Clustering and mixture models

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Outline

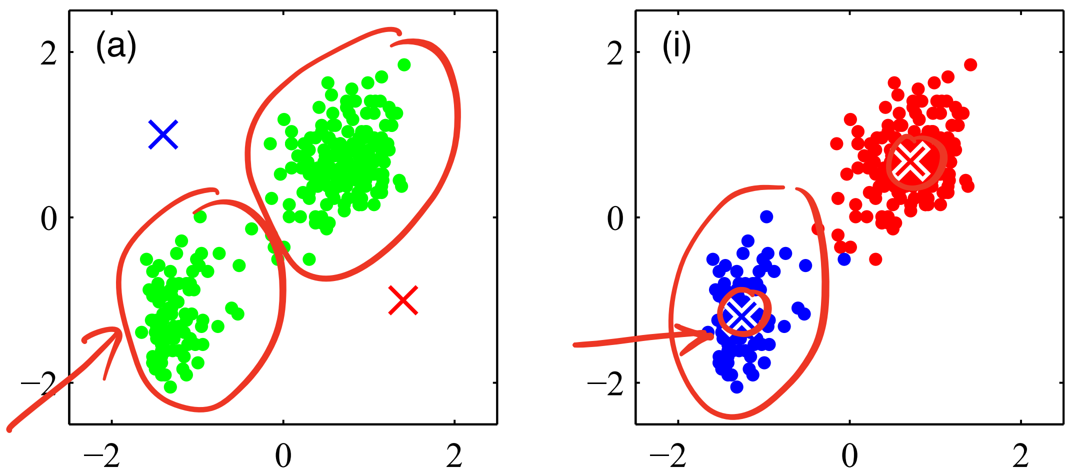
1. K-means
2. Gaussian mixture models
3. GMMs and Incomplete Data

Clustering

Setup Given $\mathcal{D} = \{\boldsymbol{x}_n\}_{n=1}^N$ and K, we want to output

- $\{\boldsymbol{\mu}_k\}_{k=1}^K$: prototypes (or centroids) of clusters
- $A(\boldsymbol{x}_n) \in \{1, 2, \ldots, K\}$: the cluster membership, i.e., the cluster ID assigned to $\boldsymbol{x}_n$

Toy Example Cluster data into two clusters.

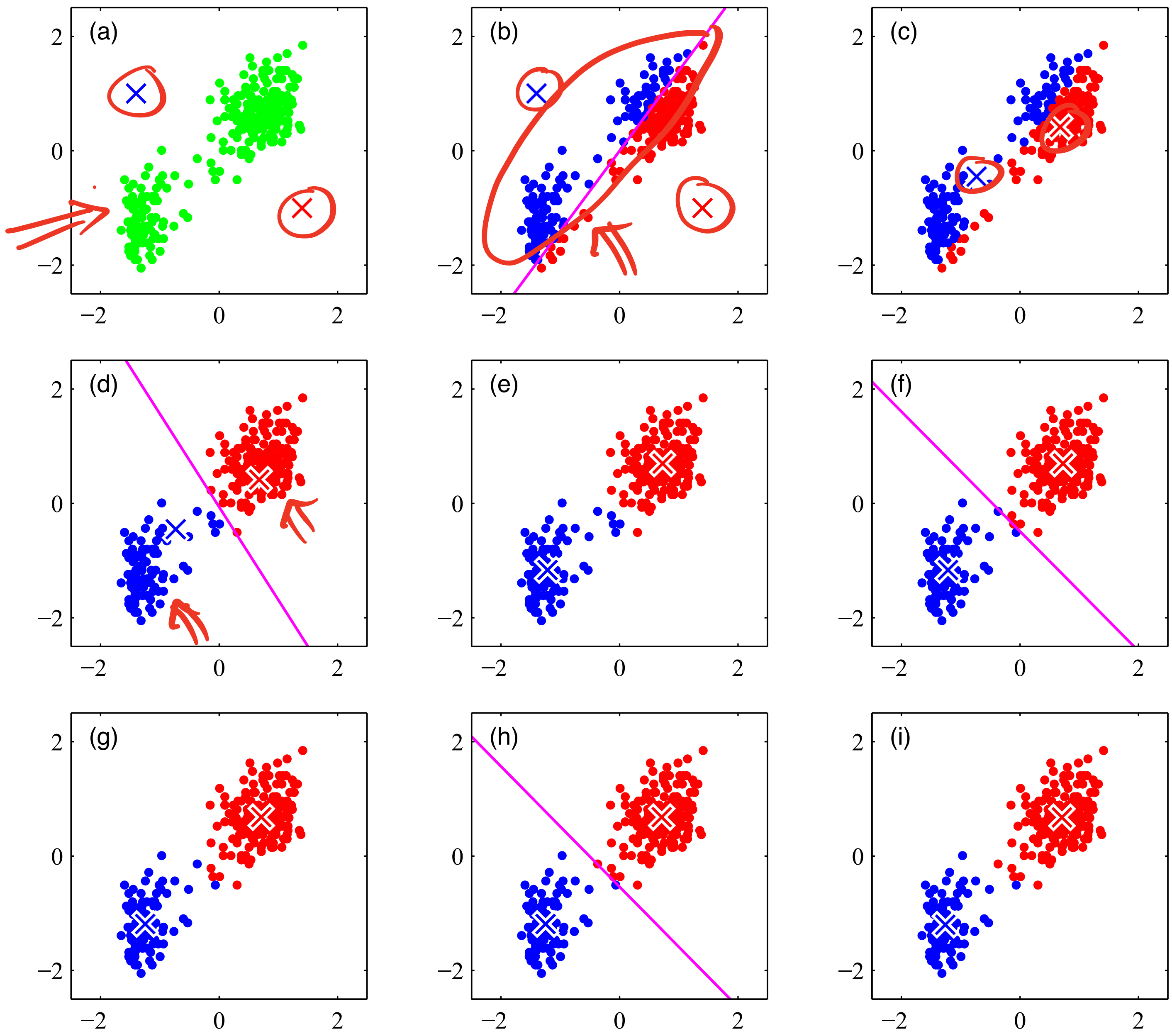


Applications

- Identify communities within social networks
- Find topics in news stories
- Group similiar sequences into gene families

K-means example

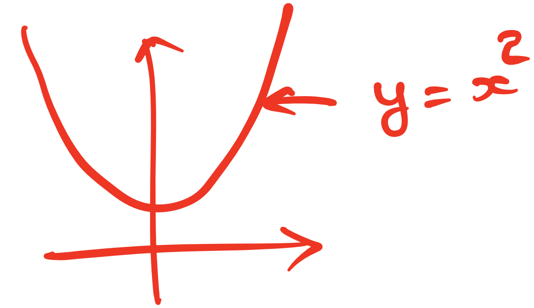
K=2



K-means clustering

Intuition Data points assigned to cluster k should be close to $\boldsymbol{\mu}_k$, the prototype.

