CSCI567 Machine Learning (Fall 2024)

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October 25, 2024

Outline

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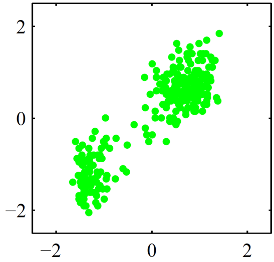
Today's focus: **clustering**, an important unsupervised learning problem

Clustering: informal definition

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



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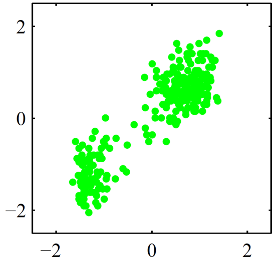

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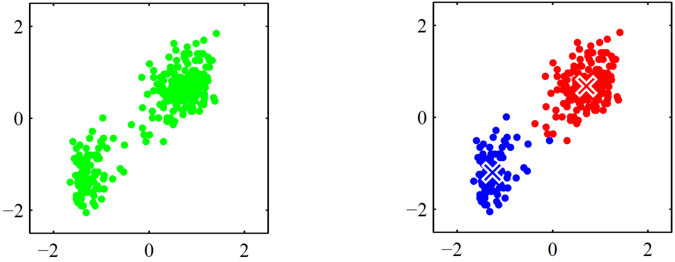
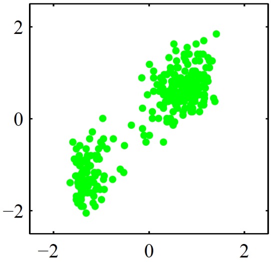
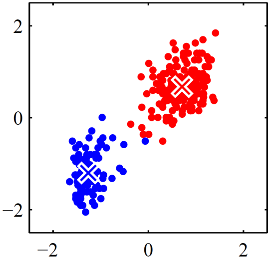
- assign each point to a specific cluster
- find the center (representative/prototype/...) of each cluster



Clustering: formal definition

Given: data points $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N \in \mathbb{R}^{\mathsf{D}}$





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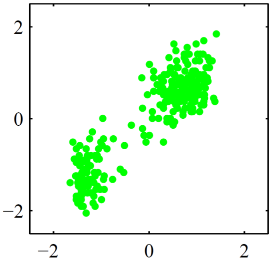

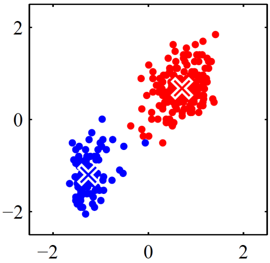

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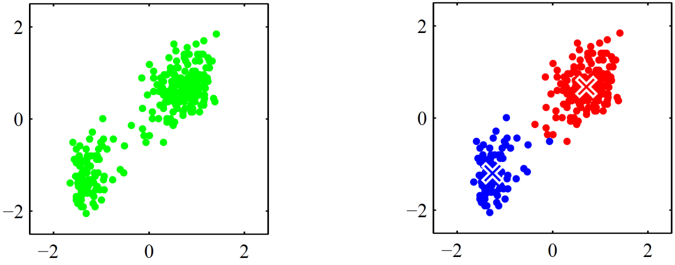
Output: group the data into K clusters, which means

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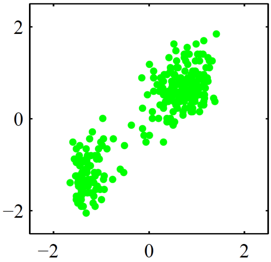
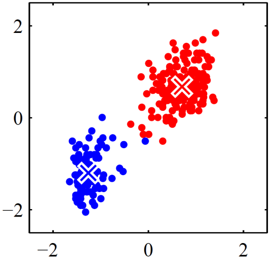
- find the cluster centers $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K \in \mathbb{R}^\mathsf{D}$





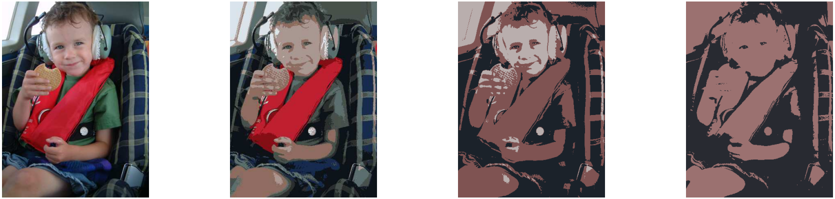
Many applications

- 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

Formal Objective

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Still, we can turn it into an optimization problem, e.g. through the popular **"K-means" objective**: find γ_{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

$$\min_{\{\gamma_{nk}\}} F\left(\{\gamma_{nk}\}, \{\boldsymbol{\mu}_k\}\right) = \min_{\{\gamma_{nk}\}} \sum_n \sum_k \gamma_{nk} \|\boldsymbol{x}_n - \boldsymbol{\mu}_k\|_2^2$$

