# CSCI567 Machine Learning (Fall 2021)

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U of Southern California

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# Administration

HW3: discuss solutions today

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HW4: to be released, due on Tue, 11/09

# Outline

1. Review of last lecture
2. Clustering
3. Gaussian mixture models

# Outline

# General training algorithm for decision trees

**DecisionTreeLearning**(Examples, Features)

- if Examples have the same class, return a leaf with this class
- else if Features is empty, return a leaf with the majority class
- else if Examples is empty, return a leaf with majority class of parent
- else

  find the best feature $A$ to split (e.g. based on conditional entropy)

  **Tree** $\leftarrow$ a root with test on $A$

  For each value $a$ of $A$:

    **Child** $\leftarrow$ **DecisionTreeLearning**(Examples with $A = a$, Features$\setminus\{A\}$)
    add **Child** to **Tree** as a new branch

- return **Tree**

# The AdaBoost Algorithm

Given a training set $S$ and a base algorithm $\mathcal{A}$, initialize $D_1$ to be uniform

For $t = 1, \ldots, T$

- obtain a weak classifier $h_t \leftarrow \mathcal{A}(S, D_t)$
- calculate the importance of $h_t$ as

$$\beta_t = \frac{1}{2} \ln \left( \frac{1 - \epsilon_t}{\epsilon_t} \right) \qquad (\beta_t > 0 \Leftrightarrow \epsilon_t < 0.5)$$

  where $\epsilon_t = \sum_{n: h_t(\boldsymbol{x}_n) \neq y_n} D_t(n)$ is the weighted error of $h_t$.

- update distributions

$$D_{t+1}(n) \propto D_t(n) e^{-\beta_t y_n h_t(\boldsymbol{x}_n)} = \begin{cases} D_t(n) e^{-\beta_t} & \text{if } h_t(x_n) = y_n \\ D_t(n) e^{\beta_t} & \text{else} \end{cases}$$

Output the final classifier $H(\boldsymbol{x}) = \text{sgn}\left( \sum_{t=1}^{T} \beta_t h_t(\boldsymbol{x}) \right)$

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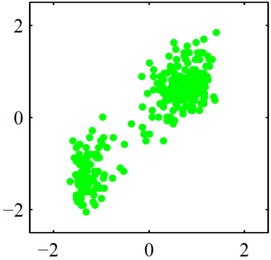
Today's focus: **clustering**, an important unsupervised learning problem

# Clustering: informal definition

**Given**: a set of data points (feature vectors), *without labels*



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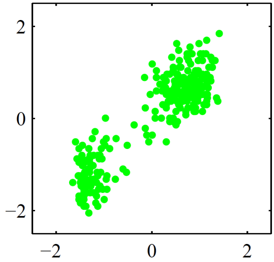

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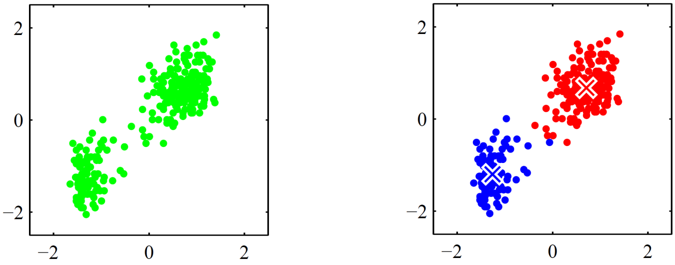
- assign each point to a specific cluster
- find the center (representative/prototype/...) of each cluster



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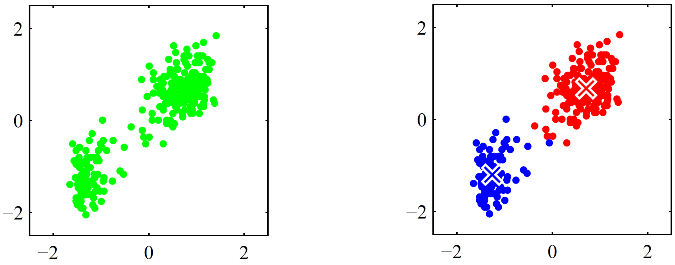

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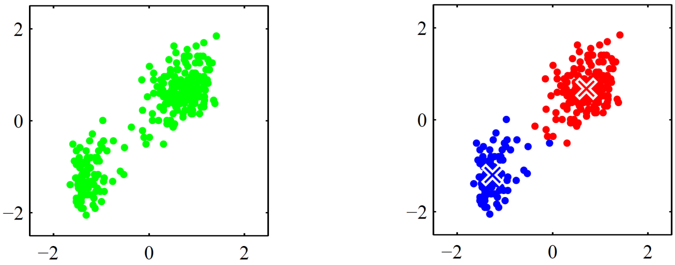

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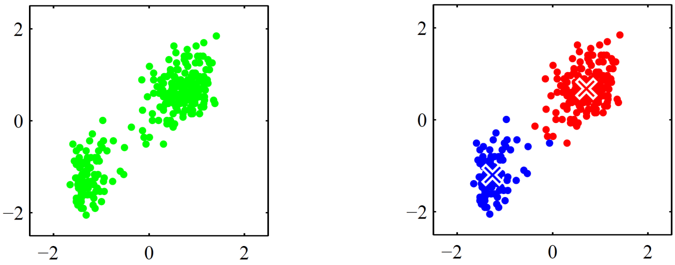
- find assignment $\gamma_{nk} \in \{0, 1\}$ for each data point $n \in [N]$ and $k \in [K]$ s.t. $\sum_{k \in [K]} \gamma_{nk} = 1$ for any fixed $n$