K-means clustering



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Distortion measure (clustering objective function, cost function)

$$J(\{r_{nk}\}, \{\boldsymbol{\mu}_k\}) = \sum_{n=1}^{N}\sum_{k=1}^{K} r_{nk}\|\boldsymbol{x}_n - \boldsymbol{\mu}_k\|_2^2$$

where $r_{nk} \in \{0, 1\}$ is an indicator variable

$$r_{nk} = 1 \quad \text{if and only if} \quad A(\boldsymbol{x}_n) = k$$

r_{nk}

$$J(\{r_{nk}\}, \{\mu_k\}) = \sum_n \sum_k r_{nk} \|x_n - \mu_k\|_2^2$$

$$J(\{r_{nk}\}, \{\mu_k\})$$

K-means clustering

K-means objective

$$argmin_{\{r_{nk}\},\{\boldsymbol{\mu}_k\}} J(\{r_{nk}\},\{\boldsymbol{\mu}_k\}) = \sum_{n=1}^{N}\sum_{k=1}^{K} r_{nk}\|\boldsymbol{x}_n - \boldsymbol{\mu}_k\|_2^2$$

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- Is a non-convex objective function.
- Minimizing the K-means objective function is NP-hard.

Llyod's algorithm for minimizing the K-means objective

Often simply called the K-means algorithm

Minimize cost function alternative optimization between $\{r_{nk}\}$ and $\{\boldsymbol{\mu}_k\}$

- **Step 0** Initialize $\{\boldsymbol{\mu}_k\}$ to some values

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- **Step 0** Initialize $\{\boldsymbol{\mu}_k\}$ to some values
- **Step 1** Assume the current value of $\{\boldsymbol{\mu}_k\}$ fixed, minimize J over $\{r_{nk}\}$, which leads to the following cluster assignment rule

$$r_{nk} = \begin{cases} 1 & \text{if } k = \arg\min_j \|\boldsymbol{x}_n - \boldsymbol{\mu}_j\|_2^2 \\ 0 & \text{otherwise} \end{cases}$$

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Minimize cost function alternative optimization between $\{r_{nk}\}$ and $\{\boldsymbol{\mu}_k\}$

$J(\{r_{nk}\}, \{\mu_k\}) = \sum_n \sum_k r_{nk} \|x_n - \mu_k\|_2^2 \Rightarrow \nabla_{\mu_k} J = 0$

- **Step 0** Initialize $\{\boldsymbol{\mu}_k\}$ to some values
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$$r_{nk} = \begin{cases} 1 & \text{if } k = \arg\min_j \|\boldsymbol{x}_n - \boldsymbol{\mu}_j\|_2^2 \\ 0 & \text{otherwise} \end{cases}$$

- **Step 2** Assume the current value of $\{r_{nk}\}$ fixed, minimize J over $\{\boldsymbol{\mu}_k\}$, which leads to the following rule to update the prototypes of the clusters

$$\Rightarrow \boldsymbol{\mu}_k = \frac{\sum_n r_{nk} \boldsymbol{x}_n}{\sum_n r_{nk}}$$

$\sum_n r_{nk}$ = # pts assigned to k

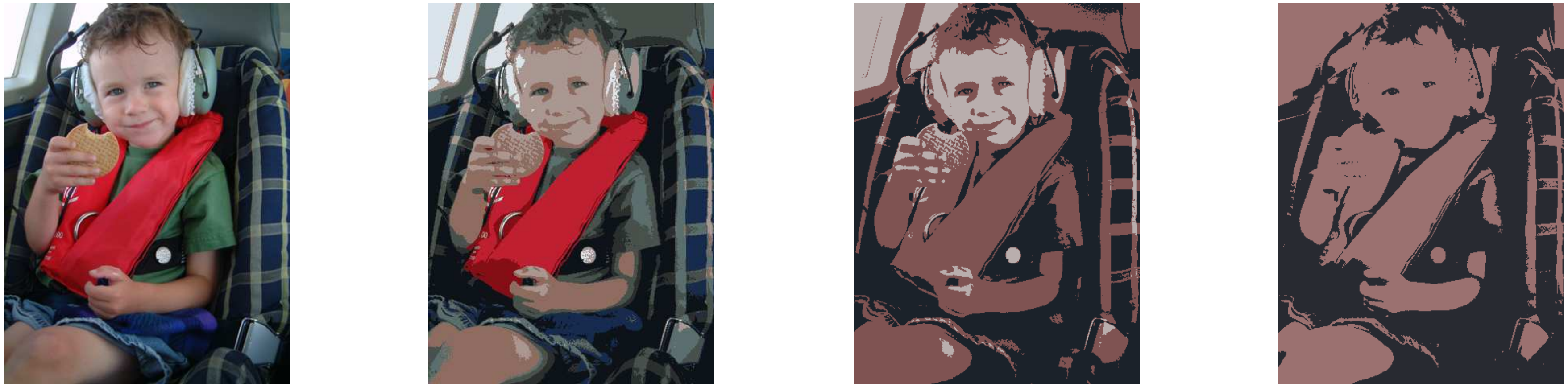
- **Step 3** Stop if the objective function J stays the same or return to Step 1

Remarks

- Prototype $\boldsymbol{\mu}_k$ is the mean of data points assigned to the cluster k, hence 'K-means'
- The procedure reduces J in both Step 1 and Step 2 and thus makes improvements on each iteration

Application: vector quantization

- Replace data point with associated prototype $\boldsymbol{\mu}_k$
- In other words, compress the data points into i) a codebook of all the prototypes; ii) a list of indices to the codebook for the data points
- Lossy compression, especially for small K



large K

small K

Clustering pixels and vector quantizing them. From left to right: Original image, quantized with large K, medium K, and a small K. Details are missing due to the higher compression (smaller K).

Properties of the K-means algorithm

$$J(\{r_{nk}\}, \{\mu_k\}) = \sum_n \sum_k r_{nk} \|x_n - \mu_k\|_2^2 \geq 0$$

$r_{nk} \in \{0,1\} \quad \geq 0$

- Does the K-means algorithm converge (*i.e.*, terminate)?
  - Yes.
- How long does it take to converge ?
  - In the worst case, exponential in the number of data points.
  - In practice, very quick.