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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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$$\min_{\{\boldsymbol{\mu}_k\}} F\left(\{\gamma_{nk}\}, \{\boldsymbol{\mu}_k\}\right) = \min_{\{\boldsymbol{\mu}_k\}} \sum_n \sum_k \gamma_{nk} \|\boldsymbol{x}_n - \boldsymbol{\mu}_k\|_2^2$$

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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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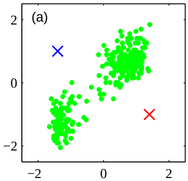
Step 3 Return to Step 1 if not converged

An example



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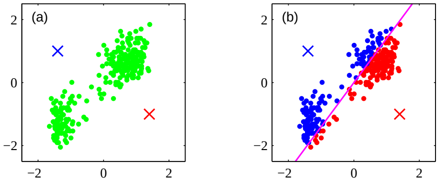

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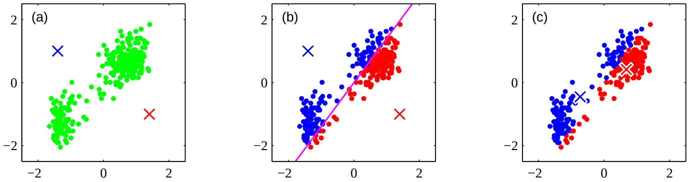

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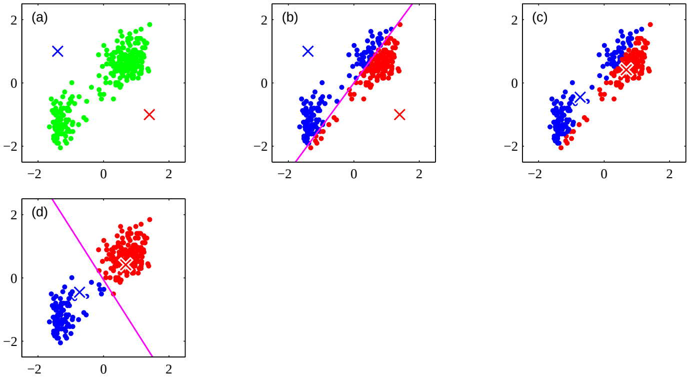

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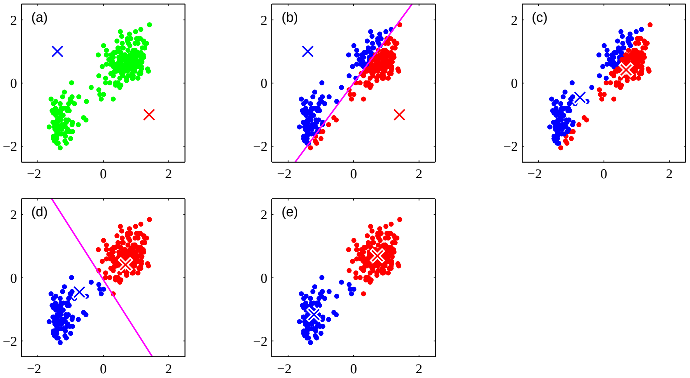

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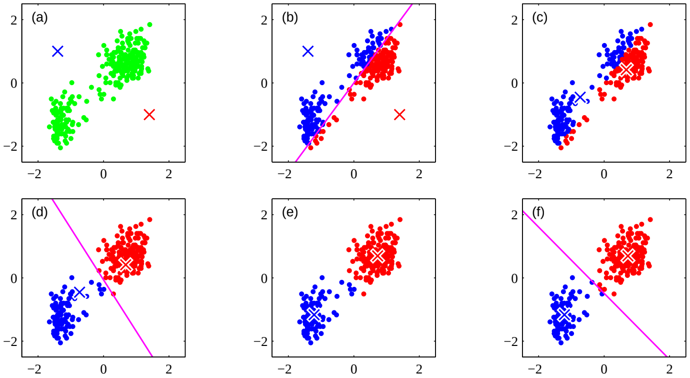