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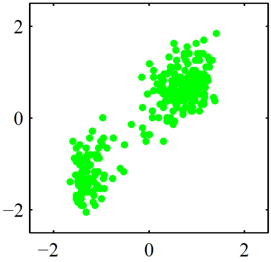
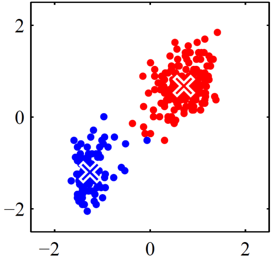
- find the cluster centers $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K \in \mathbb{R}^{\mathsf{D}}$



# Many applications

- recognize communities in a social network
- group similar customers in market research
- image segmentation
- accelerate other algorithms (e.g. NNC as in programing projects)
- ...

# One example

**image compression**:

- each pixel is a point
- perform clustering over these points
- replace each point by the center of the cluster it belongs to




Original image  Large $K \longrightarrow$ Small $K$

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Still, we can turn it into an optimization problem, e.g. through the popular **"K-means" objective**: find $\gamma_{nk}$ and $\boldsymbol{\mu}_k$ to minimize

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

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Unfortunately, finding the exact minimizer is *NP-hard!*

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# A closer look

The first step

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is simply to **assign each $x_n$ to the closest $\boldsymbol{\mu}_k$**, i.e.

$$\gamma_{nk} = \mathbb{I}\left[k == \operatorname*{argmin}_c \|\boldsymbol{x}_n - \boldsymbol{\mu}_c\|_2^2\right]$$

for all $k \in [K]$ and $n \in [N]$.

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is simply **to average the points of each cluster** (hence the name)

$$\boldsymbol{\mu}_k = \frac{\sum_{n:\gamma_{nk}=1} \boldsymbol{x}_n}{|\{n : \gamma_{nk} = 1\}|} = \frac{\sum_n \gamma_{nk} \boldsymbol{x}_n}{\sum_n \gamma_{nk}}$$

for each $k \in [K]$.

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**Step 3** Return to Step 1 if not converged

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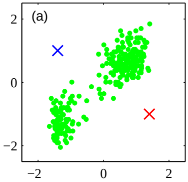

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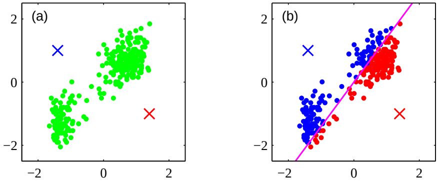

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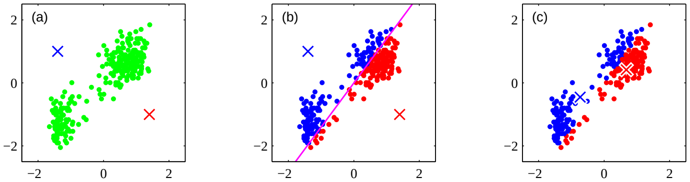

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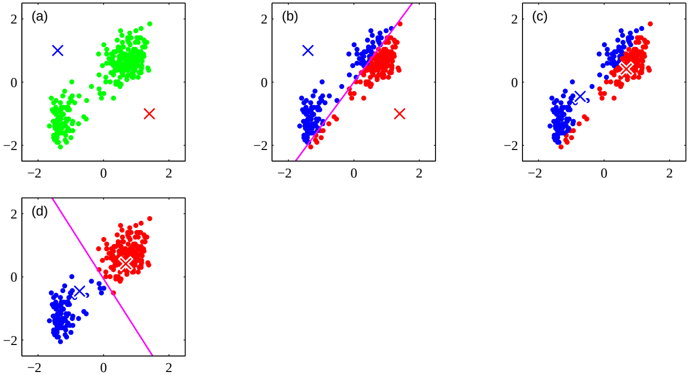

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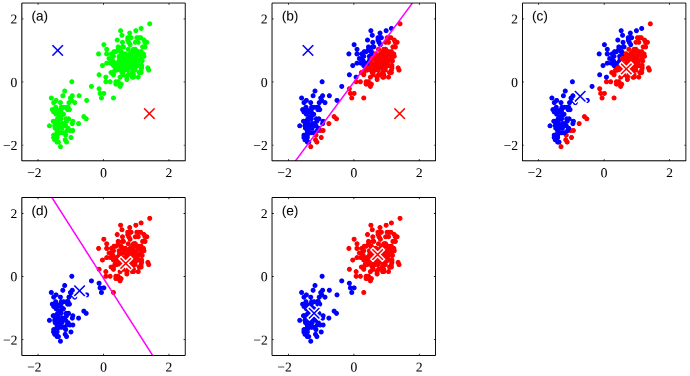

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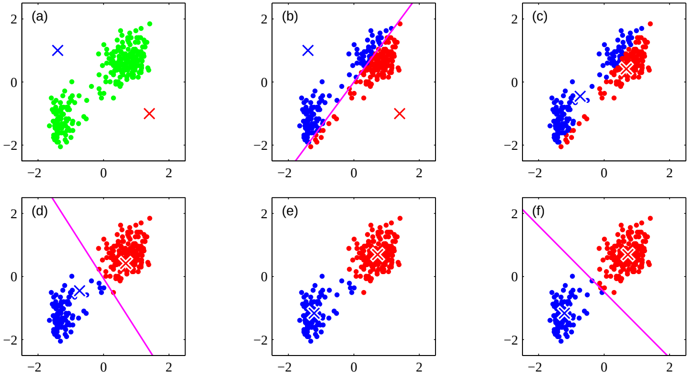