Properties of the K-means algorithm

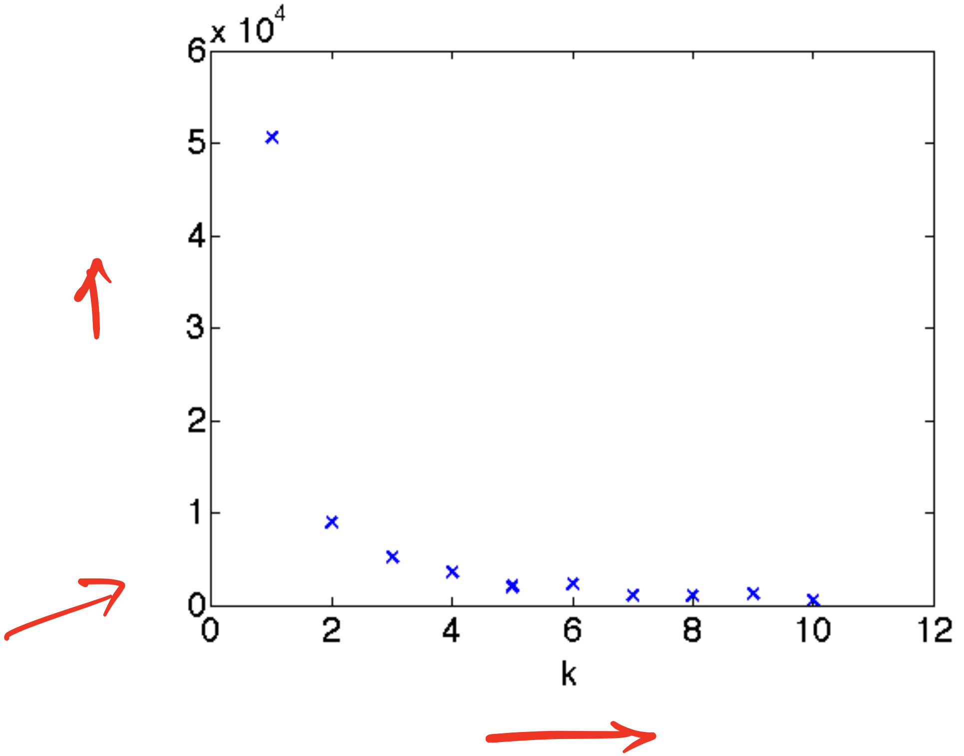
How good is the K-means solution?

- Converges to a local minimum.
- The solution depends on the initialization.
- In practice, run many times with different initializations and pick the best.
- K-means++ is a neat approximation algorithm that has theoretical guarantees on the final value of the objective.
  - Still no guarantee that you will reach the global minimum
  - You are guaranteed to get reasonably close (approximation guarantee on the final value).

Other practical issues

Choosing K

- Increasing K will always decrease the optimal value of the K-means objective.
  - Analogous to overfitting in supervised learning.
- Information criteria that effectively regularize more complex models.



K-medoids

- K-means is sensitive to outliers.
- In some applications we want the prototypes to be one of the points.
- Leads to K-medoids.

K-medoids

k-means

- **Step 0** Initialize $\{\boldsymbol{\mu}_k\}$ by randomly selecting K of the N points
- **Step 1** Assume the current value of $\{\boldsymbol{\mu}_k\}$ fixed, assign points to clusters:

$$r_{nk} = \begin{cases} 1 & \text{if } k = \arg\min_j \|\boldsymbol{x}_n - \boldsymbol{\mu}_j\|_2^2 \\ 0 & \text{otherwise} \end{cases}$$

- **Step 2** Assume the current value of $\{r_{nk}\}$ fixed, update the prototype of cluster k. In K-medoids, the prototype for a cluster is the data point that is closest to all other data points in the cluster

$$k* = \arg\min_{m:r_{mk}=1} \sum_n r_{nk} \|\boldsymbol{x}_n - \boldsymbol{x}_m\|_2^2$$

$$\boldsymbol{\mu}_k = \boldsymbol{x}_{k*}$$

- **Step 3** Stop if the objective function J stays the same or return to Step 1

Outline

RSS

Linear regression

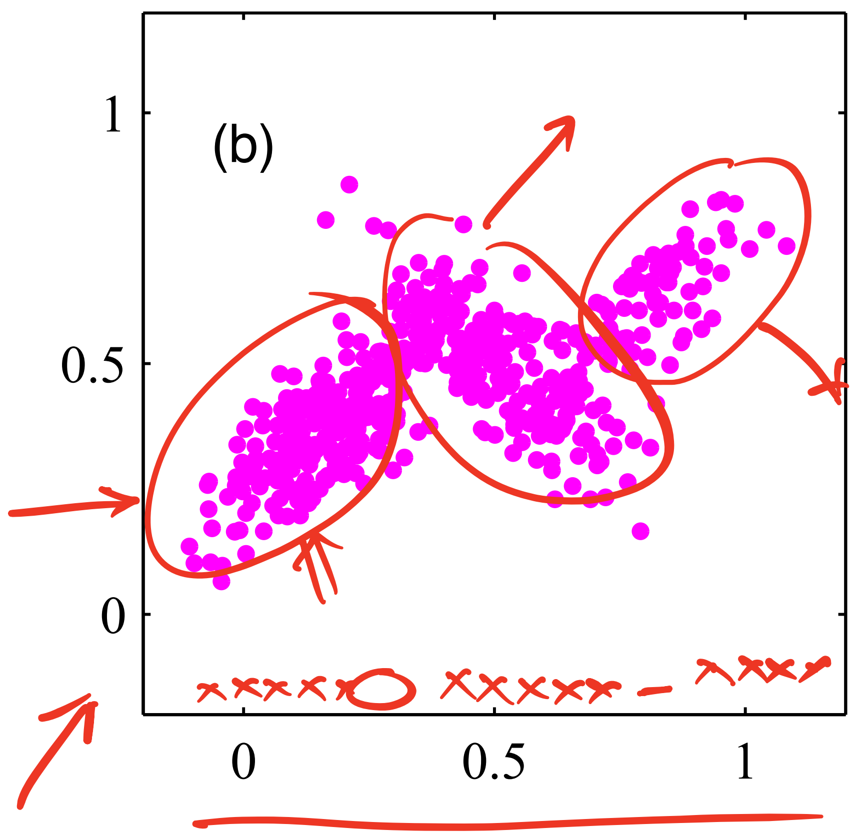
Probabilistic interpretation

1. K-means
2. Gaussian mixture models
3. GMMs and Incomplete Data

Probabilistic interpretation of clustering?

We can impose a probabilistic interpretation of our intuition that points stay close to their cluster centers

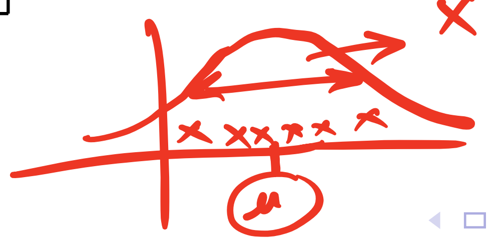
- How can we model $p(\boldsymbol{x})$ to reflect this?