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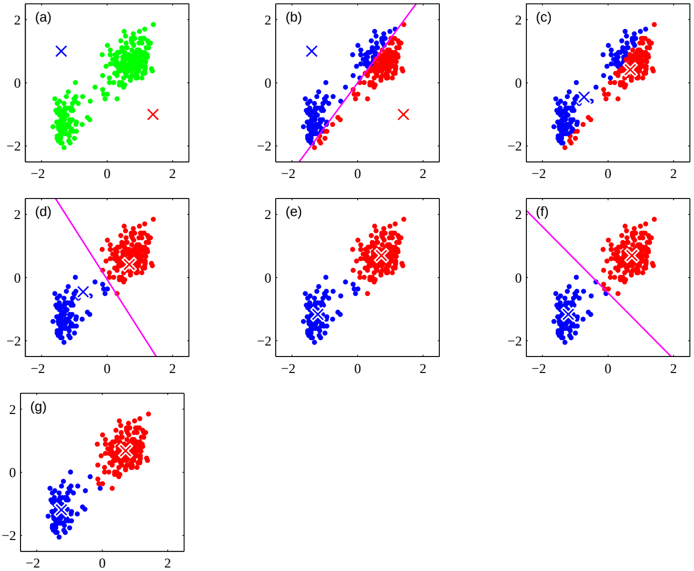

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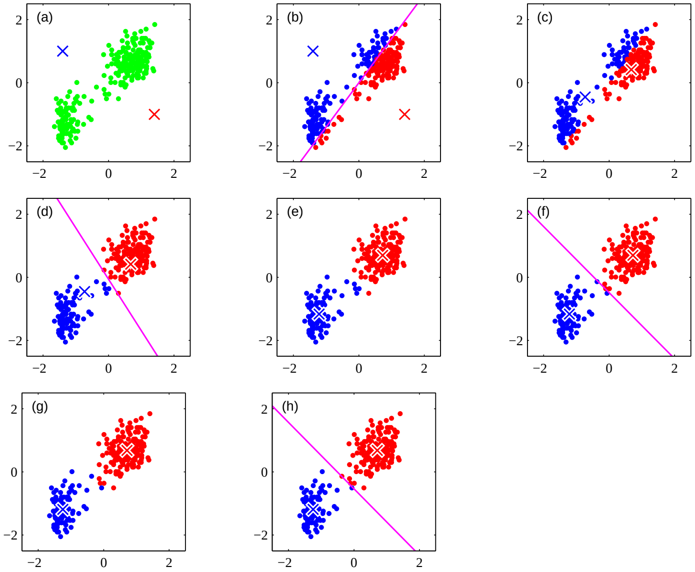

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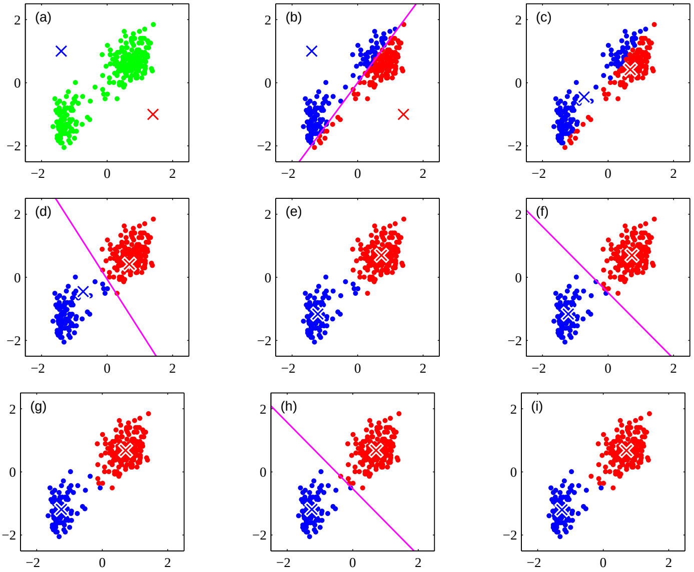

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Initialization matters for **convergence**.