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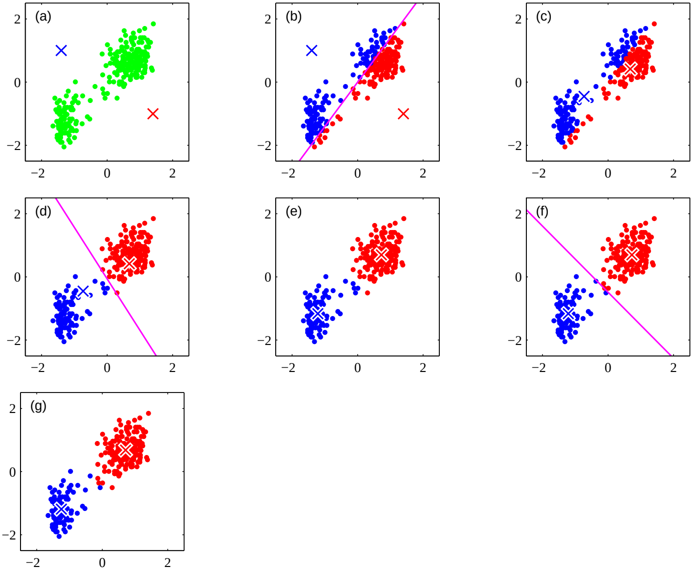

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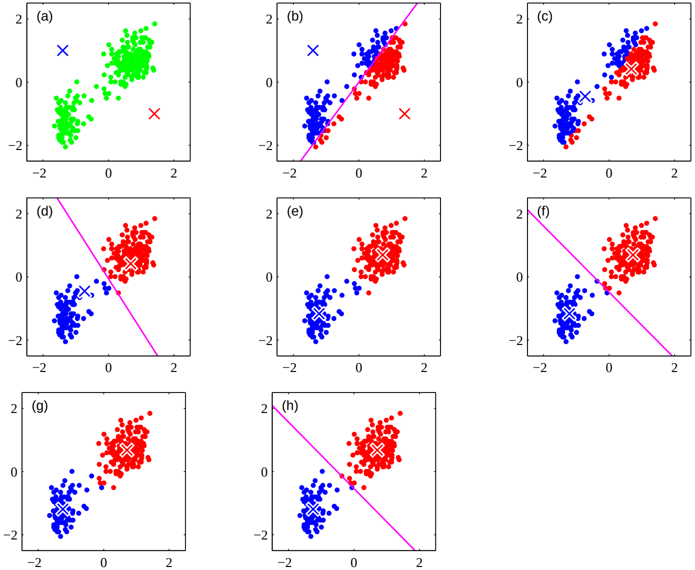

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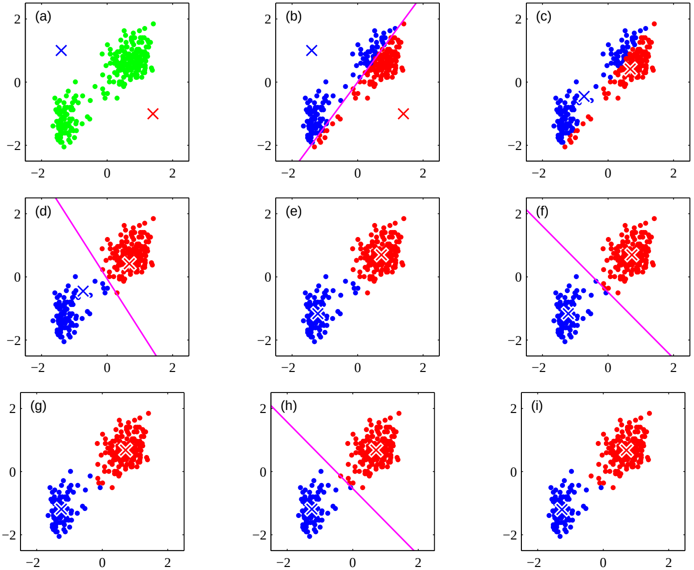

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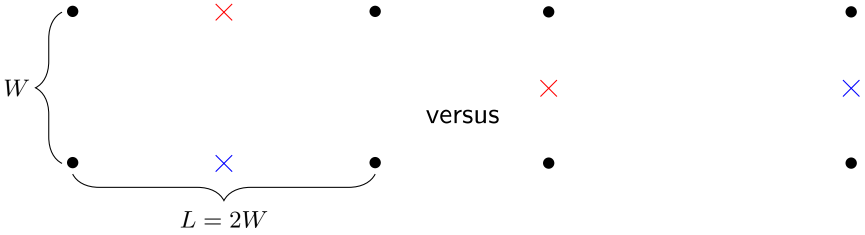
- and it *might not converge to the global minimum* of the K-means objective

# Local minimum v.s global minimum

**Simple example**: 4 data points, 2 clusters, 2 different initializations



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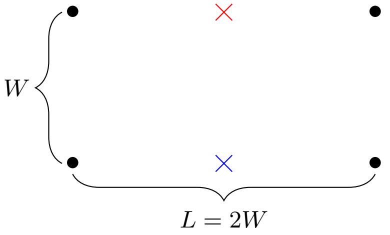


