8. Mixture Models and Expectation-Maximization

Motivation

- Often the introduction of latent (unobserved) random variables into a model can help to express complex (marginal) distributions
- A very common example are mixture models, in particular Gaussian mixture models (GMM)
- Mixture models can be used for clustering (unsupervised learning) and to express more complex probability distributions
- As we will see, the parameters of mixture models can be estimated using maximum-likelihood estimation such as expectation-maximization

K-means Clustering (Rep.)

- Given: data set $\{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$, number of clusters K
- Goal: find cluster centers $\{\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K\}$ so that

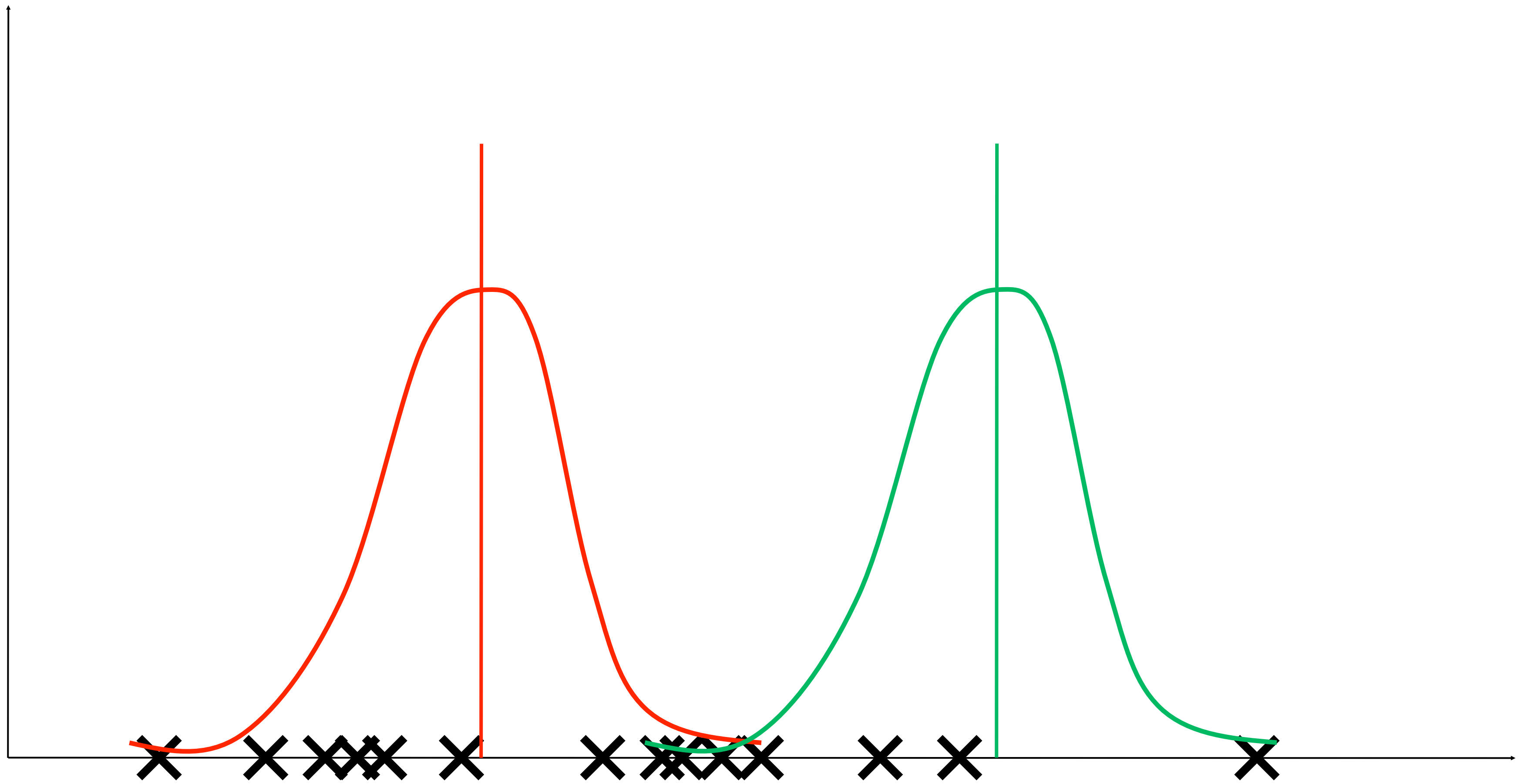
$$J = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \|\mathbf{x}_n - \boldsymbol{\mu}_k\|$$

is minimal, where $r_{nk} = 1$ if $\mathbf{x}_n$ is assigned to $\boldsymbol{\mu}_k$

- Idea: compute r_{nk} and $\boldsymbol{\mu}_k$ iteratively
- Start with some values for the cluster centers
- Find optimal assignments r_{nk}
- Update cluster centers using these assignments
- Repeat until assignments or centers don’t change

K-means Clustering

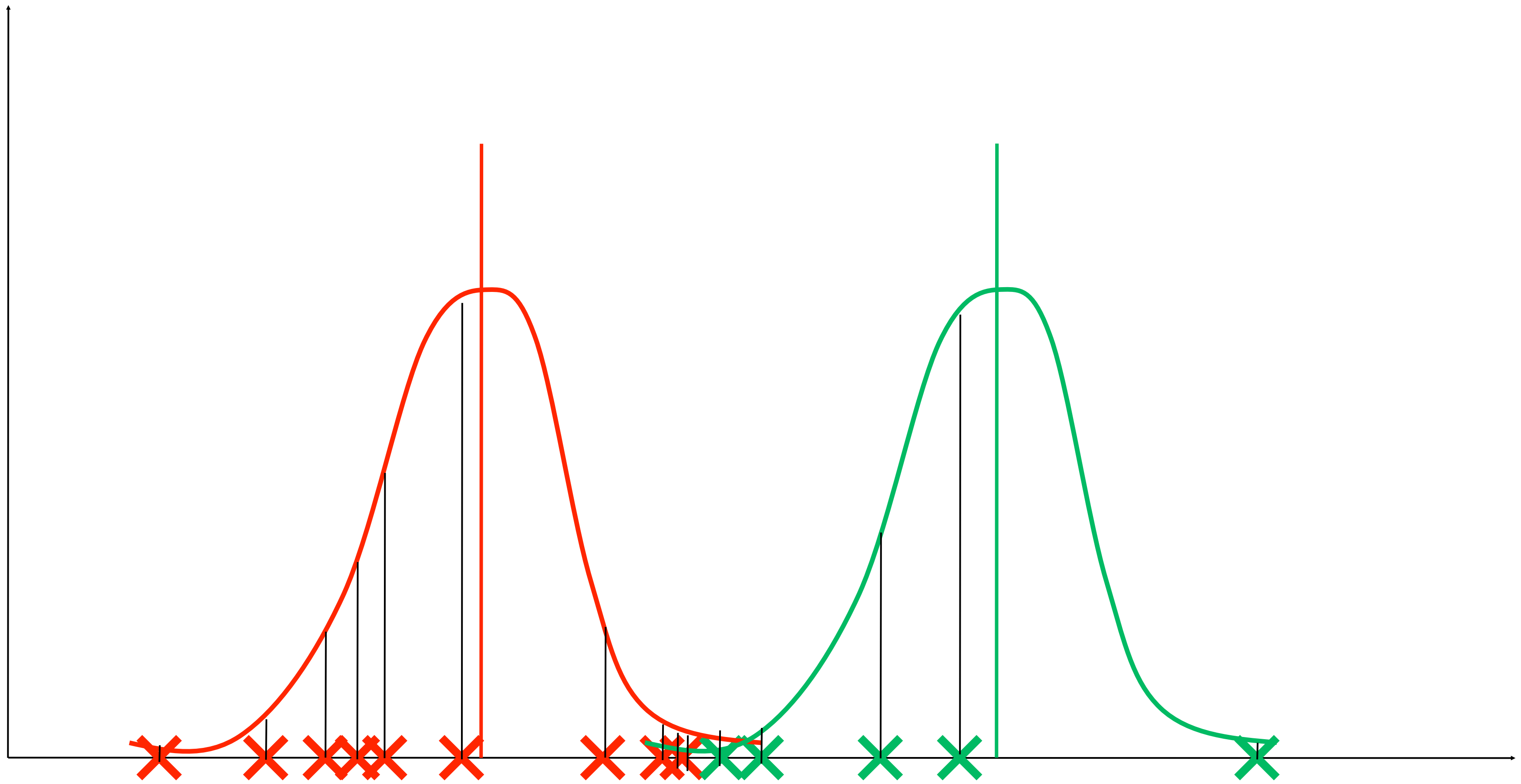
Initialize cluster means: $\{\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K\}$



K-means Clustering

Find optimal assignments:

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

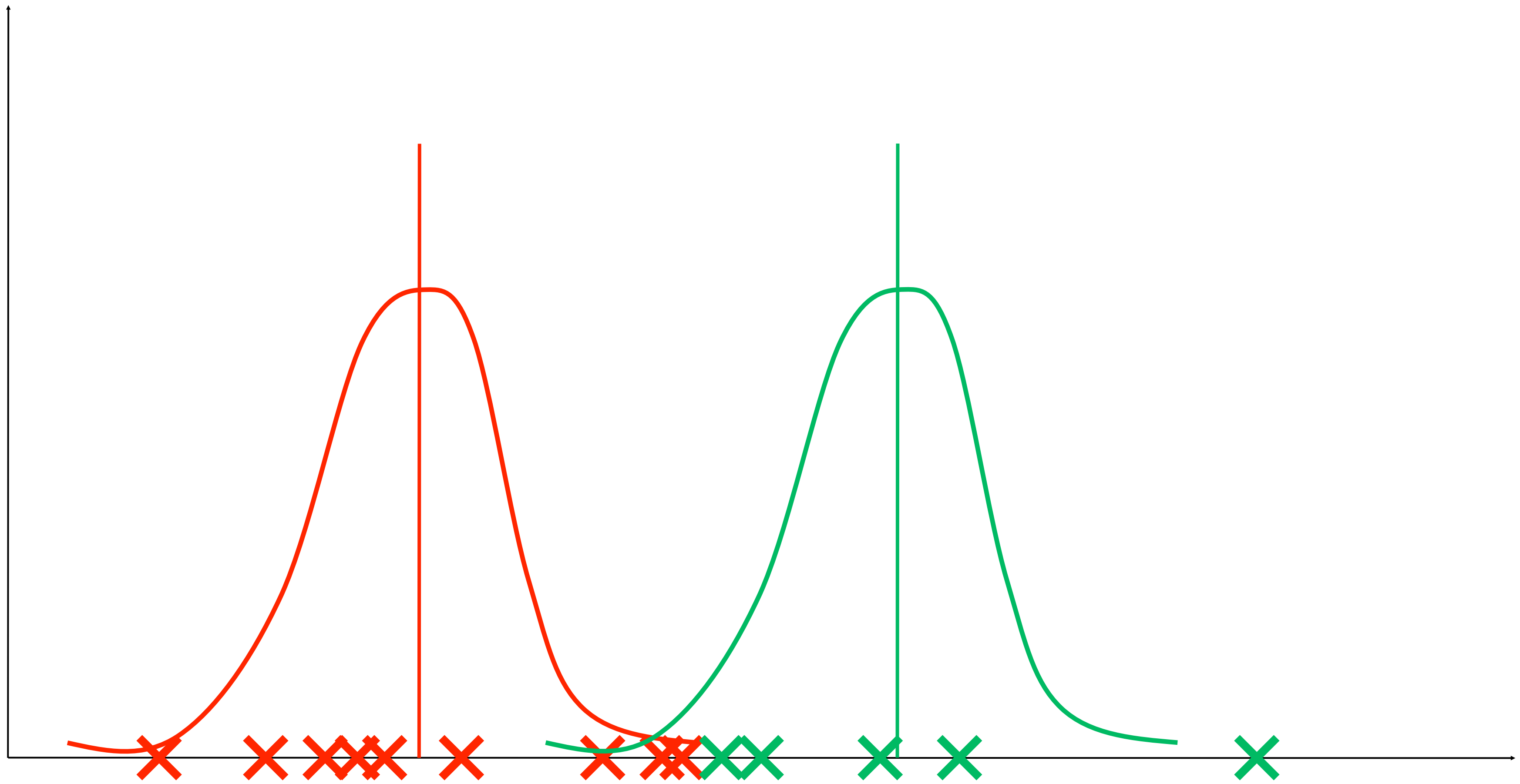


K-means Clustering

Find new optimal means:

$$\frac{\partial J}{\partial \boldsymbol{\mu}_k} = 2\sum_{n=1}^{N} r_{nk}(\mathbf{x}_n - \boldsymbol{\mu}_k) \overset{!}{=} 0$$

$$\Rightarrow \boldsymbol{\mu}_k = \frac{\sum_{n=1}^{N} r_{nk}\mathbf{x}_n}{\sum_{n=1}^{N} r_{nk}}$$



K-means Clustering

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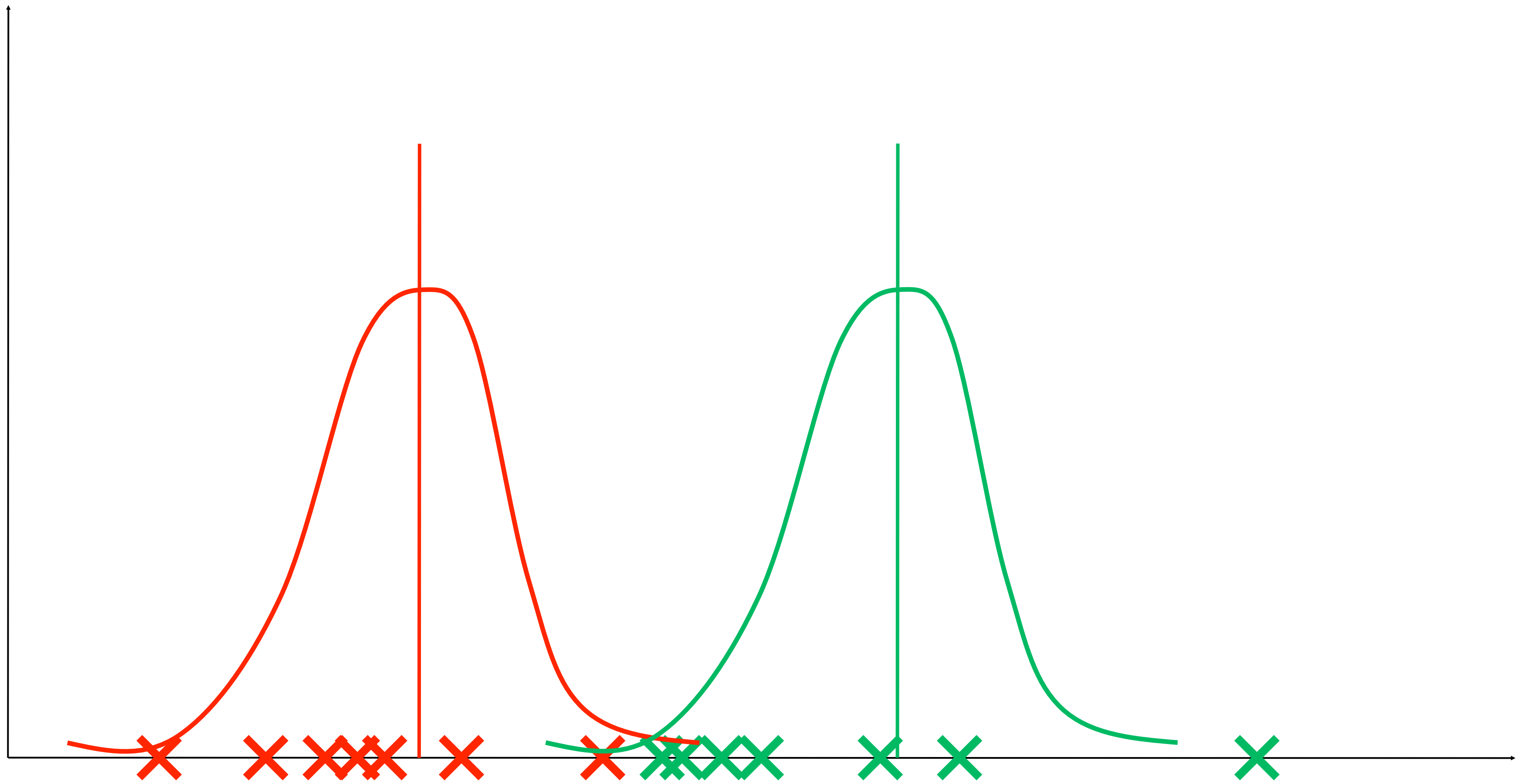
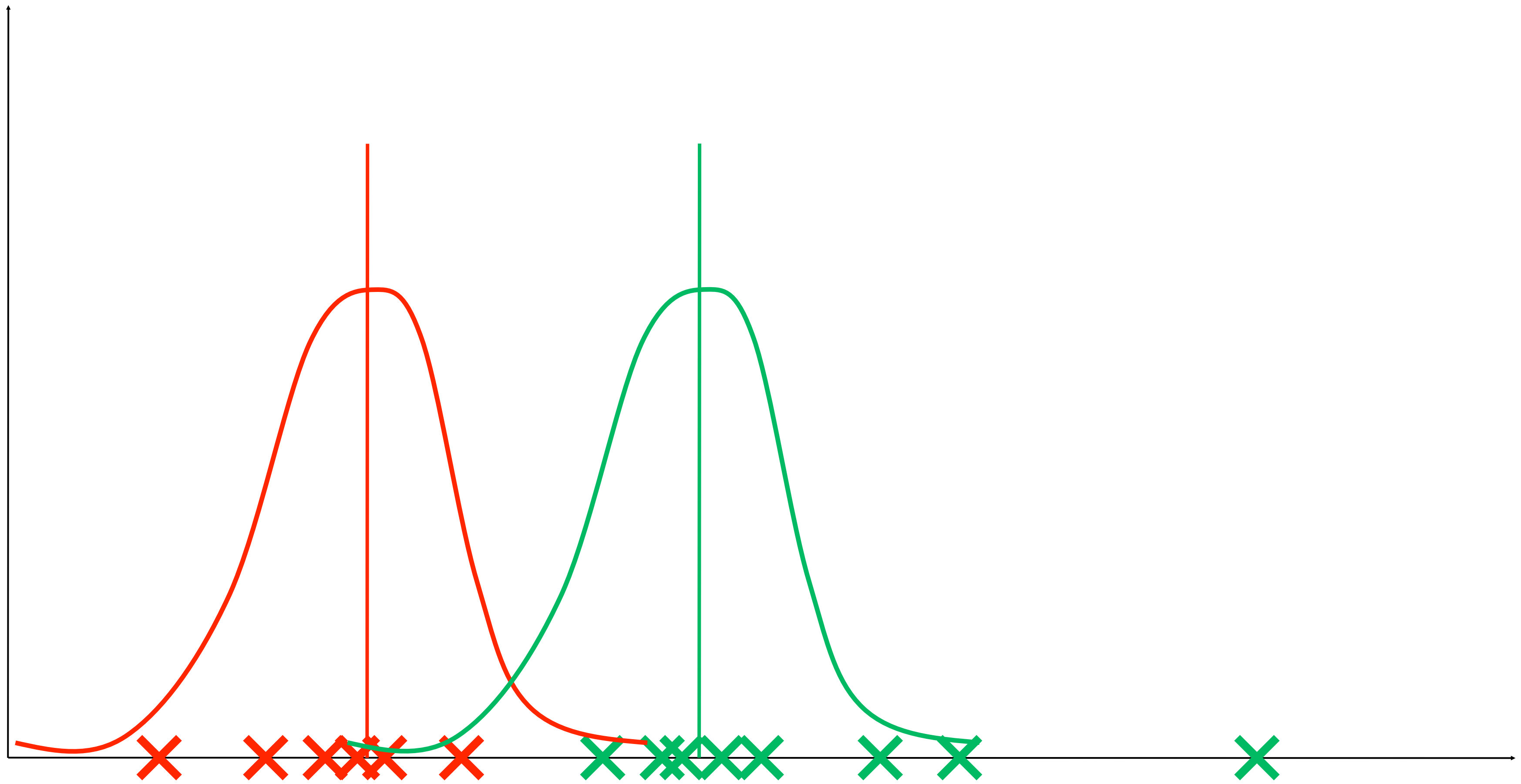
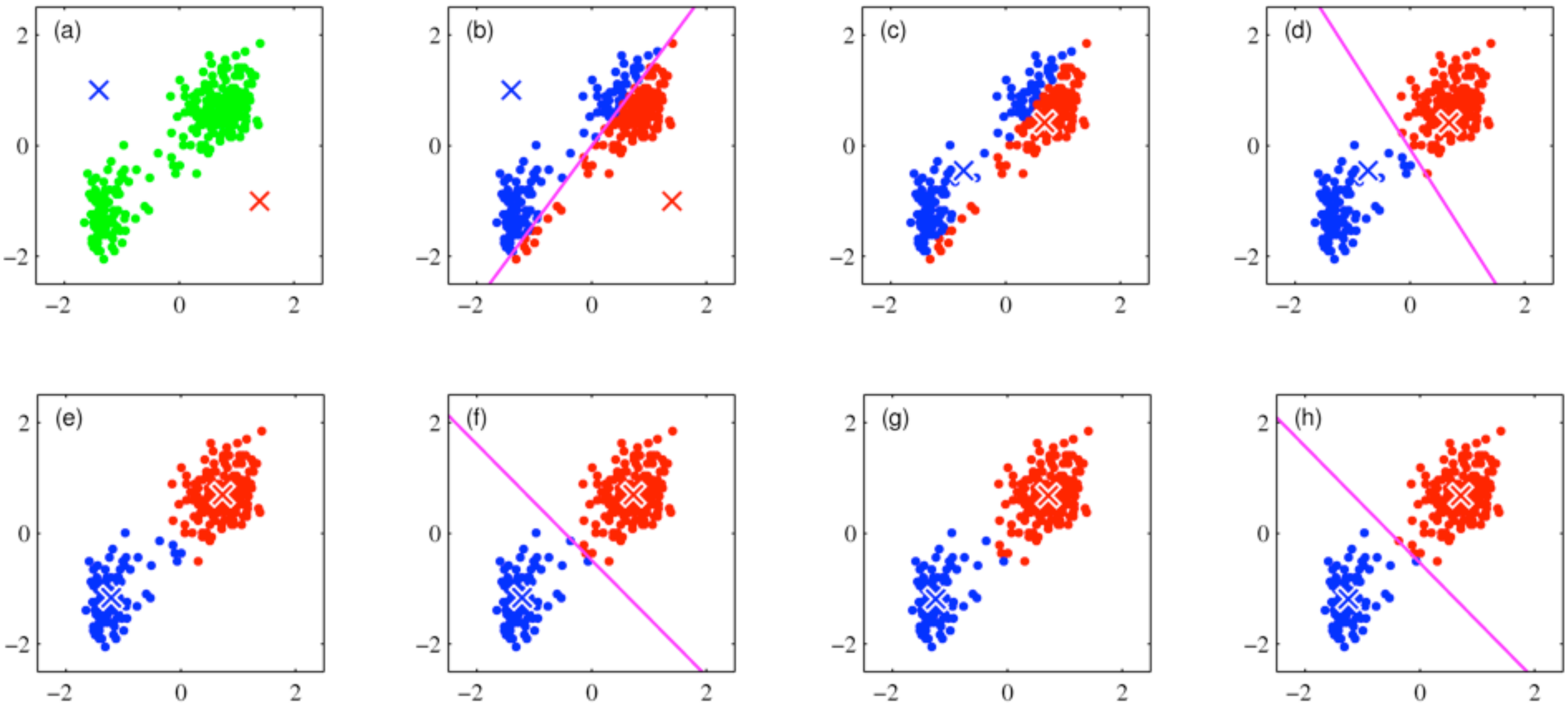