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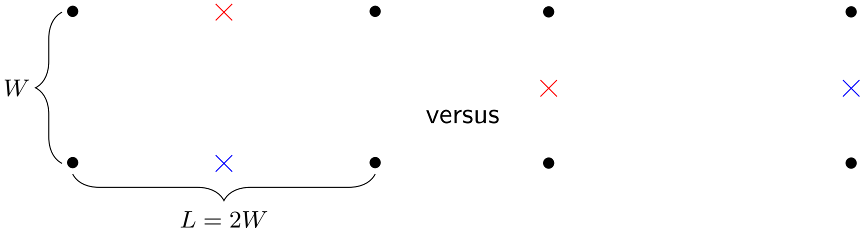
- and it *might not converge to the global minimum* of the K-means objective

Local minimum v.s global minimum

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



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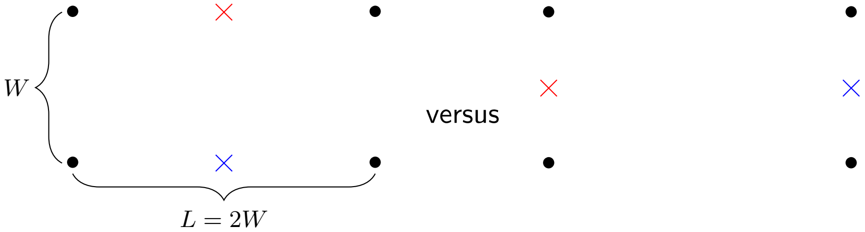

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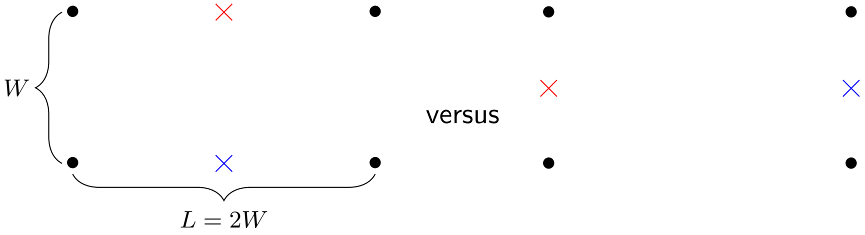

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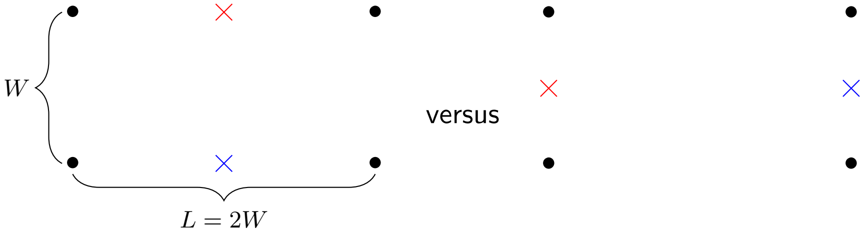

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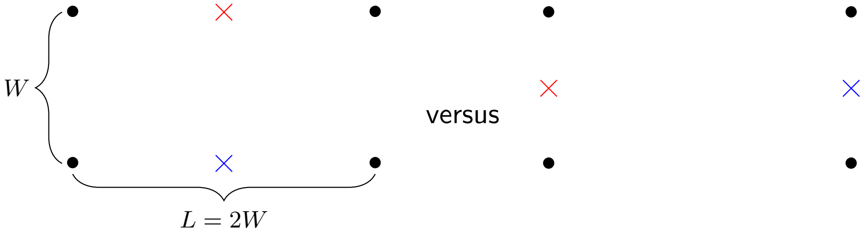

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- left has K-means objective $L^2 = 4W^2$
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- in fact, left is **local minimum**, and right is **global minimum**.

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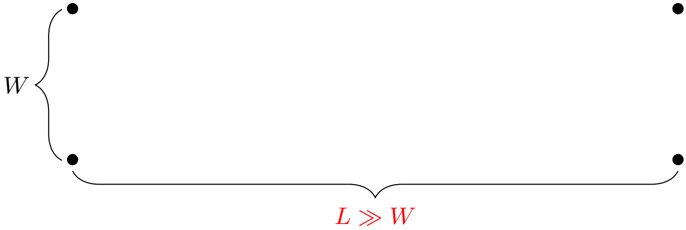

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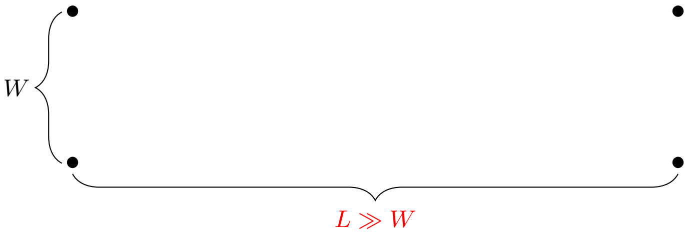