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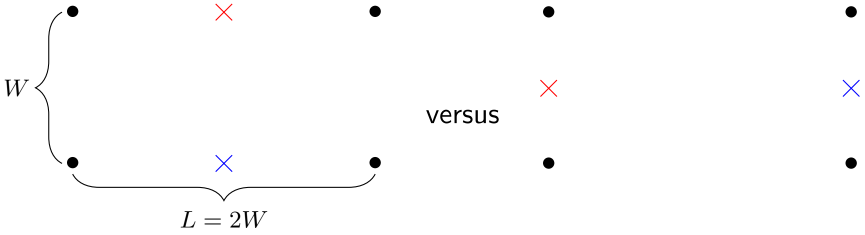


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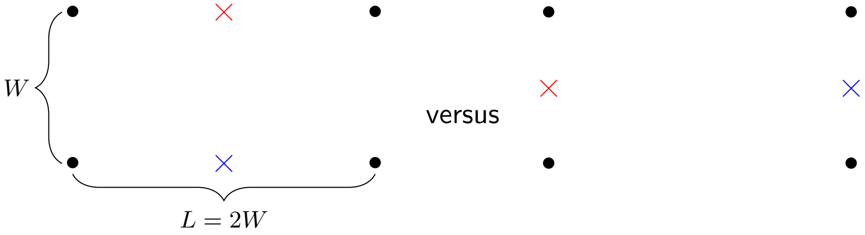


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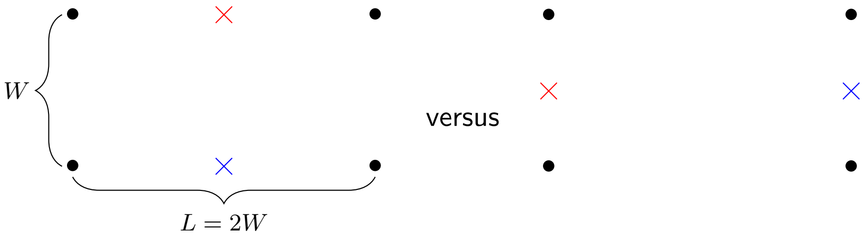


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- in fact, left is **local minimum**, and right is **global minimum**.

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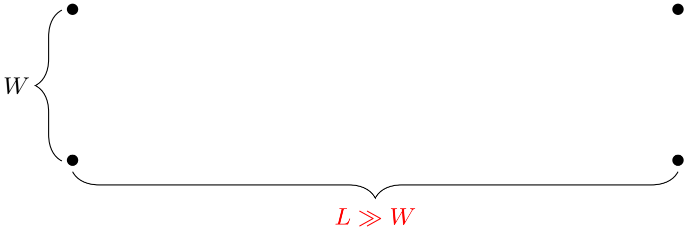

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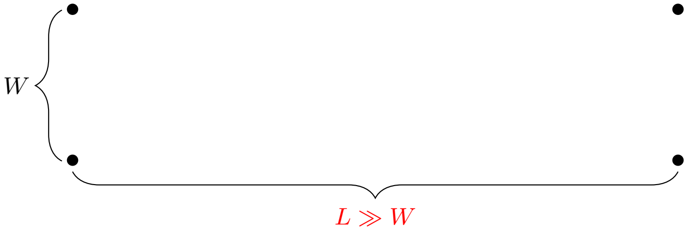


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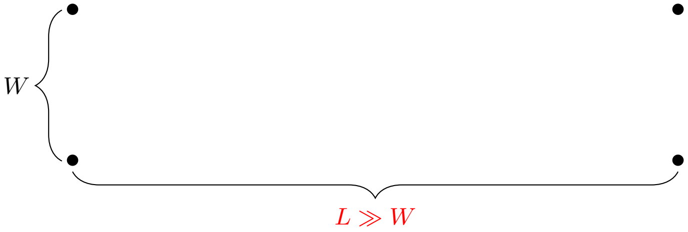
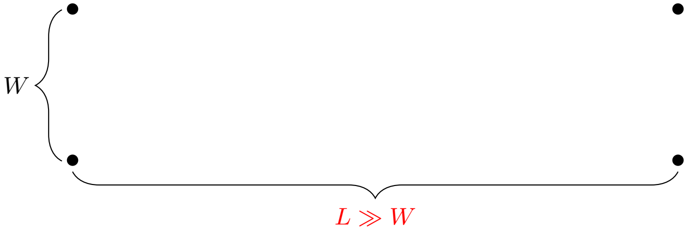



- moreover, local minimum can be *arbitrarily worse* if we increase $L$
- so *initialization matters a lot* for K-means

# How common initialization methods perform?

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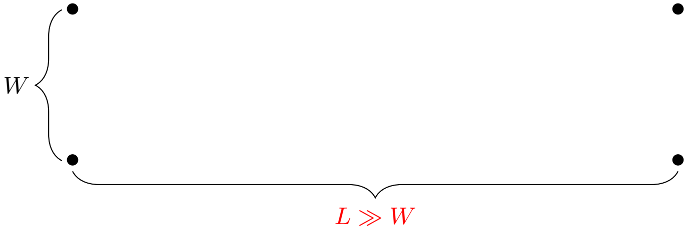


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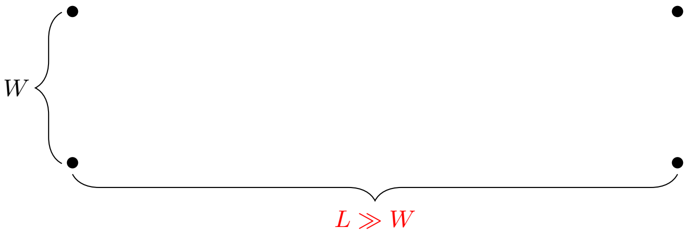