K-means Clustering

Iterate these steps until means and assignments do not change any more



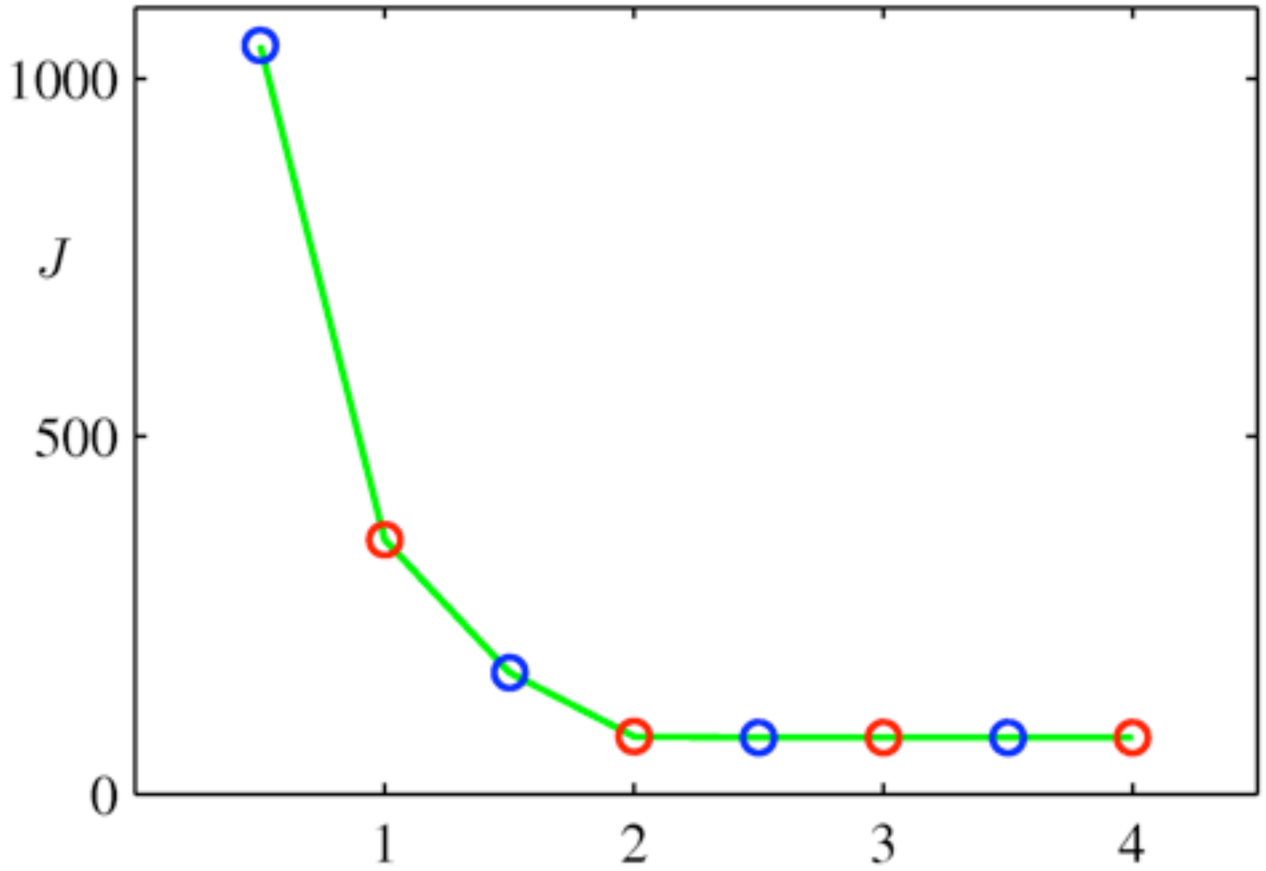
2D Example



- Real data set
- Random initialization

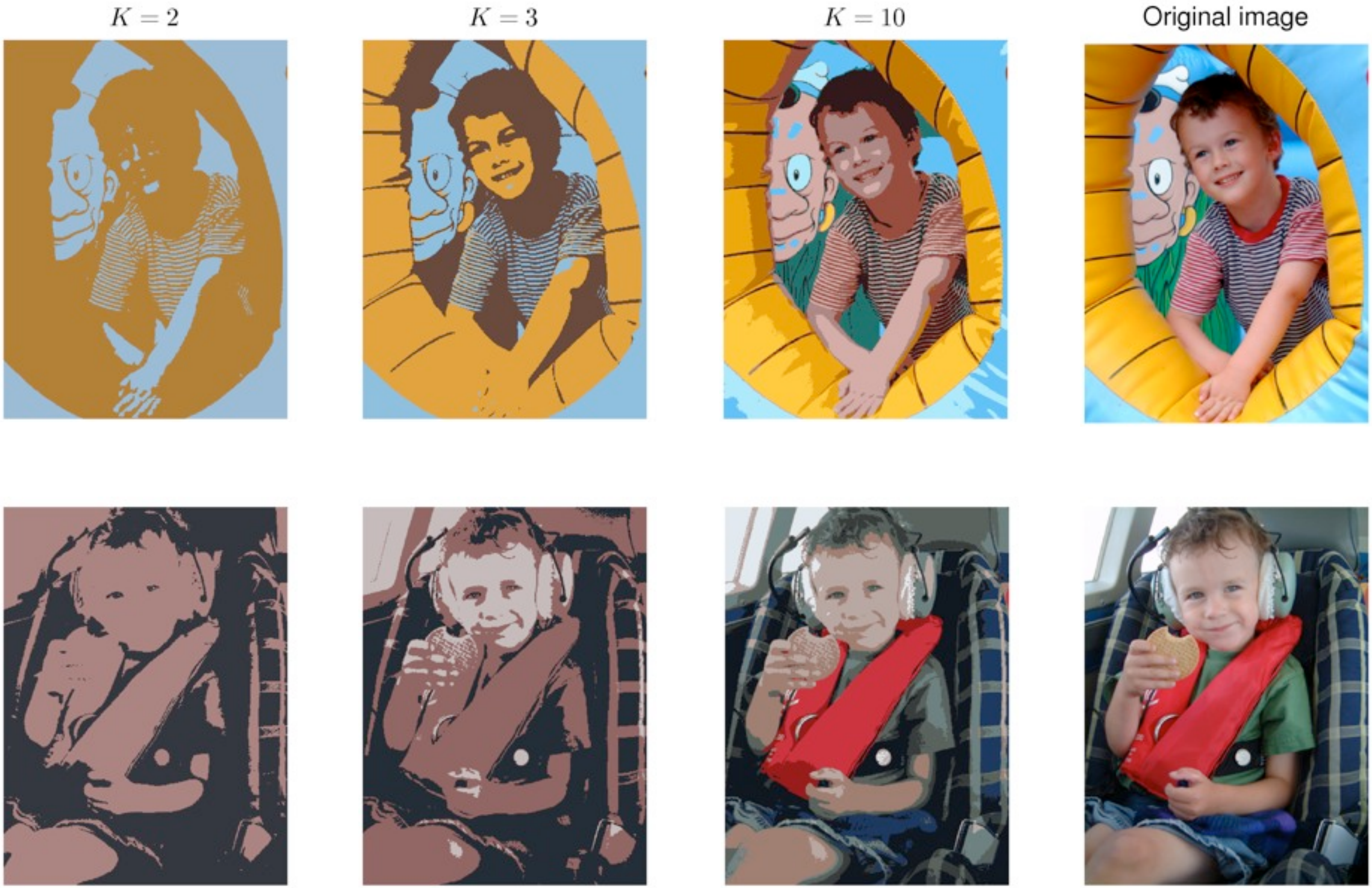
- Magenta line is “decision boundary”

The Cost Function



- After every step the cost function J is minimized
- Blue steps: update assignments
- Red steps: update means
- Convergence after 4 rounds

K-means for Segmentation



$K = 2$

$K = 3$

$K = 10$

Original image

K-Means: Additional Remarks

- There is an online version of K-means (vs. batch until now)
  - After each addition of $\mathbf{x}_i$, the nearest center c_k is updated:

$$\boldsymbol{\mu}_k^{\text{new}} = \boldsymbol{\mu}_k^{\text{old}} + \eta_n (\mathbf{x}_n - \boldsymbol{\mu}_k^{\text{old}})$$

- The K-medoid variant (see also lecture on kernels):
  - Replace the Euclidean distance by a general measure V.

$$\tilde{J} = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \mathcal{V}(\mathbf{x}_n, \boldsymbol{\mu}_k)$$