- Data points seem to form 3 clusters

$p(x) \sim \mathcal{N}(\mu, \Sigma)$

$x \sim \mathcal{N}(\mu, \sigma^2)$



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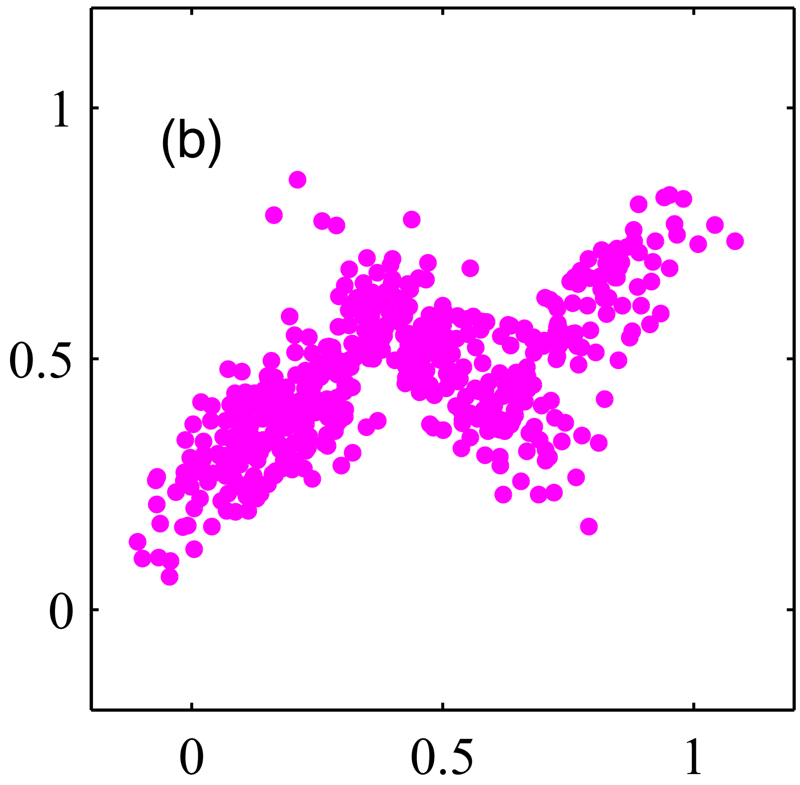
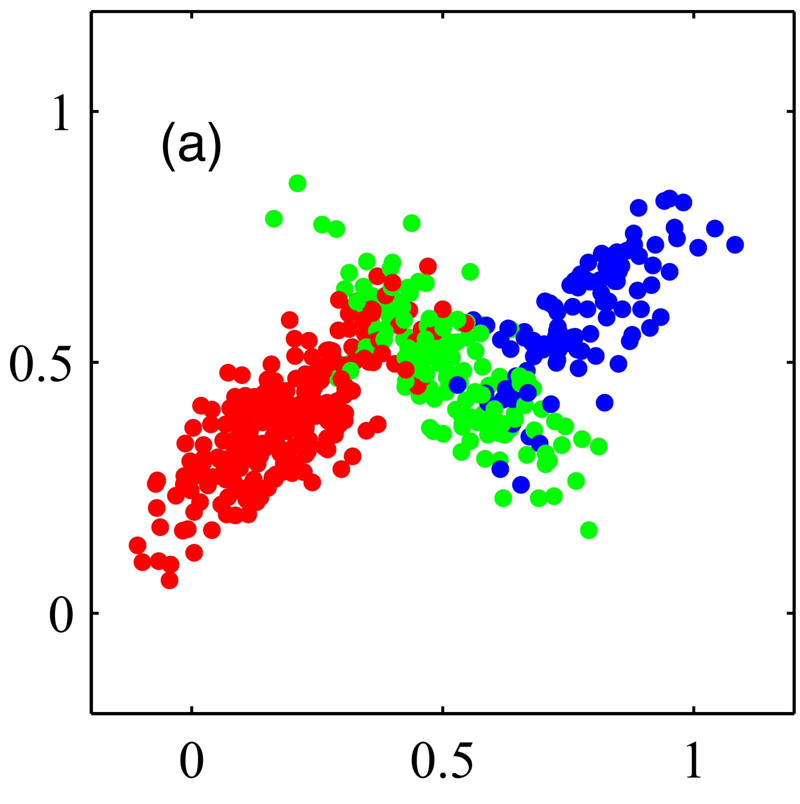


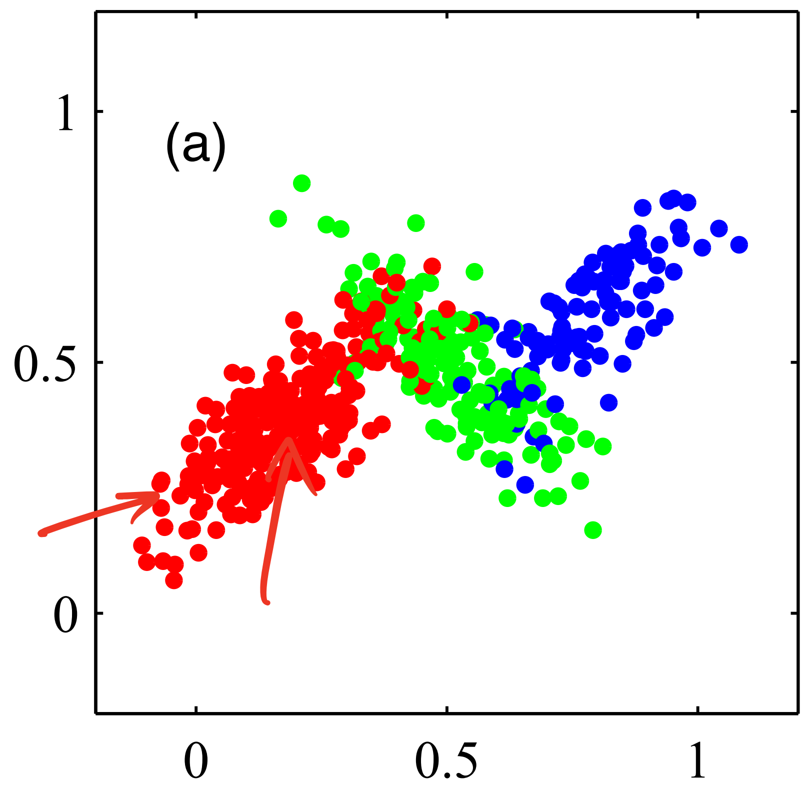
- Data points seem to form 3 clusters
- We cannot model $p(\boldsymbol{x})$ with simple and known distributions
- The data is not a Guassian as we have 3 distinct concentrated regions

Gaussian mixture models: intuition



- We can model *each* region with a distinct distribution
- Common to use Gaussians, i.e., Gaussian mixture models (GMMs) or mixture of Gaussians (MoGs).