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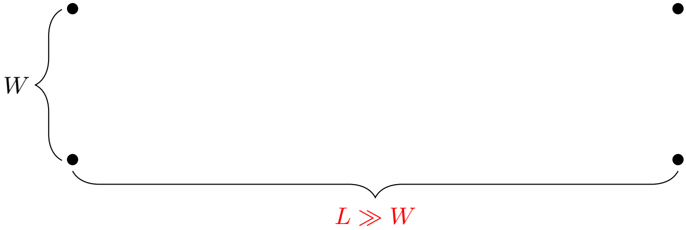
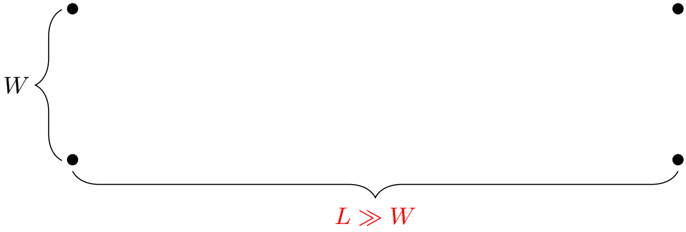


- moreover, local minimum can be *arbitrarily worse* if we increase L
- so *initialization matters a lot* for K-means

How common initialization methods perform?



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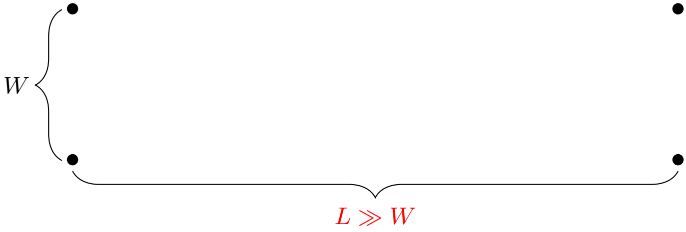

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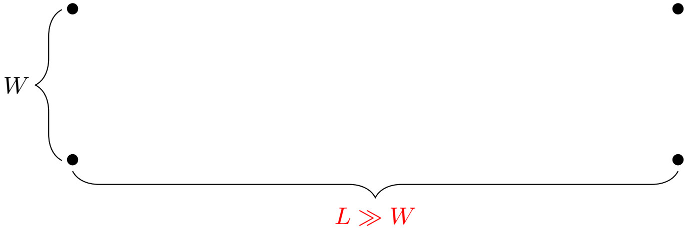

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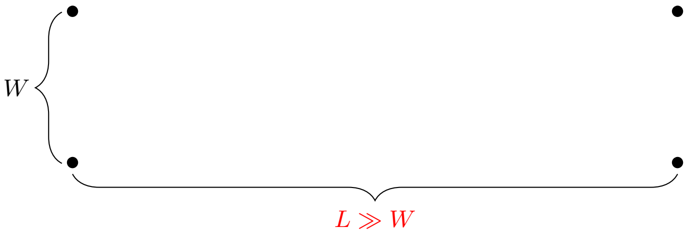

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- or randomly assign each point to a cluster, then average: similarly fail with a constant probability
- or more sophisticated approaches: **K-means++** *guarantees* to find a solution that in expectation is at most $O(\log K)$ times of the optimal

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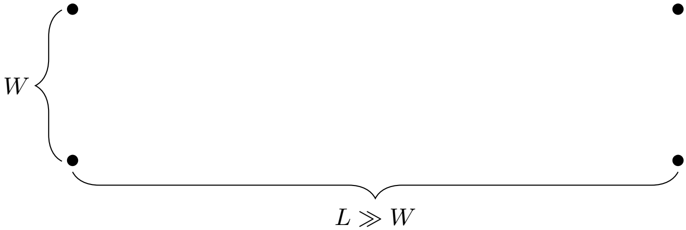
Intuitively this *spreads out the initial centers*.

K-means++ on the same example



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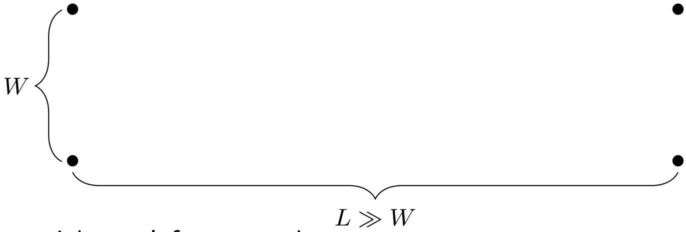