Mixtures of Gaussians

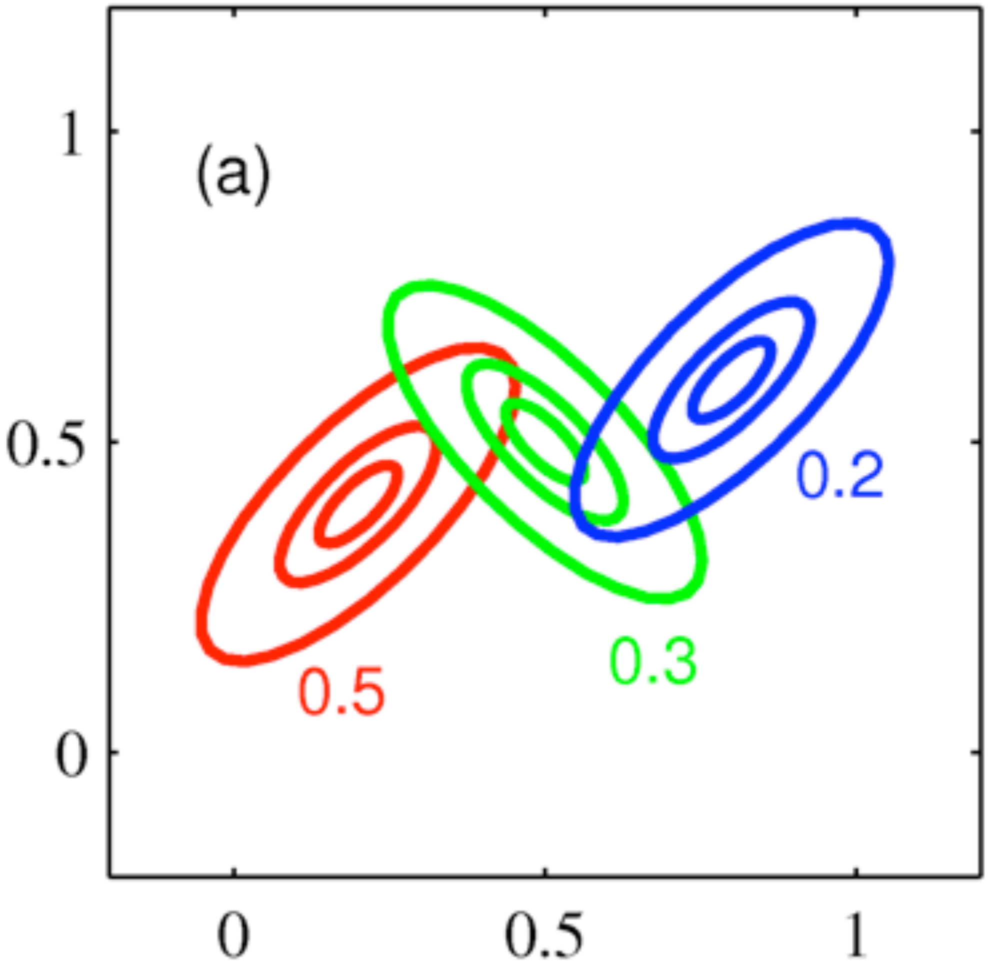
- Assume that the data consists of K clusters
- The data within each cluster is Gaussian
- For any data point $\mathbf{x}$ we introduce a K-dimensional binary random variable $\mathbf{z}$ so that:

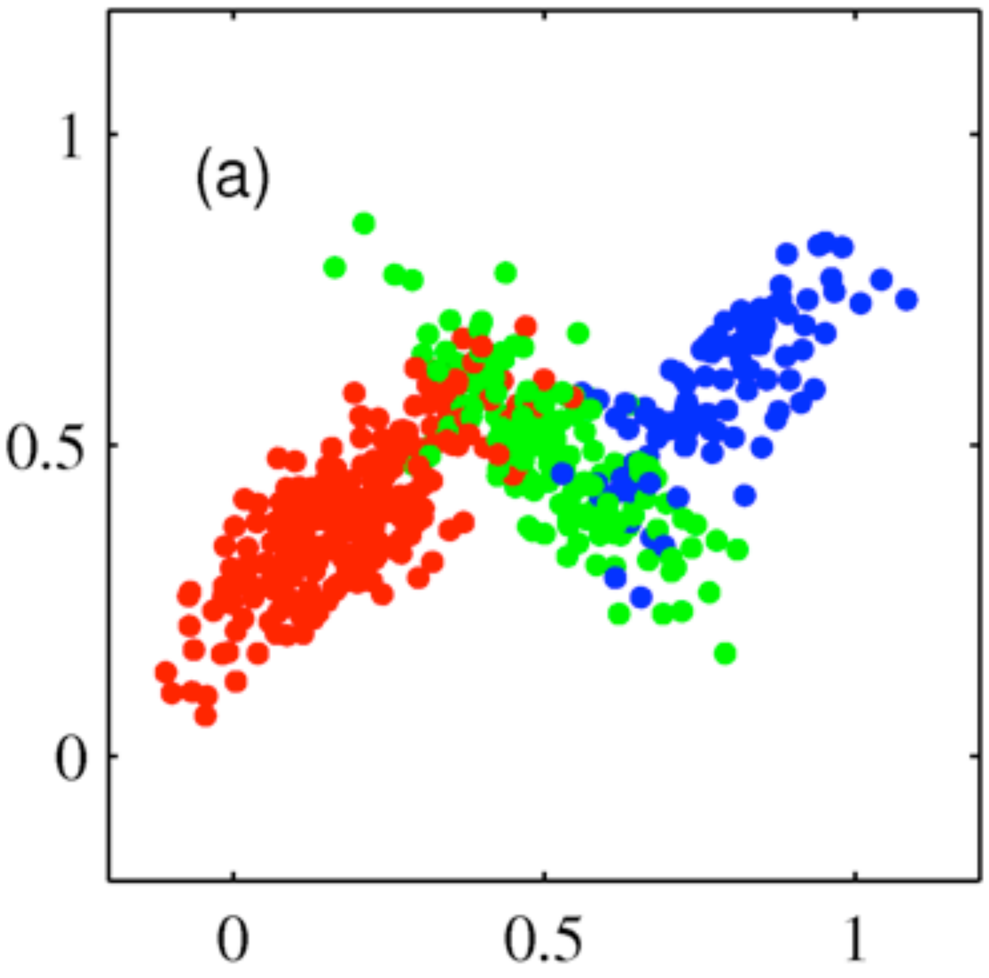
$$p(\mathbf{x}) = \sum_{k=1}^{K} \underbrace{p(z_k = 1)}_{=:\pi_k} \mathcal{N}(\mathbf{x} \mid \boldsymbol{\mu}_k, \Sigma_k)$$

where

$$z_k \in \{0, 1\}, \quad \sum_{k=1}^{K} z_k = 1$$

A Simple Example





- Mixture of three Gaussians with mixing coefficients
- Left: all three Gaussians as contour plot
- Right: samples from the mixture model, the red component has the most samples

Parameter Estimation

- From a given set of training data $\{\mathbf{x}_1, \dots, \mathbf{x}_N\}$ we want to find parameters $(\pi_{1,\dots,K}, \boldsymbol{\mu}_{1,\dots,K}, \Sigma_{1,\dots,K})$ so that the likelihood is maximized (MLE):

$$p(\mathbf{x}_1, \dots, \mathbf{x}_N \mid \pi_{1,\dots,K}, \boldsymbol{\mu}_{1,\dots,K}, \Sigma_{1,\dots,K}) = \prod_{n=1}^{N} \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \Sigma_k)$$

or, applying the logarithm:

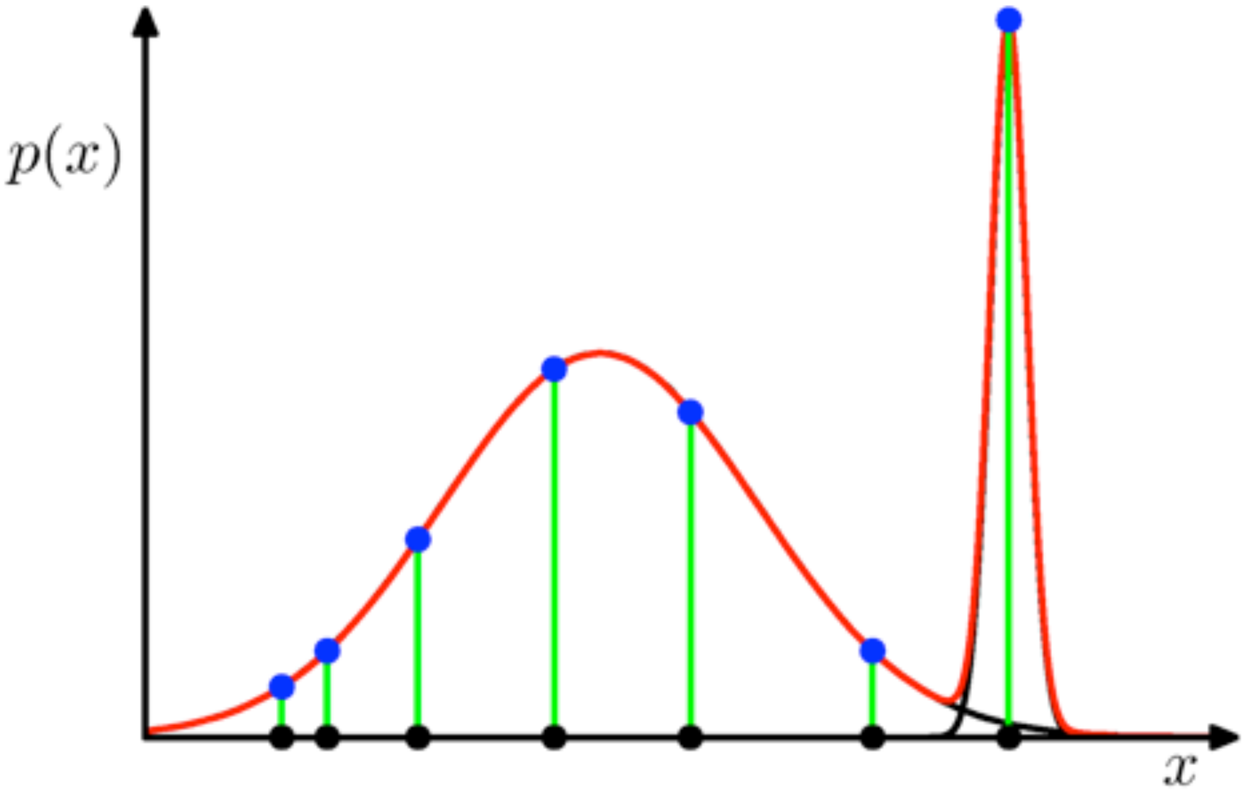
$$\log p(X \mid \boldsymbol{\pi}, \boldsymbol{\mu}, \Sigma) = \sum_{n=1}^{N} \log \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \Sigma_k)$$

- However: this is not as easy as maximum-likelihood for single Gaussians!

Problems with MLE for Gaussian Mixtures

- Assume that for one k the mean $\boldsymbol{\mu}_k$ is exactly at a data point $\mathbf{x}_n$
  - For simplicity: assume that $\Sigma_k = \sigma_k^2 I$
  - Then: $$\mathcal{N}(\mathbf{x}_n \mid \mathbf{x}_n, \sigma_k^2 I) = \frac{1}{\sqrt{2\pi}\sigma_k^D}$$
  - This means that the overall log-likelihood can be maximized arbitrarily by letting $\sigma_k \to 0$ (**overfitting**)
- Another problem is the **identifiability**:
  - The order of the Gaussians is not fixed, therefore:
  - There are $K!$ equivalent solutions to the MLE problem

Overfitting with MLE for Gaussian Mixtures



- One Gaussian fits exactly to one data point
- It has a very small variance, i.e. contributes strongly to the overall likelihood
- In standard MLE, there is no way to avoid this!