Gaussian mixture models: intuition



- We can model *each* region with a distinct distribution
- Common to use Gaussians, i.e., Gaussian mixture models (GMMs) or mixture of Gaussians (MoGs).
- We don't know *cluster assignments* (label) or *parameters* of Gaussians or *mixture components*!
- We need to learn them all from our *unlabeled* data $\mathcal{D} = \{\boldsymbol{x}_n\}_{n=1}^N$

Gaussian mixture models: formal definition

A Gaussian mixture model has the following density function for $\boldsymbol{x}$

$x \in \mathbb{R}^D$

$$p(\boldsymbol{x}) = \sum_{k=1}^{K} \omega_k N(\boldsymbol{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

- K: the number of Gaussians — they are called (mixture) components
- $\boldsymbol{\mu}_k$ and $\boldsymbol{\Sigma}_k$: mean and covariance matrix of the k-th component

$x \in \mathbb{R}^2$ $\quad \mu \in \mathbb{R}^2$ $\quad \Sigma \in \mathbb{R}^{2\times 2}$

$\Sigma = \begin{pmatrix} 3 & 0.1 \\ 0.1 & 1 \end{pmatrix}$

$\Sigma = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ $\quad \mu = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$

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- ω_k: mixture weights – they represent how much each component contributes to the final distribution. It satisfies two properties:

$\omega_k > 0$ $\qquad$ $\sum_k \omega_k = 1$

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$$\forall\, k,\ \omega_k > 0, \quad \text{and} \quad \sum_k \omega_k = 1$$

The properties ensure $p(\boldsymbol{x})$ is a properly normalized probability density function.

GMM as the marginal distribution of a joint distribution

Consider the following joint distribution

$$p(\boldsymbol{x}, z) = p(z)p(\boldsymbol{x}|z)$$

where z is a discrete random variable taking values between 1 and K.

$$p(x,z) = p(z)\,p(x|z)$$

Condition probability

GMM as the marginal distribution of a joint distribution

Consider the following joint distribution

$$p(\boldsymbol{x}, z) = p(z)p(\boldsymbol{x}|z)$$

where z is a discrete random variable taking values between 1 and K. Denote

$$\omega_k = p(z = k)$$

Now, assume the conditional distributions are Gaussian distributions

$$p(\boldsymbol{x}|z = k) = N(\boldsymbol{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

$$p(x) = p(x, z=1) + p(x, z=2) + \dots + p(x, z=K)$$

$$= \sum_k p(x, z=k) = \sum_k p(z=k)\, p(x|z=k)$$

GMM as the marginal distribution of a joint distribution

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Now, assume the conditional distributions are Gaussian distributions

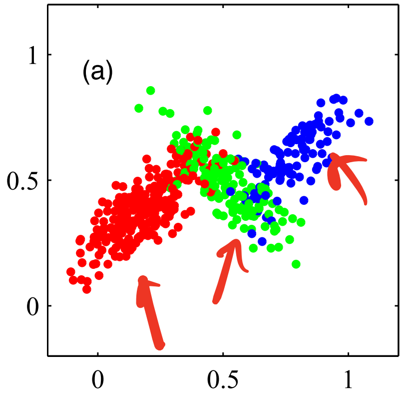
$$p(\boldsymbol{x}|z = k) = N(\boldsymbol{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

Then, the marginal distribution of $\boldsymbol{x}$ is

$$p(\boldsymbol{x}) = \sum_{k=1}^{K} \omega_k N(\boldsymbol{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

Namely, the Gaussian mixture model

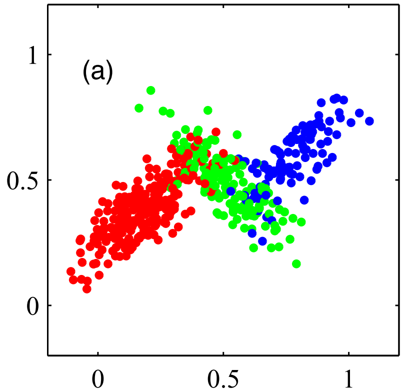
GMMs: example



The conditional distribution between $\boldsymbol{x}$ and z (representing color) are

$$
\begin{aligned}
p(\boldsymbol{x}|z = red) &= N(\boldsymbol{x}|\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1) \\
p(\boldsymbol{x}|z = blue) &= N(\boldsymbol{x}|\boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2) \\
p(\boldsymbol{x}|z = green) &= N(\boldsymbol{x}|\boldsymbol{\mu}_3, \boldsymbol{\Sigma}_3)
\end{aligned}
$$

GMMs: example



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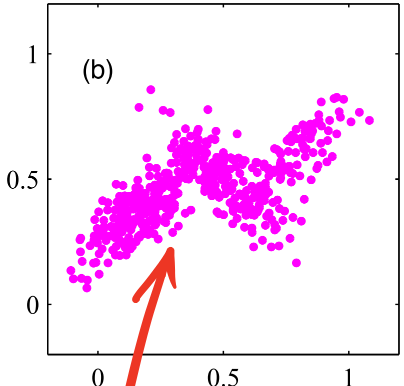

The marginal distribution is thus

$$p(\boldsymbol{x}) = p(red)N(\boldsymbol{x}|\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1) + p(blue)N(\boldsymbol{x}|\boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2) + p(green)N(\boldsymbol{x}|\boldsymbol{\mu}_3, \boldsymbol{\Sigma}_3)$$

Parameter estimation for Gaussian mixture models

The parameters in GMMs are $\boldsymbol{\theta} = \{\omega_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_{k=1}^{K}$. To estimate, consider the simple (and unrealistic) case first.

We have labels z If we assume z is observed for every $\boldsymbol{x}$, then our estimation problem is easier to solve. Our training data is augmented:

$$\mathcal{D}' = \{\boldsymbol{x}_n, z_n\}_{n=1}^{N}$$

z_n denotes the component where $\boldsymbol{x}_n$ comes from. $\mathcal{D}'$ is the *complete* data and $\mathcal{D}$ the *incomplete* data. How can we learn our parameters?

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Given $\mathcal{D}'$, the maximum likelihood estimation of the $\boldsymbol{\theta}$ is given by

$$\boldsymbol{\theta} = \arg\max \log P(\mathcal{D}') = \sum_n \log p(\boldsymbol{x}_n, z_n)$$

Parameter estimation for GMMs: complete data

The *complete* likelihood is decomposable

$$\sum_n \log p(\boldsymbol{x}_n, z_n) = \sum_n \log p(z_n)p(\boldsymbol{x}_n|z_n) = \sum_k \sum_{n:z_n=k} \log p(z_n)p(\boldsymbol{x}_n|z_n)$$

where we have grouped data by its values z_n. Let us introduce a binary variable $\gamma_{nk} \in \{0,1\}$ to indicate whether $z_n = k$. We then have

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$$\sum_n \log p(\boldsymbol{x}_n, z_n) = \sum_k \sum_n \gamma_{nk} \log p(z = k)p(\boldsymbol{x}_n|z = k)$$