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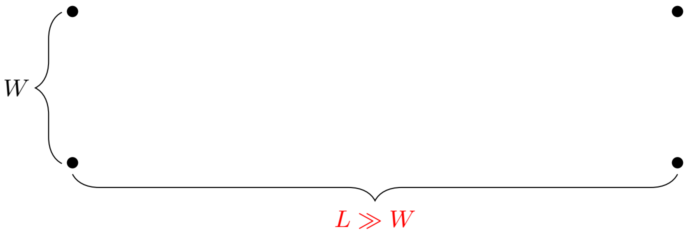


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- or randomly assign each point to a cluster, then average: similarly fail with a constant probability
- or more sophisticated approaches: **K-means++** *guarantees* to find a solution that in expectation is at most $O(\log K)$ times of the optimal

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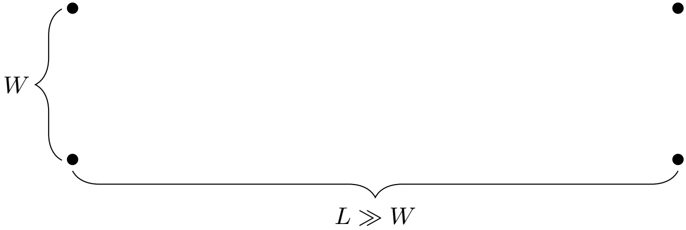
Intuitively this *spreads out the initial centers*.

# K-means++ on the same example



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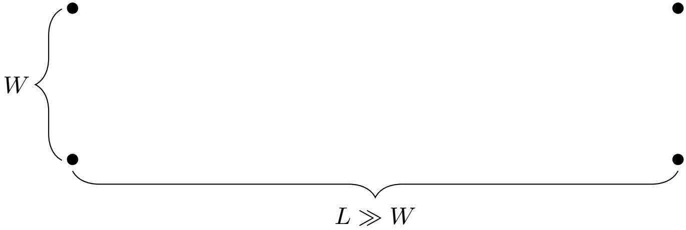


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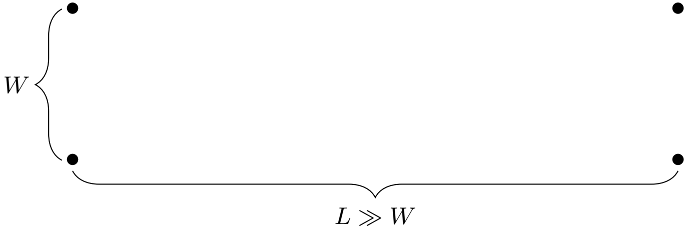


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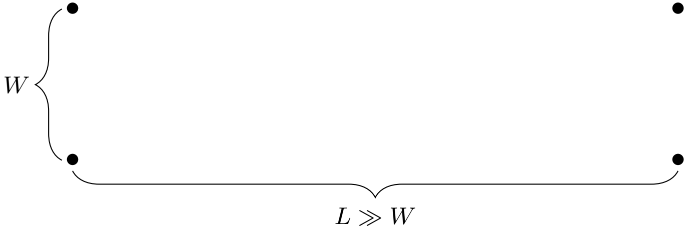


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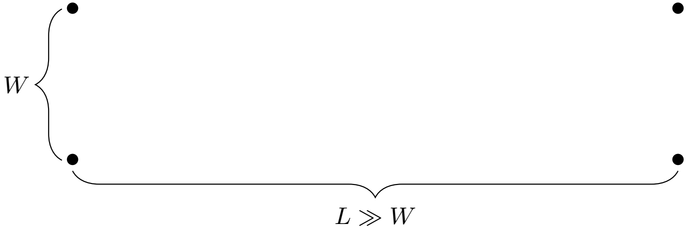


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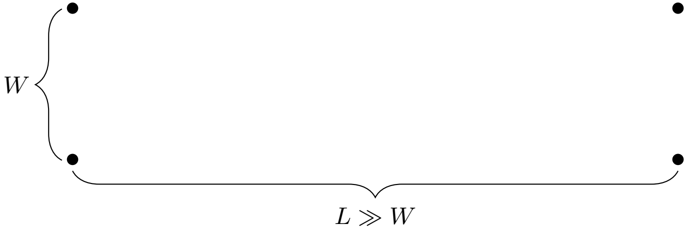


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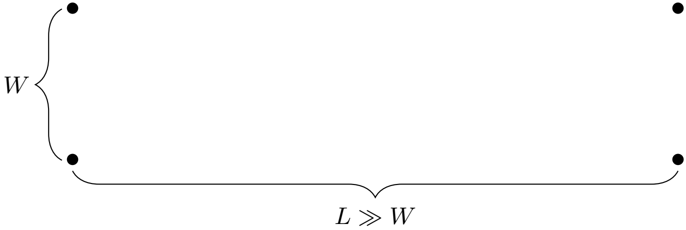


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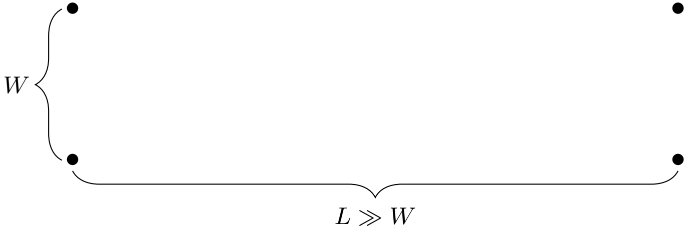


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that is, *at most 1.5 times of the optimal*.