Expectation-Maximization

- EM is an elegant and powerful method for MLE problems with latent variables
- Main idea: model parameters and latent variables are estimated iteratively, where average over the latent variables (expectation)
- A typical example application of EM is the Gaussian Mixture model (GMM)
- However, EM has many other applications
- First, we consider EM for GMMs

Expectation-Maximization for GMM

- First, we define the **responsibilities:**

$$\gamma(z_{nk}) = p(z_{nk} = 1 \mid \mathbf{x}_n)$$

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$$= \frac{\pi_k \mathcal{N}(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \Sigma_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}_n \mid \boldsymbol{\mu}_j, \Sigma_j)}$$

- Next, we derive the log-likelihood wrt. to $\boldsymbol{\mu}_k$:

$$\frac{\partial \log p(X \mid \boldsymbol{\pi}, \boldsymbol{\mu}, \Sigma)}{\partial \boldsymbol{\mu}_k} \overset{!}{=} \mathbf{0}$$

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and we obtain: $$\boldsymbol{\mu}_k = \frac{\sum_{n=1}^{N} \gamma(z_{nk}) \mathbf{x}_n}{\sum_{n=1}^{N} \gamma(z_{nk})}$$

Expectation-Maximization for GMM

- We can do the same for the covariances:

$$\frac{\partial \log p(X \mid \boldsymbol{\pi}, \boldsymbol{\mu}, \Sigma)}{\partial \Sigma_k} \overset{!}{=} \mathbf{0}$$

and we obtain:

$$\Sigma_k = \frac{\sum_{n=1}^{N} \gamma(z_{nk})(\mathbf{x}_n - \boldsymbol{\mu}_k)(\mathbf{x}_n - \boldsymbol{\mu}_k)^T}{\sum_{n=1}^{N} \gamma(z_{nk})}$$

- Finally, we derive wrt. the mixing coefficients π_k :

$$\frac{\partial \log p(X \mid \boldsymbol{\pi}, \boldsymbol{\mu}, \Sigma)}{\partial \pi_k} \overset{!}{=} \mathbf{0} \qquad \text{where:} \qquad \sum_{k=1}^{K} \pi_k = 1$$

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and the result is: $$\pi_k = \frac{1}{N} \sum_{n=1}^{N} \gamma(z_{nk})$$

Algorithm Summary

1. Initialize means $\boldsymbol{\mu}_k$ covariance matrices Σ_k and mixing coefficients $\boldsymbol{\pi}_k$
2. Compute the initial log-likelihood $\log p(X \mid \boldsymbol{\pi}, \boldsymbol{\mu}, \Sigma)$
3. **E-Step.** Compute the responsibilities:

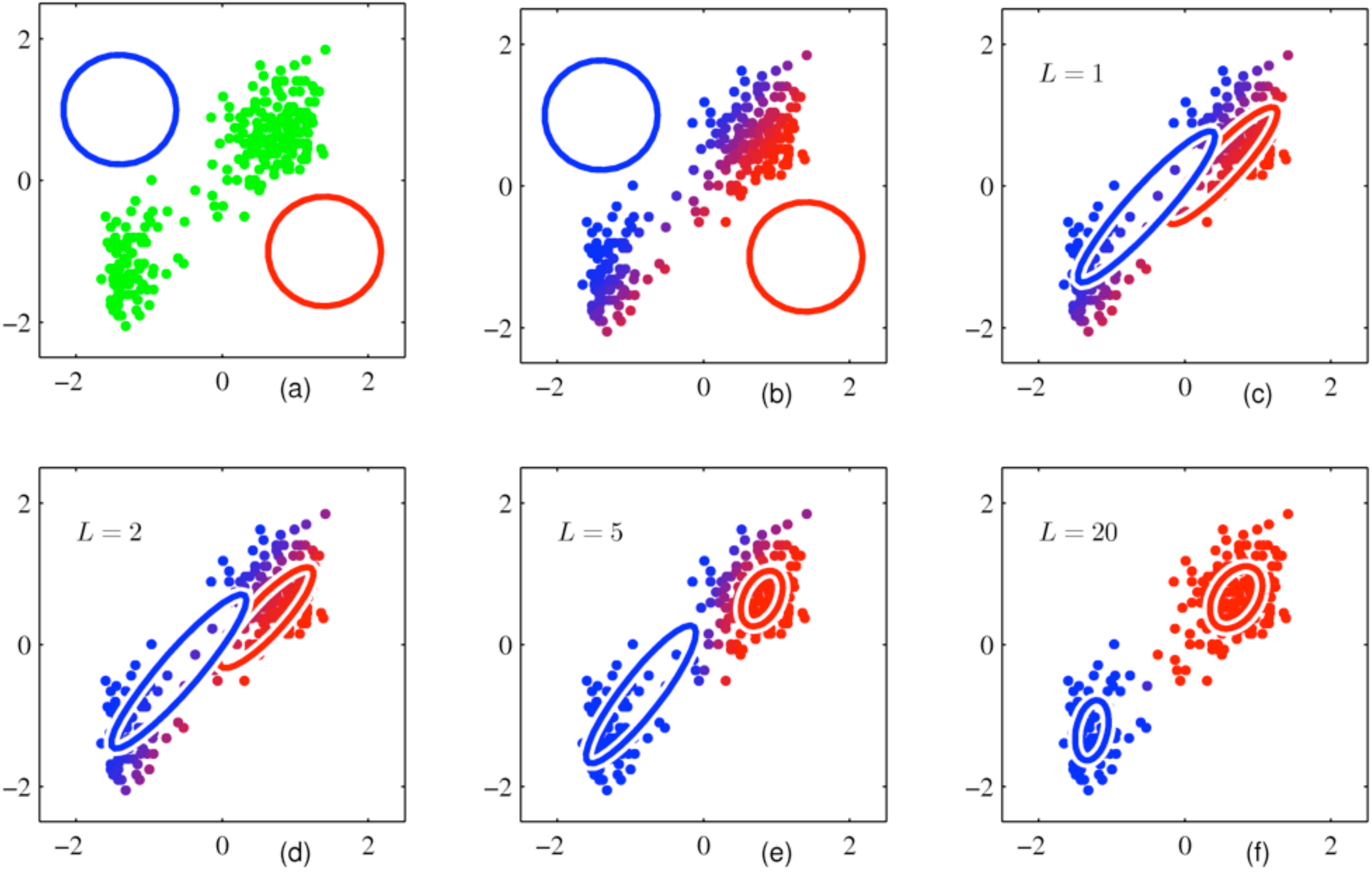
$$\gamma(z_{nk}) = \frac{\pi_k \mathcal{N}(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \Sigma_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}_n \mid \boldsymbol{\mu}_j, \Sigma_j)}$$

4. **M-Step.** Update the parameters:

$$\boldsymbol{\mu}_k^{\text{new}} = \frac{\sum_{n=1}^{N} \gamma(z_{nk}) \mathbf{x}_n}{\sum_{n=1}^{N} \gamma(z_{nk})} \quad \Sigma_k^{\text{new}} = \frac{\sum_{n=1}^{N} \gamma(z_{nk})(\mathbf{x}_n - \boldsymbol{\mu}_k^{\text{new}})(\mathbf{x}_n - \boldsymbol{\mu}_k^{\text{new}})^T}{\sum_{n=1}^{N} \gamma(z_{nk})} \quad \pi_k^{\text{new}} = \frac{1}{N} \sum_{n=1}^{N} \gamma(z_{nk})$$

5.Compute log-likelihood; if not converged go to 3.

The Same Example Again



Observations

- Compared to K-means, points can now belong to both clusters (**soft assignment**)
- In addition to the cluster center, a covariance is estimated by EM
- Initialization is the same as used for K-means
- Number of iterations needed for EM is much higher
- Also: each cycle requires much more computation
- Therefore: start with K-means and run EM on the result of K-means (covariances can be initialized to the sample covariances of K-means)
- EM only finds a **local** maximum of the likelihood!

A More General View of EM

- Assume for a moment that we observe X and the binary latent variables Z. The likelihood is then:

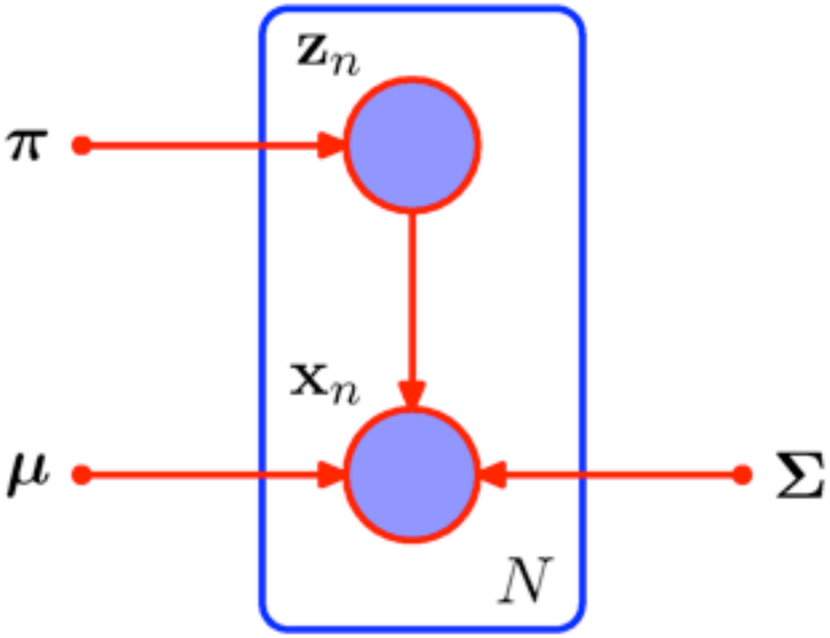
$$p(X, Z \mid \boldsymbol{\pi}, \boldsymbol{\mu}, \Sigma) = \prod_{n=1}^{N} p(\mathbf{z}_n \mid \boldsymbol{\pi}) p(\mathbf{x}_n \mid \mathbf{z}_n, \boldsymbol{\mu}, \Sigma)$$

Remember:

$$z_{nk} \in \{0, 1\}, \quad \sum_{k=1}^{K} z_{nk} = 1$$

where $p(\mathbf{z}_n \mid \boldsymbol{\pi}) = \prod_{k=1}^{K} \pi_k^{z_{nk}}$ and

$$p(\mathbf{x}_n \mid \mathbf{z}_n, \boldsymbol{\mu}, \Sigma) = \prod_{k=1}^{K} \mathcal{N}(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \Sigma_k)^{z_{nk}}$$



which leads to the log-formulation:

$$\log p(X, Z \mid \boldsymbol{\pi}, \boldsymbol{\mu}, \Sigma) = \sum_{n=1}^{N} \sum_{k=1}^{K} z_{nk} (\log \pi_k + \log \mathcal{N}(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \Sigma_k))$$

The Complete-Data Log-Likelihood

$$\log p(X, Z \mid \boldsymbol{\pi}, \boldsymbol{\mu}, \Sigma) = \sum_{n=1}^{N} \sum_{k=1}^{K} z_{nk} (\log \pi_k + \log \mathcal{N}(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \Sigma_k))$$

- This is called the **complete-data log-likelihood**
- Advantage: solving for the parameters $(\pi_k, \boldsymbol{\mu}_k, \Sigma_k)$ is much simpler, as the log is inside the sum!
- We could switch the sums and then for every mixture component k only look at the points that are associated with that component.
- This leads to simple closed-form solutions for the parameters
- However: the latent variables Z are not observed!