We use a "dummy" variable z to denote all the possible values cluster assignment values for $\boldsymbol{x}_n$

$$\sum_k \sum_n \gamma_{nk} \log p(z=k)\, p(x_n | z=k)$$

$\mathcal{D}'$ specifies this value in the complete data setting

$$\log(\omega_k \, \mathcal{N}(x_n; \mu_k, \Sigma_k))$$

$$= (\log(\omega_k) + \log \mathcal{N}(x_n; \mu_k, \Sigma_k))$$

Parameter estimation for GMMs: complete data

We now have

$$\sum_n \log p(\boldsymbol{x}_n, z_n) = \sum_k \sum_n \gamma_{nk} [\log \omega_k + \log N(\boldsymbol{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)]$$

Regrouping, we have

$$\sum_n \log p(\boldsymbol{x}_n, z_n) = \sum_k \sum_n \gamma_{nk} \log \omega_k + \sum_k \left\{ \sum_n \gamma_{nk} \log N(\boldsymbol{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \right\}$$

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The term inside the braces depends on k-th component's parameters. It can be shown that the MLE is:

$\gamma_{nk} \in \{0,1\}$

$$\omega_k = \frac{\sum_n \gamma_{nk}}{\sum_k \sum_n \gamma_{nk}}, \quad \boldsymbol{\mu}_k = \frac{1}{\sum_n \gamma_{nk}} \sum_n \gamma_{nk} \boldsymbol{x}_n$$

$N =$

$$\boldsymbol{\Sigma}_k = \frac{1}{\sum_n \gamma_{nk}} \sum_n \gamma_{nk} (\boldsymbol{x}_n - \boldsymbol{\mu}_k)(\boldsymbol{x}_n - \boldsymbol{\mu}_k)^{\mathrm{T}}$$

What's the intuition?

Intuition

Since γ_{nk} is binary, the previous solution is nothing but

- For ω_k: count the number of data points whose z_n is k and divide by the total number of data points (note that $\sum_k \sum_n \gamma_{nk} = N$)
- For $\boldsymbol{\mu}_k$: get all the data points whose z_n is k, compute their mean
- For $\boldsymbol{\Sigma}_k$: get all the data points whose z_n is k, compute their covariance matrix

This intuition is going to help us to develop an algorithm for estimating $\boldsymbol{\theta}$ when we do not know z_n (incomplete data).

Parameter estimation for GMMs: incomplete data

$P(z_n = k \mid x_n)$

When z_n is not given, we can guess it via the posterior probability

$$p(z_n = k|\boldsymbol{x}_n) = \frac{p(\boldsymbol{x}_n|z_n = k)p(z_n = k)}{p(\boldsymbol{x}_n)} = \frac{p(\boldsymbol{x}_n|z_n = k)p(z_n = k)}{\sum_{k'=1}^{K} p(\boldsymbol{x}_n|z_n = k')p(z_n = k')}$$

$$P(Y|X) = \frac{P(X|Y)\,P(Y)}{P(X)}$$

(Bayes theorem)

Random variable   Random variable

$$P(z_n = k \mid x_n) = \frac{P(x_n \mid z_n = k)\, P(z_n = k)}{P(x_n)}$$

$$= \mathcal{N}(x_n; \mu_k, \Sigma_k)$$

ω_k

Parameter estimation for GMMs: incomplete data

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To compute the posterior probability, we need to know the parameters $\boldsymbol{\theta}$!

Let's pretend we know the value of the parameters so we can compute the posterior probability.

How is that going to help us?

Estimation with soft γ_{nk}

We define $\gamma_{nk} = p(z_n = k|\boldsymbol{x}_n)$

Estimation with soft γ_{nk}

We define $\gamma_{nk} = p(z_n = k|\boldsymbol{x}_n)$

- Recall that γ_{nk} was binary.
- Now it's a "soft" assignment of $\boldsymbol{x}_n$ to k-th component
- Each $\boldsymbol{x}_n$ is assigned to a component fractionally according to $p(z_n = k|\boldsymbol{x}_n)$

Parameter estimation for GMMs: incomplete data

With the soft assignment γ_{nk} plugged into the complete data log likelihood, we now have:

$$\sum_k \sum_n \gamma_{nk} [\log \omega_k + \log N(\boldsymbol{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)]$$

Regrouping, we have

$$\sum_k \sum_n \gamma_{nk} \log \omega_k + \sum_k \left\{ \sum_n \gamma_{nk} \log N(\boldsymbol{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \right\}$$

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Regrouping, we have

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We now get the same expression for the MLE as before!

$$\omega_k = \frac{\sum_n \gamma_{nk}}{\sum_k \sum_n \gamma_{nk}}, \quad \boldsymbol{\mu}_k = \frac{1}{\sum_n \gamma_{nk}} \sum_n \gamma_{nk} \boldsymbol{x}_n$$

$$\boldsymbol{\Sigma}_k = \frac{1}{\sum_n \gamma_{nk}} \sum_n \gamma_{nk} (\boldsymbol{x}_n - \boldsymbol{\mu}_k)(\boldsymbol{x}_n - \boldsymbol{\mu}_k)^{\mathrm{T}}$$

But remember, we're 'cheating' by using $\boldsymbol{\theta}$ to compute γ_{nk}!

Iterative procedure

$\theta = (\omega_k, \mu_k, \Sigma_k)_{k=1}^{K}$

We can alternate between estimating γ_{nk} and using the estimated γ_{nk} to compute the parameters (same idea as with K-means!)

- Step 0: initialize $\boldsymbol{\theta}$ with some values (random or otherwise)
- Step 1: compute γ_{nk} using the current $\boldsymbol{\theta}$
- Step 2: update $\boldsymbol{\theta}$ using the just computed γ_{nk}
- Step 3: go back to Step 1

Questions:

- Is this procedure reasonable, i.e., are we optimizing a sensible criteria?
- Will this procedure converge?

The answers lie in the *EM algorithm* — a powerful procedure for model estimation with unknown data.

Outline

1 K-means

2 Gaussian mixture models

3 GMMs and Incomplete Data

Parameter estimation for GMMs: complete data

GMM Parameters

$$\boldsymbol{\theta} = \{\omega_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_{k=1}^{K}$$

Complete Data: We (unrealistically) assume z is observed for every $\boldsymbol{x}$,

$$\mathcal{D}' = \{\boldsymbol{x}_n, z_n\}_{n=1}^{N}$$

MLE: Maximize the complete likelihood

$$\boldsymbol{\theta} = \arg\max \log P(\mathcal{D}') = \sum_n \log p(\boldsymbol{x}_n, z_n)$$

Leads to closed-form solution!

Parameter estimation for GMMs: Incomplete data

GMM Parameters

$$\boldsymbol{\theta} = \{\omega_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_{k=1}^K$$

Incomplete Data

Our data contains observed and unobserved random variables, and hence is incomplete

- Observed: $\mathcal{D} = \{\boldsymbol{x}_n\}$
- Unobserved (hidden): $\{\boldsymbol{z}_n\}$

Goal Obtain the maximum likelihood estimate of $\boldsymbol{\theta}$:

$$\widehat{\boldsymbol{\theta}} = \arg\max \ell(\boldsymbol{\theta}) = \arg\max \log P(\mathcal{D}) = \arg\max \sum_n \log p(\boldsymbol{x}_n|\boldsymbol{\theta})$$

$$= \arg\max \sum_n \log \sum_{\boldsymbol{z}_n} p(\boldsymbol{x}_n, \boldsymbol{z}_n|\boldsymbol{\theta})$$

The objective function $\ell(\boldsymbol{\theta})$ is called the *incomplete* log-likelihood.