# Summary for K-means

K-means is alternating minimization for the K-means objective.

The initialization matters a lot for the convergence.

K-means++ uses a theoretically (and often empirically) better initialization.

# Outline

# Gaussian mixture models

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To solve GMM, we will introduce a powerful method for learning probabilistic model: **Expectation–Maximization (EM) algorithm**

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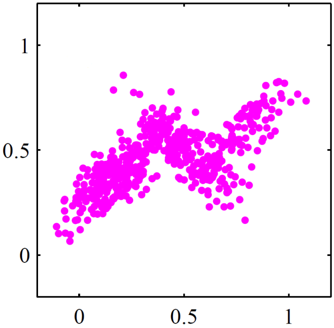

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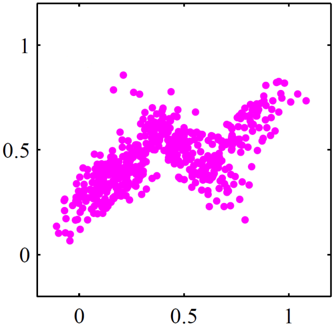
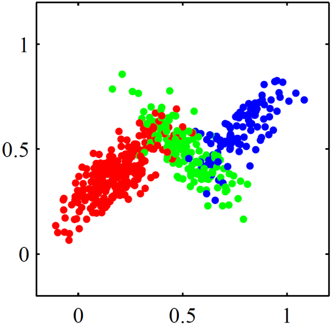
*What probabilistic model generates data like this?*



# GMM: intuition

GMM is a natural model to explain such data

Assume there are 3 ground-truth Gaussian models.



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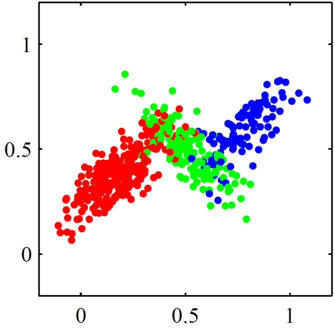

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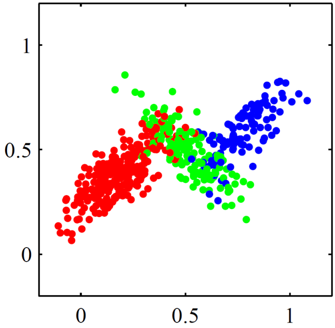

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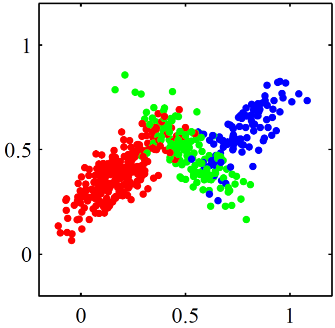


Hence the name "**Gaussian mixture model**".

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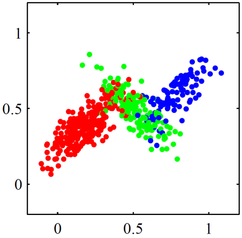
$\boldsymbol{x}$ and $z$ are both random variables drawn from the model

- $\boldsymbol{x}$ is observed
- $z$ is unobserved/latent

# An example




The conditional distributions are

$$p(\boldsymbol{x} \mid z = \text{red}) = N(\boldsymbol{x} \mid \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1)$$
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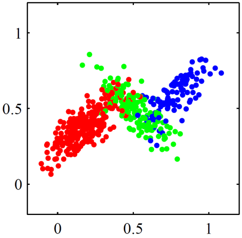


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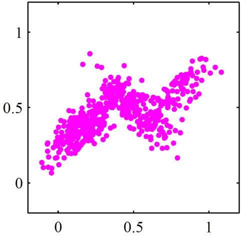


The marginal distribution is

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

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- both learn the cluster centers $\boldsymbol{\mu}_k$'s
- in addition, GMM learns cluster weight $\omega_k$ and covariance $\boldsymbol{\Sigma}_k$, thus
  - we can *predict probability of seeing a new point*
  - we can *generate synthetic data*

# How to learn these parameters?

An obvious attempt is **maximum-likelihood estimation (MLE)**: find

$$\operatorname*{argmax}_{\boldsymbol{\theta}} \ \ln \prod_{n=1}^{N} p(\boldsymbol{x}_n \ ; \boldsymbol{\theta}) = \operatorname*{argmax}_{\boldsymbol{\theta}} \sum_{n=1}^{N} \ln p(\boldsymbol{x}_n \ ; \boldsymbol{\theta}) \triangleq \operatorname*{argmax}_{\boldsymbol{\theta}} P(\boldsymbol{\theta})$$

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One solution is to still apply GD/SGD, but a much more effective approach is the **Expectation–Maximization (EM) algorithm**.

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We will see how this is a special case of EM.