The Main Idea of EM

- Instead of maximizing the joint log-likelihood, we maximize its **expectation** under the latent variable distribution:

$$\mathbb{E}_Z[\log p(X, Z \mid \boldsymbol{\pi}, \boldsymbol{\mu}, \Sigma)] = \sum_{n=1}^{N} \sum_{k=1}^{K} \mathbb{E}_Z[z_{nk}](\log \pi_k + \log \mathcal{N}(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \Sigma_k))$$

where the latent variable distribution per point is:

$$p(\mathbf{z}_n \mid \mathbf{x}_n, \boldsymbol{\theta}) = \frac{p(\mathbf{x}_n \mid \mathbf{z}_n, \boldsymbol{\theta}) p(\mathbf{z}_n \mid \boldsymbol{\theta})}{p(\mathbf{x}_n \mid \boldsymbol{\theta})} \qquad \boldsymbol{\theta} = (\boldsymbol{\pi}, \boldsymbol{\mu}, \Sigma)$$

$$= \frac{\prod_{l=1}^{K} (\pi_l \mathcal{N}(\mathbf{x}_n \mid \boldsymbol{\mu}_l, \Sigma_l))^{z_{nl}}}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}_n \mid \boldsymbol{\mu}_j, \Sigma_j)}$$

The Main Idea of EM

The expected value of the latent variables is:

$$\mathbb{E}[z_{nk}] = \gamma(z_{nk})$$

plugging in we obtain:

$$\mathbb{E}_Z[\log p(X, Z \mid \boldsymbol{\pi}, \boldsymbol{\mu}, \Sigma)] = \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma(z_{nk})(\log \pi_k + \log \mathcal{N}(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \Sigma_k))$$

We compute this iteratively:

1. Initialize $i = 0, \quad (\pi_k^i, \boldsymbol{\mu}_k^i, \Sigma_k^i)$
2. Compute $\mathbb{E}[z_{nk}] = \gamma(z_{nk})$
3. Find parameters $(\pi_k^{i+1}, \boldsymbol{\mu}_k^{i+1}, \Sigma_k^{i+1})$ that maximize this
4. Increase i; if not converged, goto 2.

The Theory Behind EM

- We have seen that EM maximizes the **expected complete-data log-likelihood**, but:
- Actually, we need to maximize the log-marginal

$$\log p(X \mid \boldsymbol{\theta}) = \log \sum_{Z} p(X, Z \mid \boldsymbol{\theta})$$

- It turns out that the log-marginal is maximized **implicitly!**

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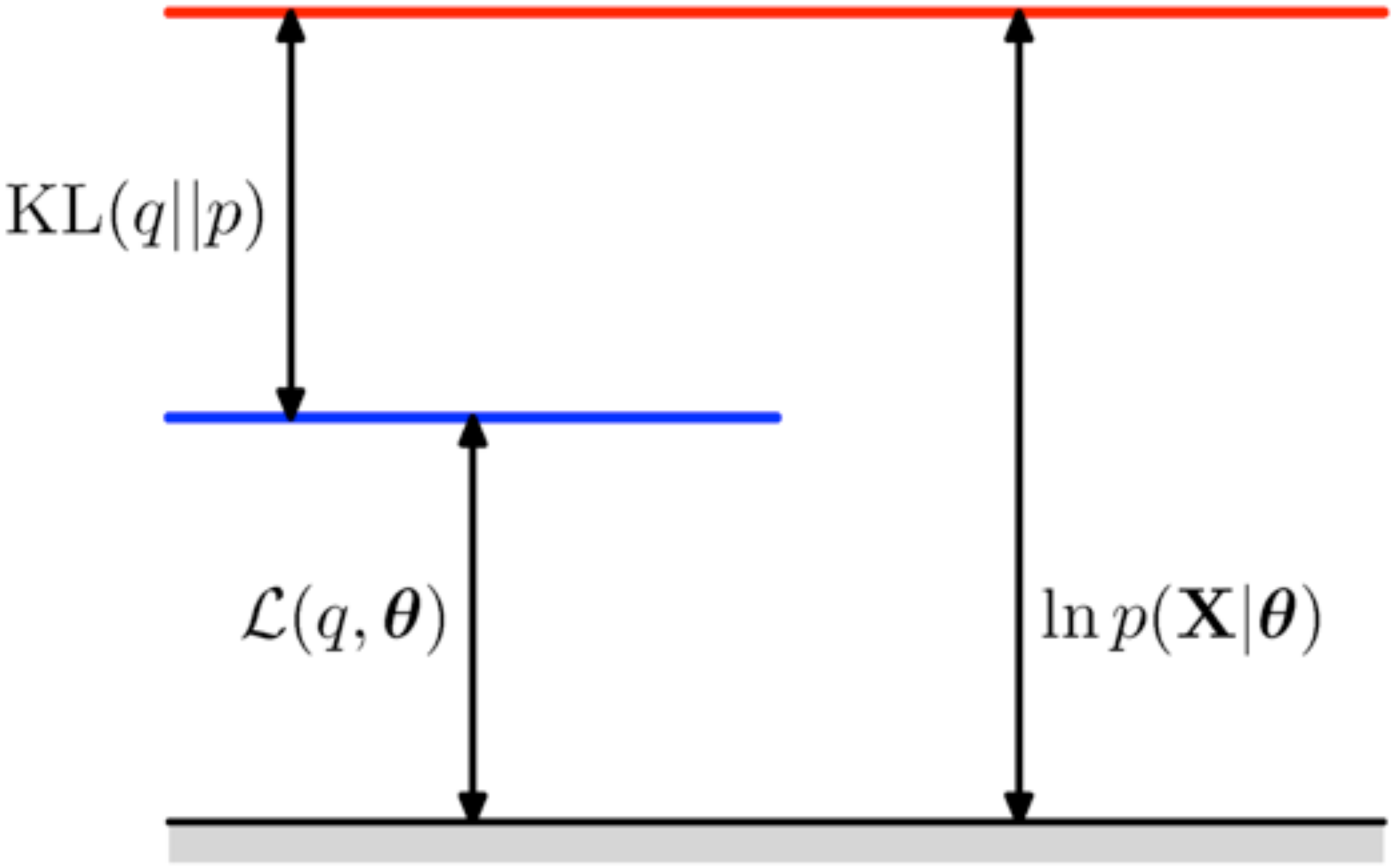
- It turns out that the log-marginal is maximized **implicitly!**

$$\log p(X \mid \boldsymbol{\theta}) = \mathcal{L}(q, \boldsymbol{\theta}) + \mathrm{KL}(q \| p)$$

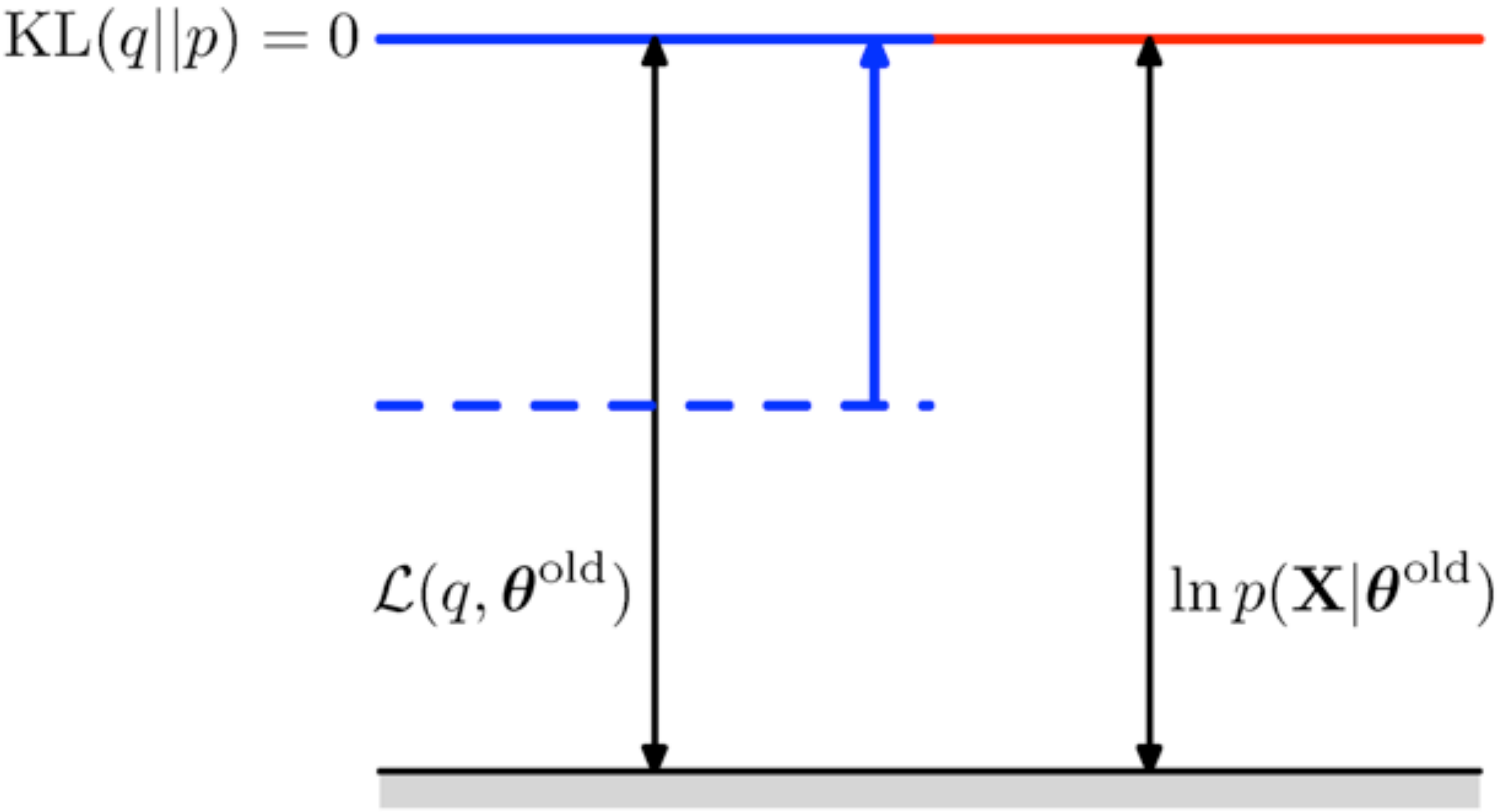
$$\mathcal{L}(q, \boldsymbol{\theta}) = \sum_{Z} q(Z) \log \frac{p(X, Z \mid \boldsymbol{\theta})}{q(Z)} \qquad \mathrm{KL}(q \| p) = -\sum_{Z} q(Z) \log \frac{p(Z \mid X, \boldsymbol{\theta})}{q(Z)}$$

Visualization


$\mathrm{KL}(q||p)$
$\mathcal{L}(q, \boldsymbol{\theta})$
$\ln p(\mathbf{X}|\boldsymbol{\theta})$