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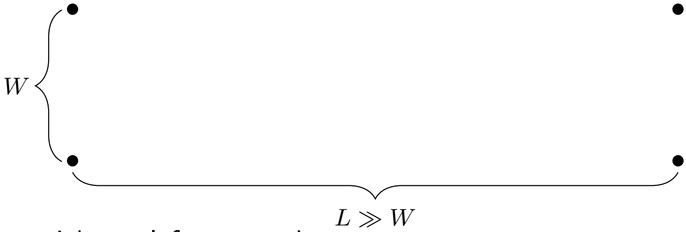

Suppose we pick top left as $\boldsymbol{\mu}_1$, then

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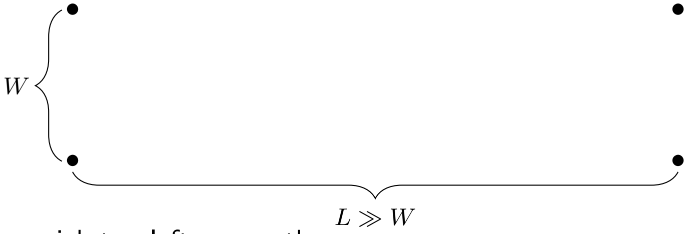
K-means++ on the same example



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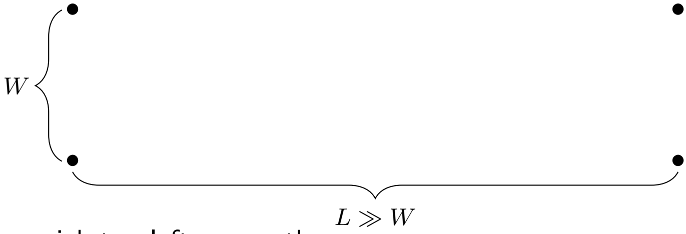

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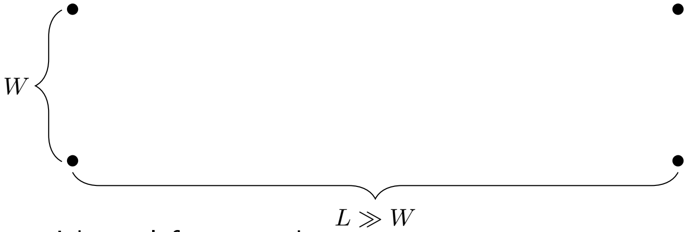

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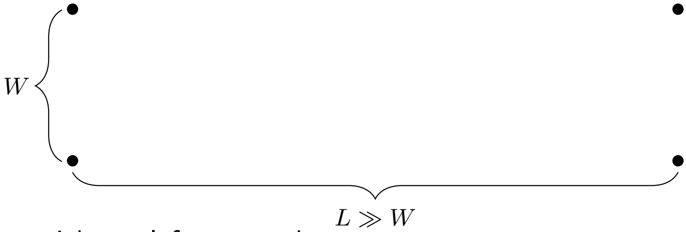

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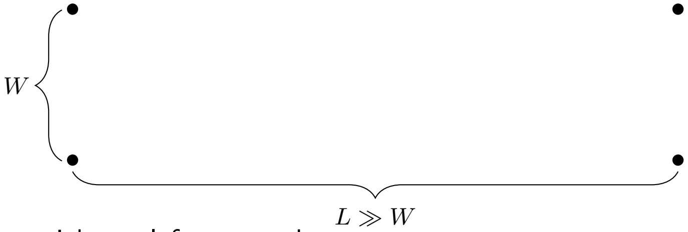

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that is, *at most 1.5 times of the optimal*.

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

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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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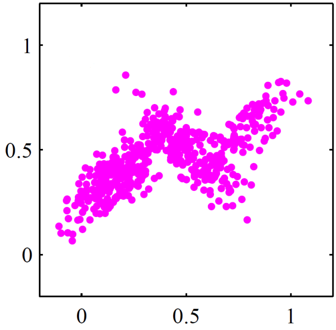

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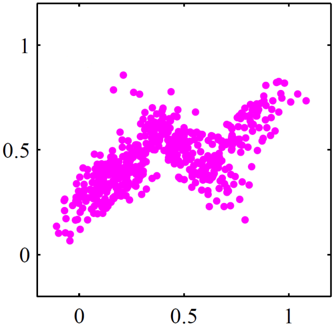
What probabilistic model generates data like this?



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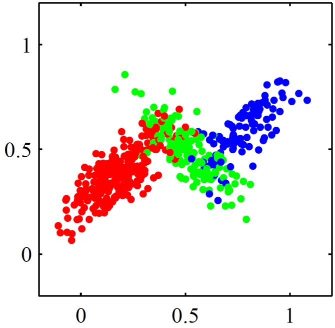
GMM is a natural model to explain such data

Assume there are 3 ground-truth Gaussian models.