Issue with Incomplete log-likelihood

No simple way to optimize the incomplete log-likelihood

Expectation-Maximization (EM) algorithm provides a strategy for iteratively optimizing this function

Two steps as they apply to GMM:

- E-step: 'guess' values of the z_n using existing values of $\boldsymbol{\theta}$
- M-step: solve for new values of $\boldsymbol{\theta}$ given imputed values for z_n (maximize complete likelihood!)

E-step: Soft cluster assignments

We define γ_{nk} as $p(z_n = k|\boldsymbol{x}_n, \boldsymbol{\theta})$

- This is the posterior distribution of z_n given $\boldsymbol{x}_n$ and $\boldsymbol{\theta}$
- Recall that in complete data setting γ_{nk} was binary
- Now it's a "soft" assignment of $\boldsymbol{x}_n$ to k-th component, with $\boldsymbol{x}_n$ assigned to each component with some probability

E-step: Soft cluster assignments

$0 \leq \gamma_{nk} \leq 1$

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Given $\boldsymbol{\theta} = \{\omega_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_{k=1}^K$, we can compute γ_{nk} using Bayes theorem:

$$\begin{aligned}
\gamma_{nk} &= p(z_n = k|\boldsymbol{x}_n) \\
&= \frac{p(\boldsymbol{x}_n|z_n = k)p(z_n = k)}{p(\boldsymbol{x}_n)} \\
&= \frac{p(\boldsymbol{x}_n|z_n = k)p(z_n = k)}{\sum_{k'=1}^K p(\boldsymbol{x}_n|z_n = k')p(z_n = k')} \quad = \frac{\mathcal{N}(\boldsymbol{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)\omega_k}{\sum_{k'=1}^K \mathcal{N}(\boldsymbol{x}_n|\boldsymbol{\mu}_{k'}, \boldsymbol{\Sigma}_{k'})\omega_{k'}}
\end{aligned}$$

M-step: Maximimize complete likelihood

Recall definition of complete likelihood from earlier:

$$\sum_n \log p(\boldsymbol{x}_n, z_n) = \sum_k \sum_n \gamma_{nk} \log \omega_k + \sum_k \left\{ \sum_n \gamma_{nk} \log \mathcal{N}(\boldsymbol{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \right\}$$

Previously γ_{nk} was binary, but now we define $\gamma_{nk} = p(z_n = k | \boldsymbol{x}_n)$ (E-step)

M-step: Maximimize complete likelihood

Recall definition of complete likelihood from earlier:

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Previously γ_{nk} was binary, but now we define $\gamma_{nk} = p(z_n = k | \boldsymbol{x}_n)$ (E-step)

We get the same simple expression for the MLE as before!

$$\left\{ \begin{array}{l} \omega_k = \frac{\sum_n \gamma_{nk}}{\sum_k \sum_n \gamma_{nk}}, \quad \boldsymbol{\mu}_k = \frac{1}{\sum_n \gamma_{nk}} \sum_n \gamma_{nk} \boldsymbol{x}_n \\ \boldsymbol{\Sigma}_k = \frac{1}{\sum_n \gamma_{nk}} \sum_n \gamma_{nk} (\boldsymbol{x}_n - \boldsymbol{\mu}_k)(\boldsymbol{x}_n - \boldsymbol{\mu}_k)^{\mathrm{T}} \end{array} \right.$$

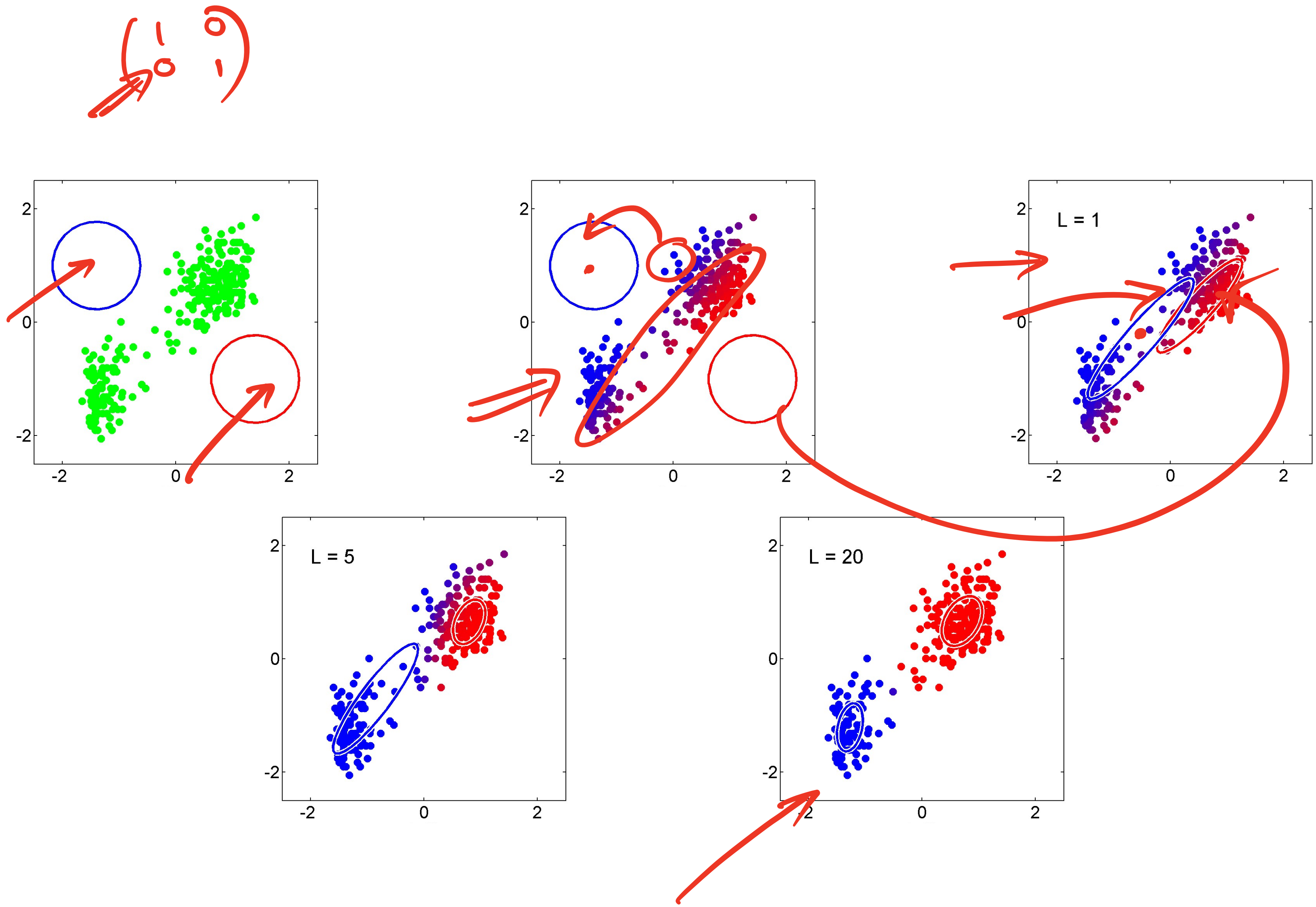
Intuition: Each point now contributes some fractional component to each of the parameters, with weights determined by γ_{nk}

