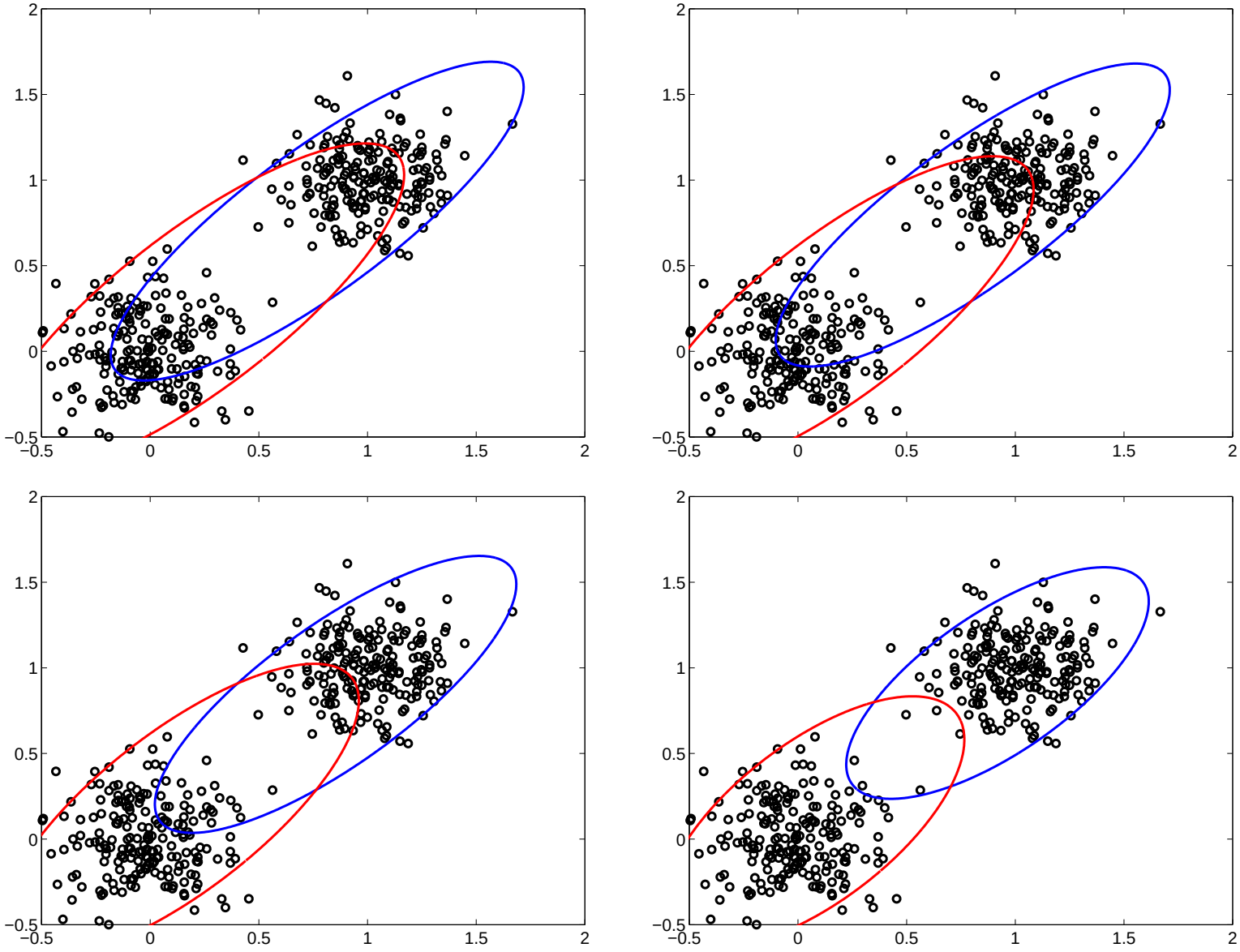
$$\hat{\mu}_j \leftarrow \frac{1}{\hat{n}_j} \sum_{i=1}^{n} \hat{p}(j|i)\, \mathbf{x}_i$$

$$\hat{\Sigma}_j \leftarrow \frac{1}{\hat{n}_j} \sum_{i=1}^{n} \hat{p}(j|i)\, (\mathbf{x}_i - \hat{\mu}_j)(\mathbf{x}_i - \hat{\mu}_j)^T$$