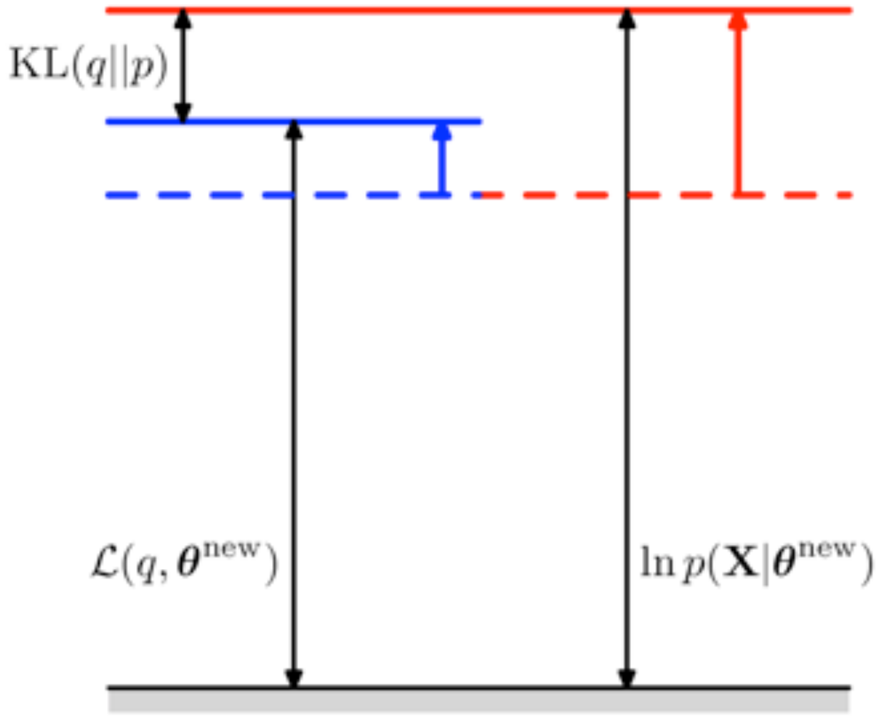
- The KL-divergence is positive or 0
- Thus, the log-likelihood is at least as large as L or:
- *L* is a lower bound of the log-likelihood

What Happens in the E-Step?


$\mathrm{KL}(q\|p) = 0$
$\mathcal{L}(q, \boldsymbol{\theta}^{\text{old}})$
$\ln p(\mathbf{X}|\boldsymbol{\theta}^{\text{old}})$

- The log-likelihood is independent of q
- Thus: L is maximized iff KL is minimal
- This is the case iff $q(Z) = p(Z \mid X, \boldsymbol{\theta})$

What Happens in the M-Step?

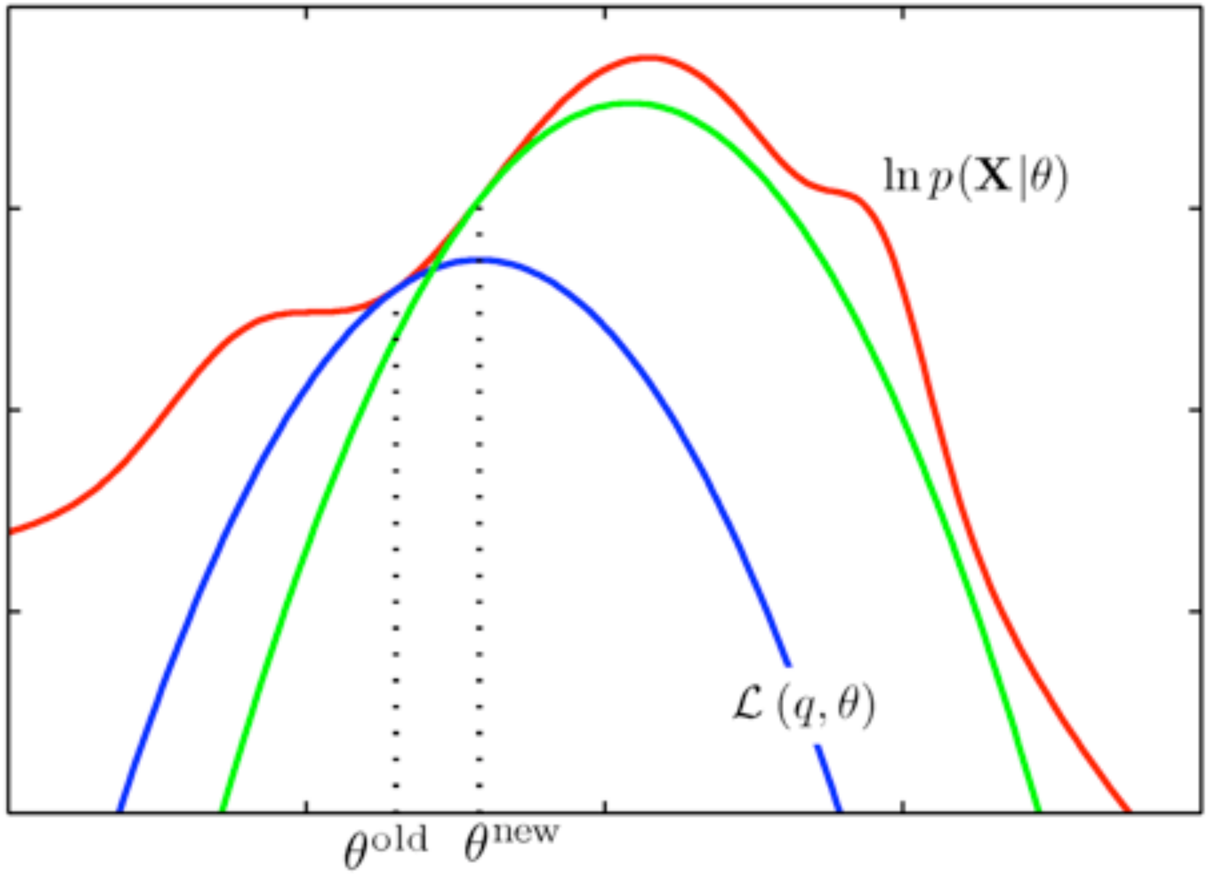

$\mathrm{KL}(q||p)$
$\mathcal{L}(q, \boldsymbol{\theta}^{\mathrm{new}})$
$\ln p(\mathbf{X}|\boldsymbol{\theta}^{\mathrm{new}})$

- In the M-step we keep q fixed and find new $\boldsymbol{\theta}$

$$\mathcal{L}(q, \boldsymbol{\theta}) = \sum_Z p(Z \mid X, \boldsymbol{\theta}^{\mathrm{old}}) \log p(X, Z \mid \boldsymbol{\theta}) - \sum_Z q(Z) \log q(Z)$$

- We maximize the first term, the second is indep.
- This implicitly makes KL non-zero
- The log-likelihood is maximized even more!

Visualization in Parameter-Space



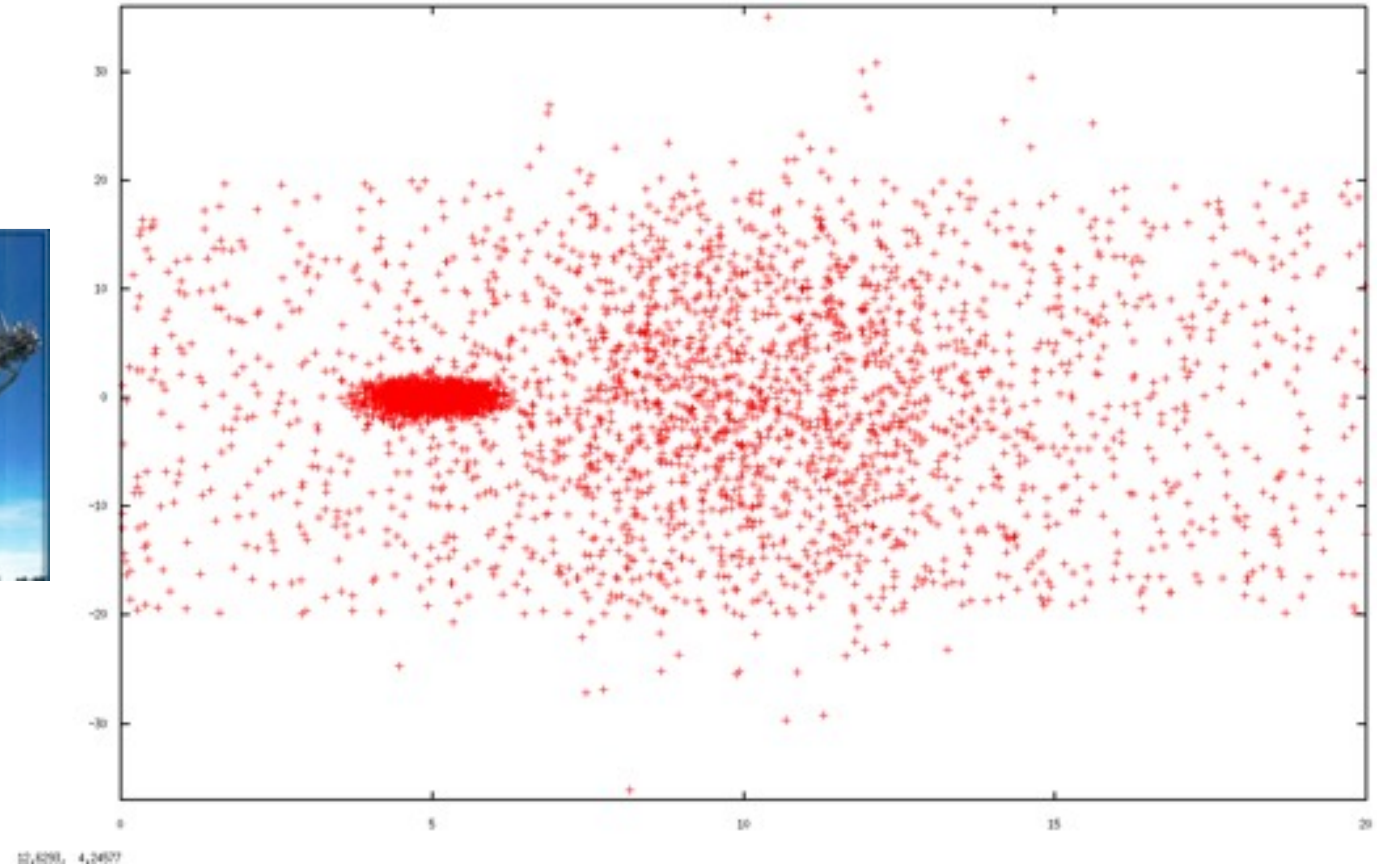
- In the E-step we compute the concave lower bound for given old parameters θ^{old} (blue curve)
- In the M-step, we maximize this lower bound and obtain new parameters θ^{new}
- This is repeated (green curve) until convergence

Variants of EM

- Instead of maximizing the log-likelihood, we can use EM to maximize a **posterior** when a prior is given (MAP instead of MLE) ⇒ less overfitting
- In Generalized EM, the M-step only increases the lower bound instead of maximization (useful if standard M-step is intractable)
- Similarly, the E-step can be generalized in that the optimization wrt. *q* is not complete
- Furthermore, there are incremental versions of EM, where data points are given sequentially and the parameters are updated after each data point.