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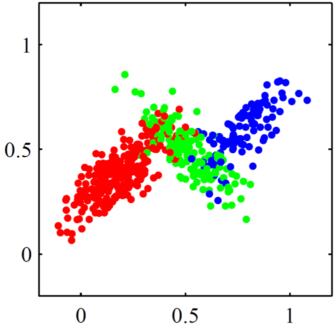

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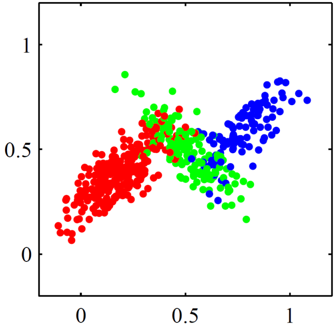

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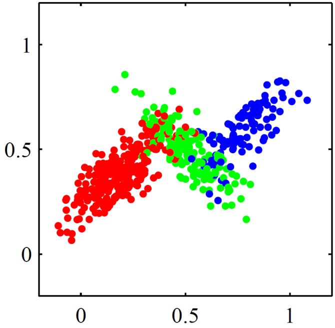

Hence the name "**Gaussian mixture model**".

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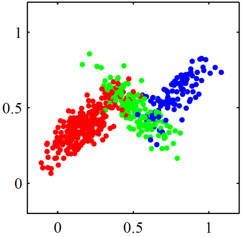
$\boldsymbol{x}$ and z are both random variables drawn from the model

- $\boldsymbol{x}$ 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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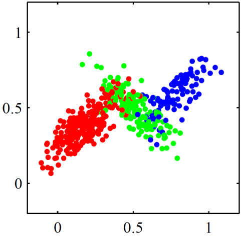

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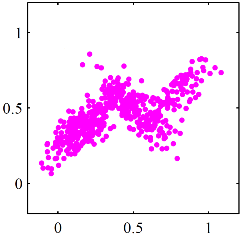

The marginal distribution is

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

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- in addition, GMM learns cluster weight ω_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**.

Preview of EM for learning GMMs

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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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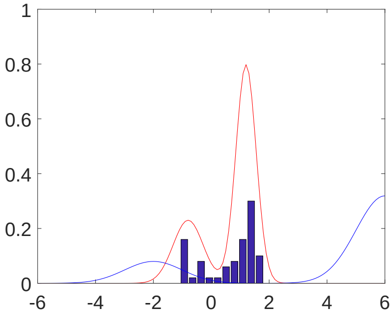

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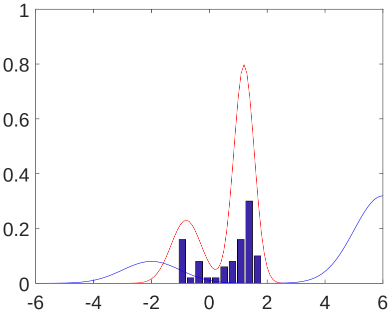

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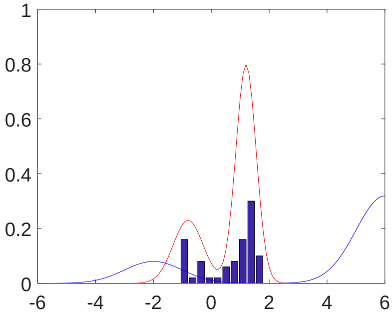

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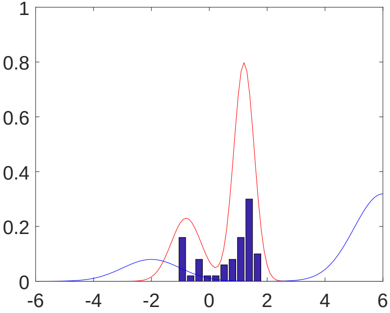

EM_demo.pdf shows how the blue curve moves towards red curve quickly via EM

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EM algorithm

In general EM is **a heuristic to solve MLE with latent variables** (not just GMM), i.e. find the maximizer of