# Demo

Generate 50 data points from a mixture of 2 Gaussians with

- $\omega_1 = 0.3, \mu_1 = -0.8, \Sigma_1 = 0.52$
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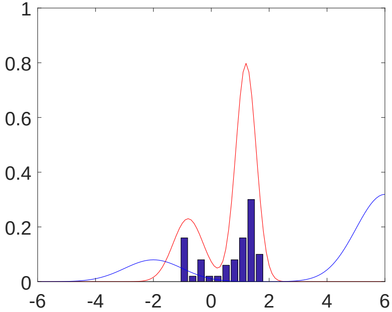

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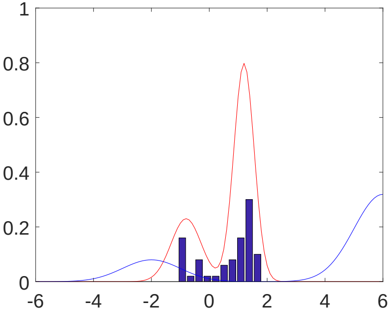

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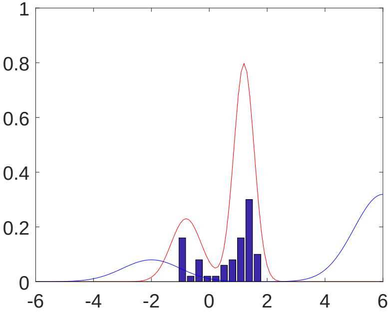

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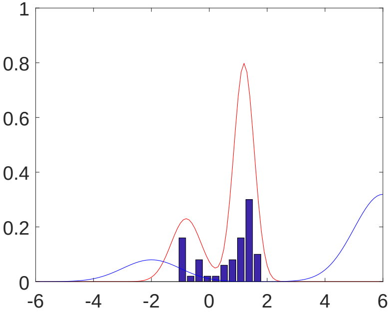


EM_demo.pdf shows how the blue curve moves towards red curve quickly via EM

# EM algorithm

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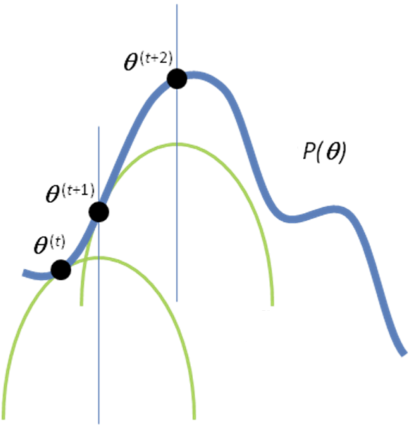
Again, directly solving the objective is intractable.

# High level idea

Keep maximizing **a lower bound of $P$ that is more manageable**



# Derivation of EM

**Finding the lower bound of $P$:**

$$\ln p(\boldsymbol{x}\ ;\boldsymbol{\theta}) = \ln \frac{p(\boldsymbol{x}, z\ ;\boldsymbol{\theta})}{p(z|\boldsymbol{x}\ ;\boldsymbol{\theta})} \qquad \text{(true for any } z\text{)}$$

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# Alternatively maximize the lower bound

Therefore, we obtain a lower bound for the log-likelihood function

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&\geq \sum_{n=1}^{N} \left(\mathbb{E}_{z_n \sim q_n}\left[\ln p(\boldsymbol{x}_n, z_n \,; \boldsymbol{\theta})\right] + H(q_n)\right) = F(\boldsymbol{\theta}, \{q_n\})
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Equivalently, this is the same as alternatingly maximizing $F$ over $\{q_n\}$ and $\boldsymbol{\theta}$ (similar to K-means).

# Maximizing over $\{q_n\}$

Fix $\boldsymbol{\theta}^{(t)}$, the solution to

$$\operatorname*{argmax}_{q_n} \mathbb{E}_{z_n \sim q_n}\left[\ln p(\boldsymbol{x}_n, z_n\ ; \boldsymbol{\theta}^{(t)})\right] + H(q_n)$$

is $q_n^{(t)}$ s.t.

$$q_n^{(t)}(z_n) = p(z_n \mid \boldsymbol{x}_n\ ; \boldsymbol{\theta}^{(t)})$$

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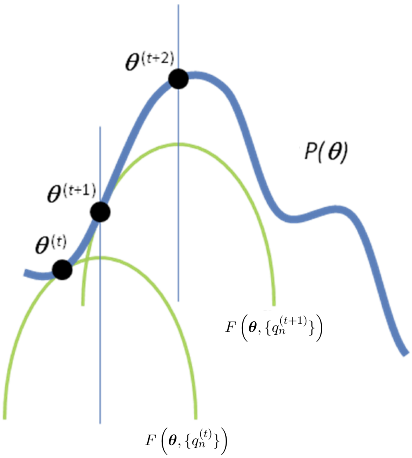
**Step 2 (M-Step)** **update the model parameter** via **Maximization**

$$\boldsymbol{\theta}^{(t+1)} \leftarrow \operatorname*{argmax}_{\boldsymbol{\theta}} Q(\boldsymbol{\theta} \,; \boldsymbol{\theta}^{(t)})$$

**Step 3** $t \leftarrow t + 1$ and return to Step 1 if not converged

# Pictorial explanation

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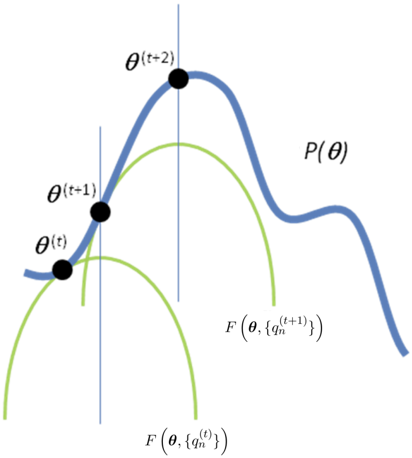