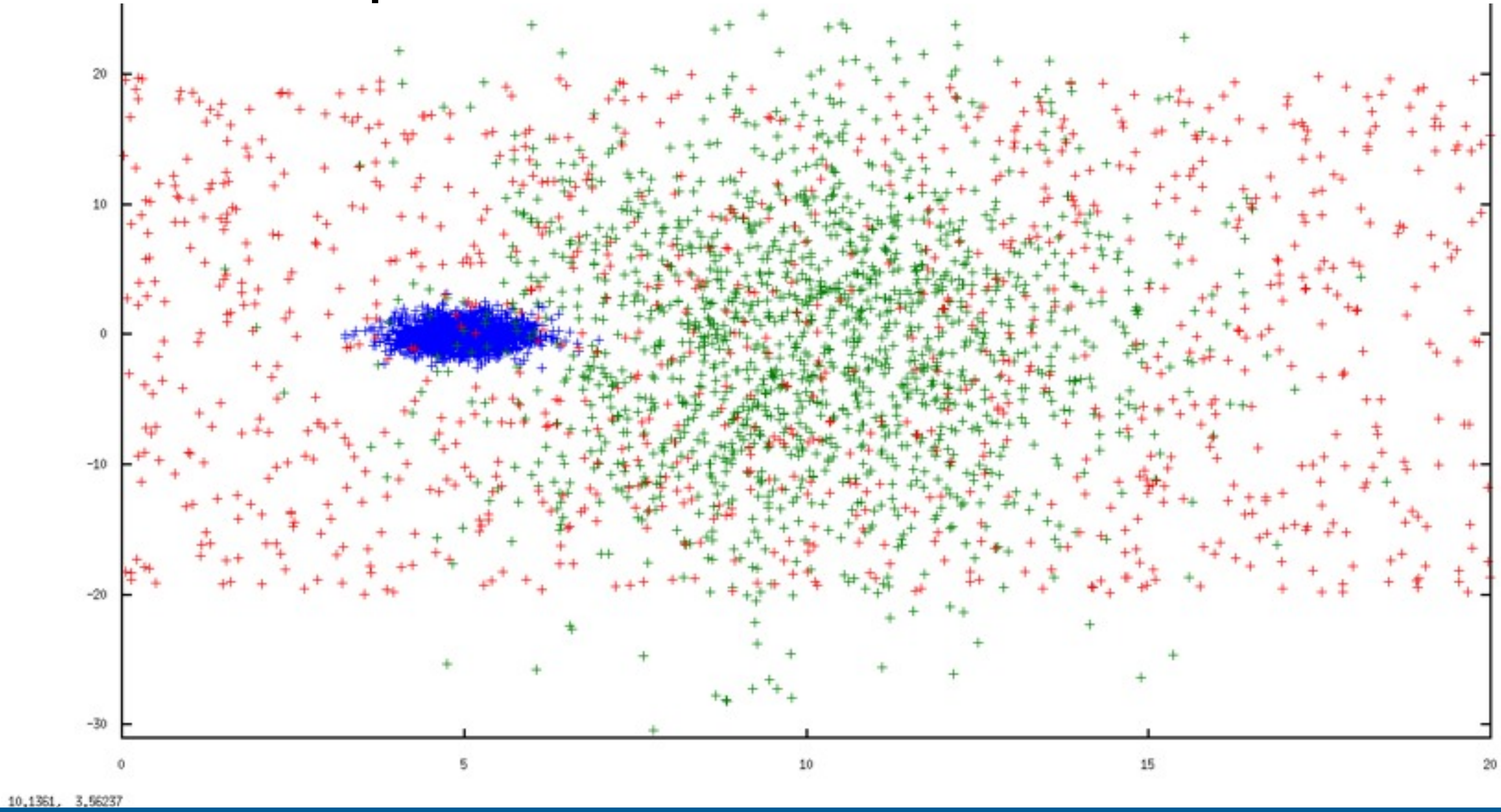
Example 1: Learn a Sensor Model

- A Radar range finder on a metallic target will returns 3 types of measurement:
  - The distance to target
  - The distance to the wall behind the target
  - A completely random value



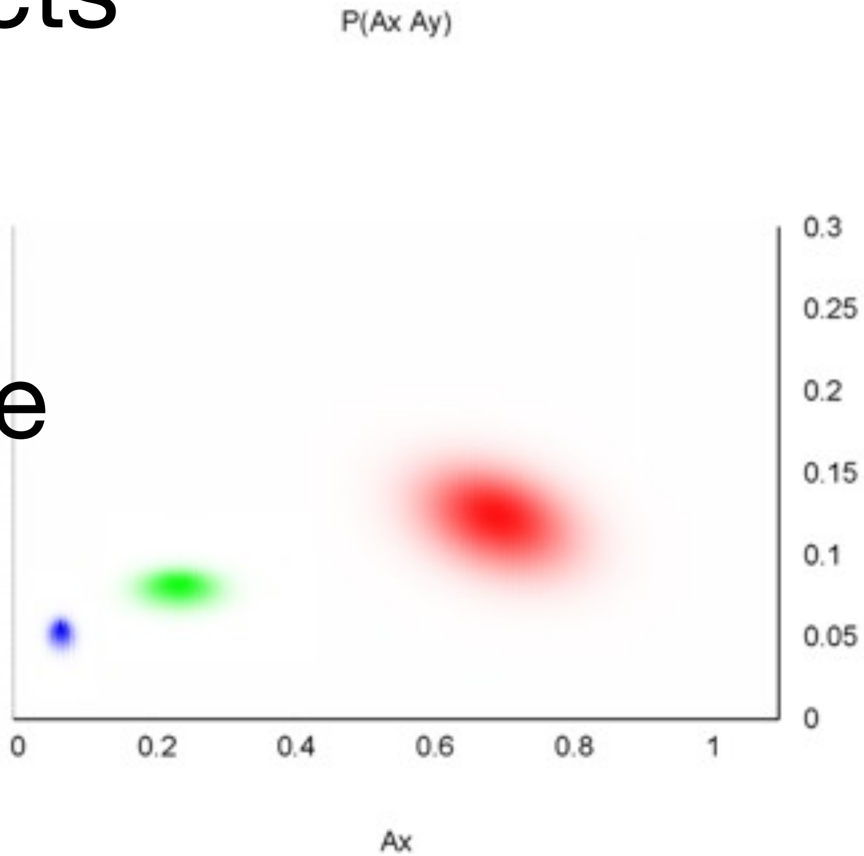
Example 1: Learn a Sensor Model

- Which point corresponds to from which model?
- What are the different model parameters?
- Solution: Expectation-Maximization



Example 2: Environment Classification

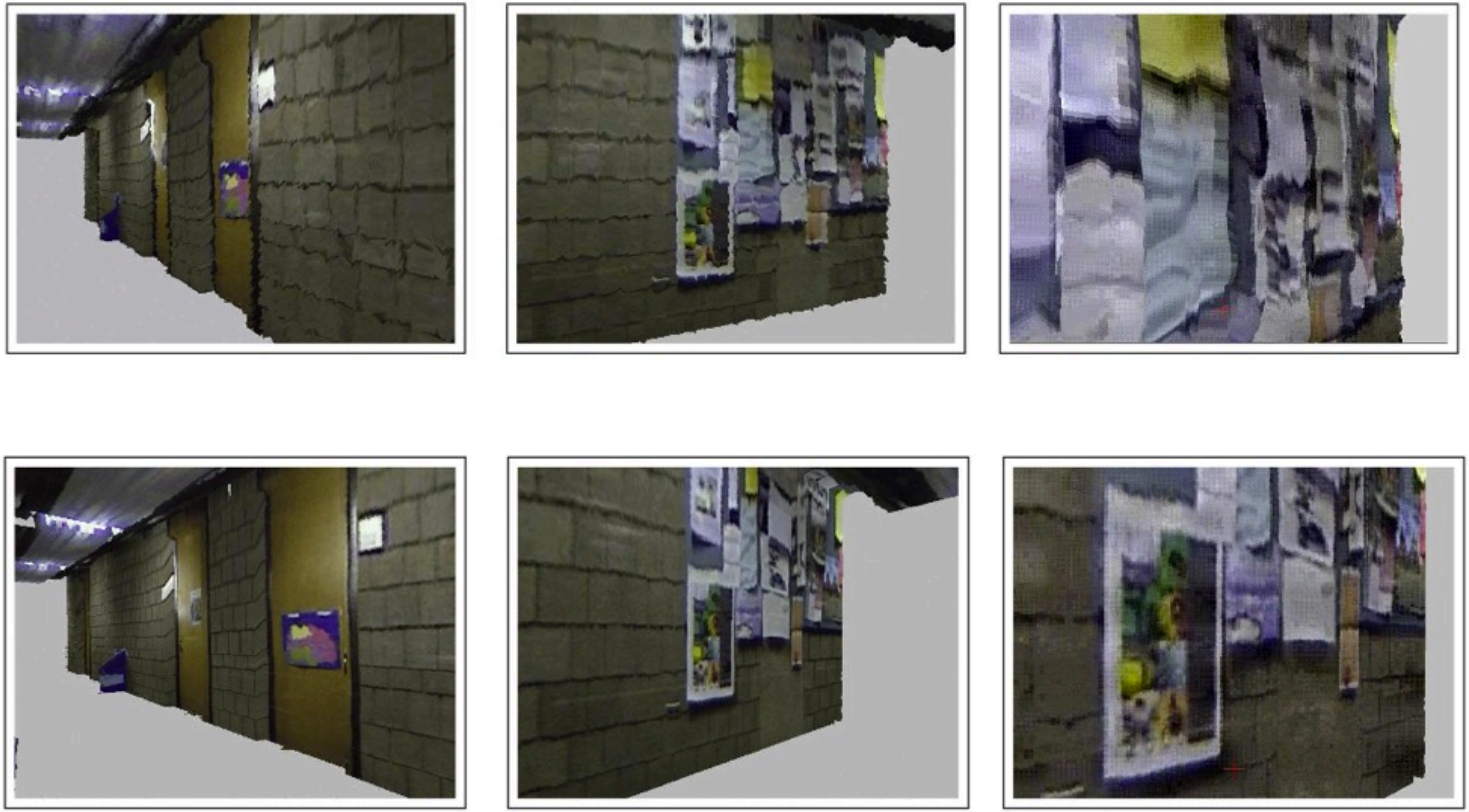
- From each image, the robot extracts features: => points in nD space
- K-means only finds the cluster centers, not their extent and shape
- The centers and covariances can be obtained with EM



Example 3: Plane Fitting in 3D

- Has been done in this paper
- Given a set of 3D points, fit planes into the data
- Idea: Model parameters θ are normal vectors and distance to origin for a set of planes
- Gaussian noise model: $$p(z \mid \theta) = \mathcal{N}(\underset{\substack{\uparrow \\ \text{point-to-plane} \\ \text{distance}}}{d}(\mathbf{z}, \theta) \mid 0, \underset{\substack{\uparrow \\ \text{noise} \\ \text{variance}}}{\sigma})$$
- Introduce latent correspondence variables C_{ij} and maximize the expected log-lik.: $$\mathbb{E}[\log p(Z, C \mid \theta)]$$
- Maximization can be done in closed form

Example 3: Plane Fitting in 3D



Summary

- K-means is an iterative method for clustering
- Mixture models can be formalized using latent (unobserved) variables
- A very common example are Gaussian mixture models (GMMs)
- To estimate the parameters of a GMM we can use expectation-maximization (EM)
- In general EM can be interpreted as maximizing a lower bound to the complete-data loglikelihood
- EM is guaranteed to converge, but it may run into local maxima