Mixture density estimation: example



Mixture density estimation



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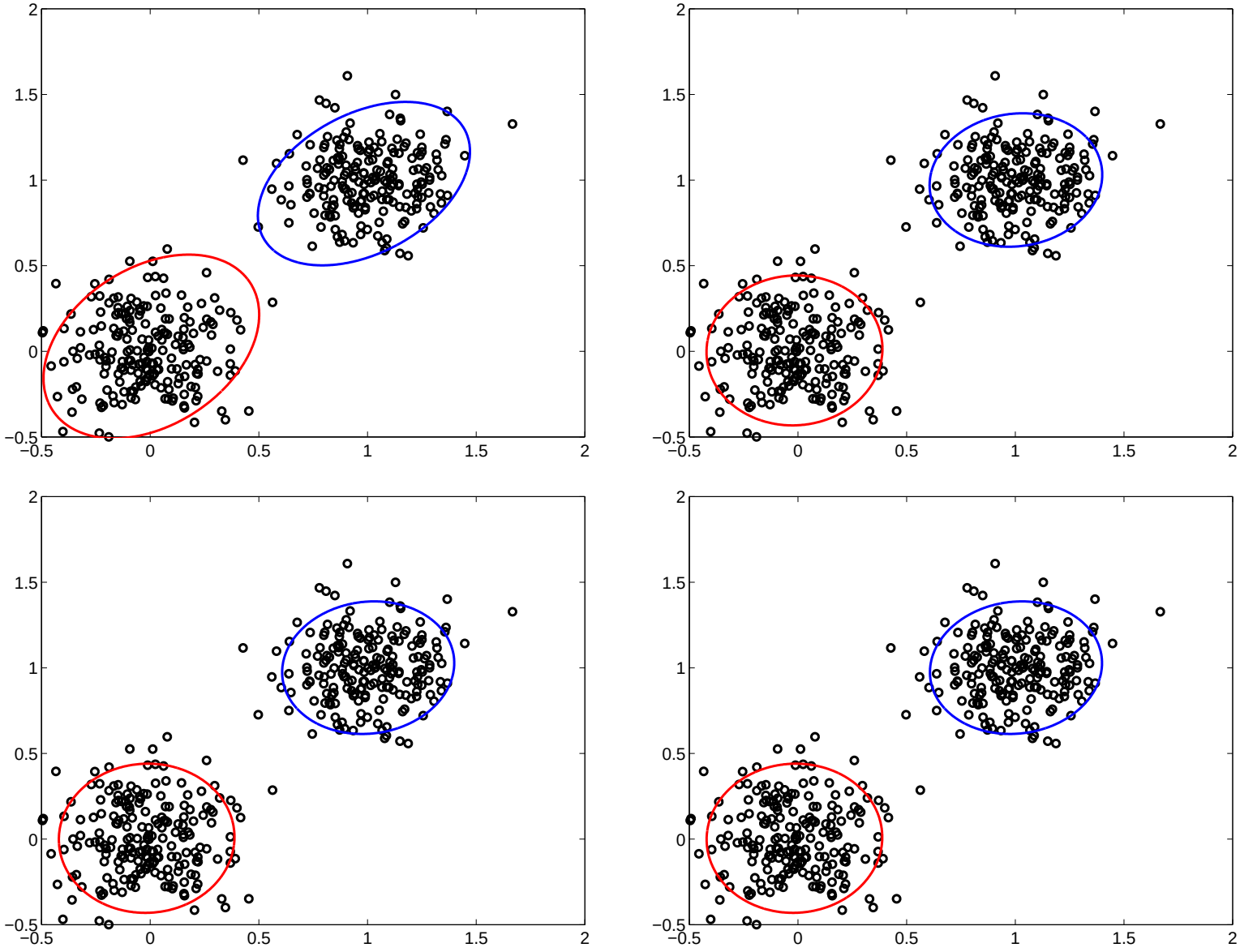

The EM-algorithm

- Each iteration of the EM-algorithm *monotonically* increases the (log-)likelihood of the n training examples $\mathbf{x}_1, \ldots, \mathbf{x}_n$:

$$\log p(\text{ data } | \theta^{(k)}) = \sum_{i=1}^{n} \log \left(\overbrace{p_1\, p(\mathbf{x}_i | \mu_1, \Sigma_1) + p_2\, p(\mathbf{x}_i | \mu_2, \Sigma_2)}^{p(\mathbf{x}_i | \theta^{(k)})} \right)$$

where $\theta^{(k)} = \{p_1, p_2, \mu_1, \mu_2, \Sigma_1, \Sigma_2\}$ specifies the parameters of the mixture model at the k^{th} iteration.