EM procedure for GMM

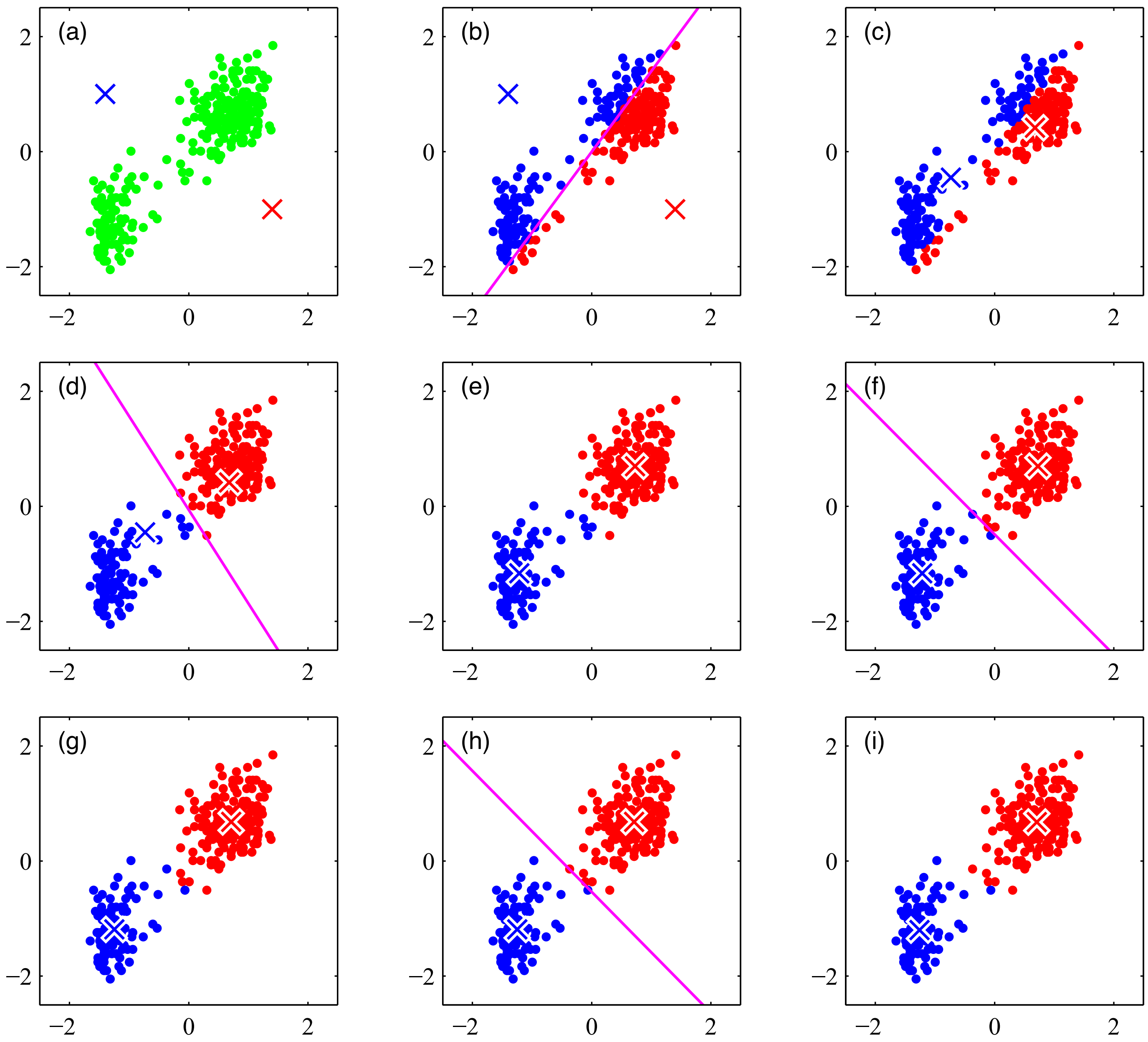
Alternate between estimating γ_{nk} and estimating $\boldsymbol{\theta}$

- Initialize $\boldsymbol{\theta}$ with some values (random or otherwise)
- Repeat
  - E-Step: Compute γ_{nk} using the current $\boldsymbol{\theta}$
  - M-Step: Update $\boldsymbol{\theta}$ using the γ_{nk} we just computed
- Until Convergence

Example of GMM



Compare to K-means example



EM procedure for GMM

Questions to be answered next

- How does GMM relate to K-means?
- Is this procedure reasonable, i.e., are we optimizing a sensible criterion?
- Will this procedure converge?

GMMs and K-means

GMMs provide probabilistic interpretation for K-means

GMMs reduce to K-means under the following assumptions (in which case EM for GMM parameter estimation simplifies to K-means):

- Assume all mixture weights ω_k are equal
- Assume all Gaussians have $\sigma^2 \boldsymbol{I}$ covariance matrices
- Further assume $\sigma \rightarrow 0$, so we only need to estimate $\boldsymbol{\mu}_k$, i.e., means
- GMMs are more general model.

$$\begin{pmatrix} \sigma^2 & & & 0 \\ & \sigma^2 & & \\ & & \sigma^2 & \\ 0 & & & \ddots \end{pmatrix}$$

K-means is often called "hard" GMM or GMMs is called "soft" K-means

The posterior γ_{nk} provides a probabilistic assignment for $\boldsymbol{x}_n$ to cluster k

EM algorithm

- The estimates of the parameter $\boldsymbol{\theta}$ in each iteration increase the likelihood.
- EM algorithm converges but only to a local optimum.

Summary

Clustering

- Group similar instances
- K-means
  - Minimize a cost function that measures the sum of squared distances from the cluster prototypes.
  - Iterative algorithm for minimizing the cost function.
- Variants: K-medoids
- Probabilistic interpretation of K-means: Gaussian Mixture Model
- Can define a number of mixture models for other kinds of data.
- Probabilistic interpretation: GMMs
  - Generalization of K-means
  - Estimation using an iterative EM algorithm.