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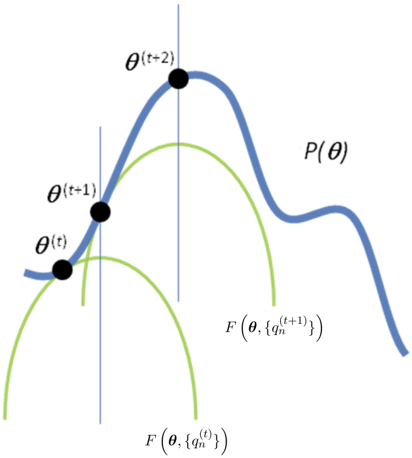


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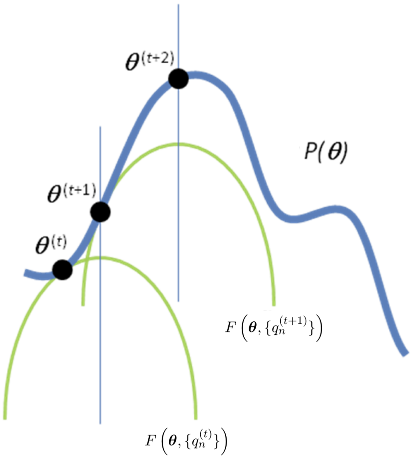


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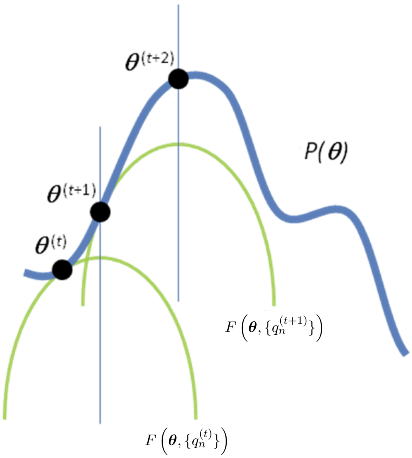


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So EM always increases the objective value and will converge to some local maximum (similar to K-means).

# Apply EM to learn GMMs

**E-Step**:

$$
\begin{aligned}
q_n^{(t)}(z_n = k) &= p\left(z_n = k \mid \boldsymbol{x}_n \,; \boldsymbol{\theta}^{(t)}\right) \\
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This computes the "soft assignment" $\gamma_{nk} = q_n^{(t)}(z_n = k)$, i.e. conditional probability of $\boldsymbol{x}_n$ belonging to cluster $k$.

# Apply EM to learn GMMs

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$$\operatorname*{argmax}_{\boldsymbol{\theta}} Q(\boldsymbol{\theta}, \boldsymbol{\theta}^{(t)}) = \operatorname*{argmax}_{\boldsymbol{\theta}} \sum_{n=1}^{N} \mathbb{E}_{z_n \sim q_n^{(t)}} [\ln p(\boldsymbol{x}_n, z_n \; ; \boldsymbol{\theta})]$$

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&= \operatorname*{argmax}_{\{\omega_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}} \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma_{nk} \left(\ln \omega_k + \ln N(\boldsymbol{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)\right)
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# Apply EM to learn GMMs

**M-Step**:

$$\begin{aligned}
\underset{\boldsymbol{\theta}}{\operatorname{argmax}}\, Q(\boldsymbol{\theta}, \boldsymbol{\theta}^{(t)}) &= \underset{\boldsymbol{\theta}}{\operatorname{argmax}} \sum_{n=1}^{N} \mathbb{E}_{z_n \sim q_n^{(t)}} \left[\ln p(\boldsymbol{x}_n, z_n \, ; \boldsymbol{\theta})\right] \\
&= \underset{\boldsymbol{\theta}}{\operatorname{argmax}} \sum_{n=1}^{N} \mathbb{E}_{z_n \sim q_n^{(t)}} \left[\ln p(z_n \, ; \boldsymbol{\theta}) + \ln p(\boldsymbol{x}_n | z_n \, ; \boldsymbol{\theta})\right] \\
&= \underset{\{\omega_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}}{\operatorname{argmax}} \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma_{nk} \left(\ln \omega_k + \ln N(\boldsymbol{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)\right)
\end{aligned}$$

To find $\omega_1, \ldots, \omega_K$, solve

$$\underset{\boldsymbol{\omega}}{\operatorname{argmax}} \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma_{nk} \ln \omega_k$$

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To find $\omega_1, \ldots, \omega_K$, solve

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\operatorname*{argmax}_{\boldsymbol{\omega}} \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma_{nk} \ln \omega_k
$$

To find each $\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k$, solve

$$
\operatorname*{argmax}_{\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k} \sum_{n=1}^{N} \gamma_{nk} \ln N(\boldsymbol{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)
$$

# M-Step (continued)

Solutions to previous two problems are very natural, for each $k$

$$\omega_k = \frac{\sum_n \gamma_{nk}}{N}$$

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

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You will verify some of these in HW4.

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EM for learning GMMs:

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**Step 1 (E-Step) update the "soft assignment"** (fixing parameters)

$$\gamma_{nk} = p(z_n = k \mid \boldsymbol{x}_n) \propto \omega_k N\left(\boldsymbol{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right)$$

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**Step 2 (M-Step)** **update the model parameter** (fixing assignments)

$$\omega_k = \frac{\sum_n \gamma_{nk}}{N} \qquad \boldsymbol{\mu}_k = \frac{\sum_n \gamma_{nk} \boldsymbol{x}_n}{\sum_n \gamma_{nk}}$$

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**Step 3** return to Step 1 if not converged

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GMM is a soft version of K-means and it provides a probabilistic interpretation of the data, which means we can predict and generate data after learning.