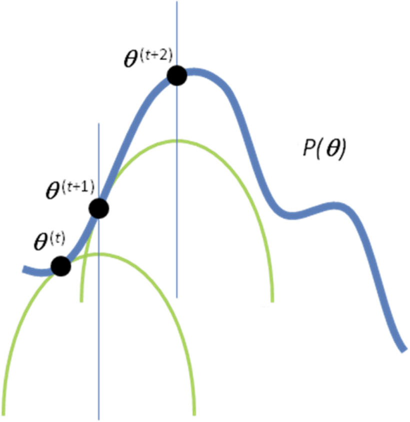
$$P(\boldsymbol{\theta}) = \sum_{n=1}^{N} \ln p(\boldsymbol{x}_n \ ; \boldsymbol{\theta}) = \sum_{n=1}^{N} \ln \int_{z_n} p(\boldsymbol{x}_n, z_n \ ; \boldsymbol{\theta}) dz_n$$

- $\boldsymbol{\theta}$ is the parameters for a general probabilistic model
- $\boldsymbol{x}_n$'s are observed random variables
- z_n's are latent variables

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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$$= \mathbb{E}_{z\sim q}\left[\ln p(\boldsymbol{x}, z\,;\boldsymbol{\theta})\right] + H(q) - \mathbb{E}_{z\sim q}\left[\ln \frac{p(z|\boldsymbol{x}\,;\boldsymbol{\theta})}{q(z)}\right] \qquad (H \text{ is entropy})$$

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\end{aligned}$$

(Jensen's inequality)

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$$= \mathbb{E}_{z\sim q}\left[\ln p(\boldsymbol{x}, z\,;\boldsymbol{\theta})\right] + H(q)$$

Alternatively maximize the lower bound

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

$$
\begin{aligned}
P(\boldsymbol{\theta}) &= \sum_{n=1}^{N} \ln p(\boldsymbol{x}_n\ ; \boldsymbol{\theta}) \\
&\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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This holds for *any* $\{q_n\}$, so how do we choose?

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This holds for *any* $\{q_n\}$, so how do we choose? Naturally, *the one that maximizes the lower bound* (i.e. the tightest lower bound)!

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

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

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

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

i.e., the *posterior distribution of z_n* given $\boldsymbol{x}_n$ and $\boldsymbol{\theta}^{(t)}$. (Verified in HW4)

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- versus the incomplete likelihood: $P(\boldsymbol{\theta}) = \sum_{n=1}^{N} \ln p(\boldsymbol{x}_n \,; \boldsymbol{\theta})$

General EM algorithm

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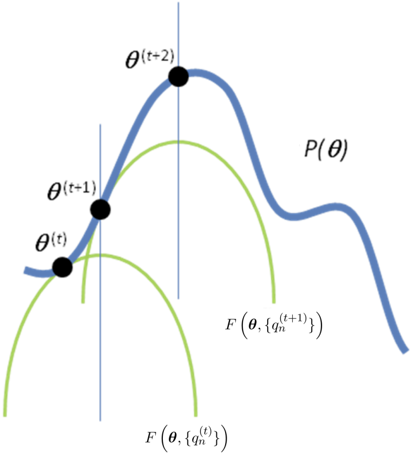
Step 2 (M-Step) **update the model parameter** via **Maximization**

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

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

Pictorial explanation



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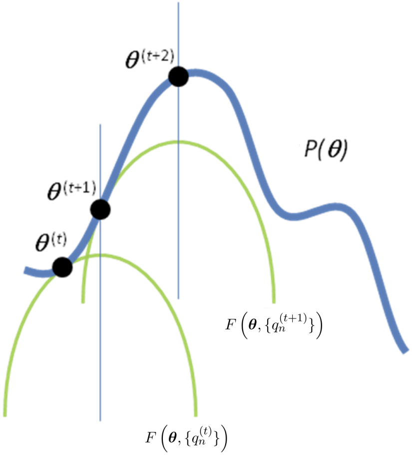

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$$P(\boldsymbol{\theta}^{(\mathrm{t+1})}) \geq F\left(\boldsymbol{\theta}^{(\mathrm{t+1})}; \{q_n^{(t)}\}\right)$$

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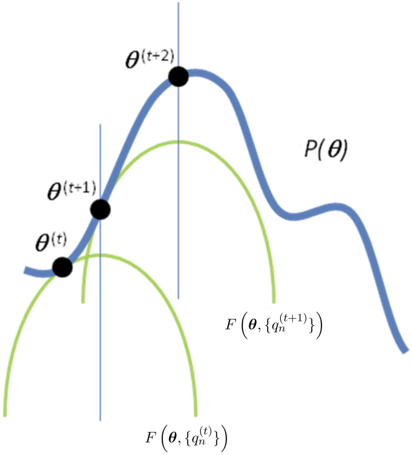

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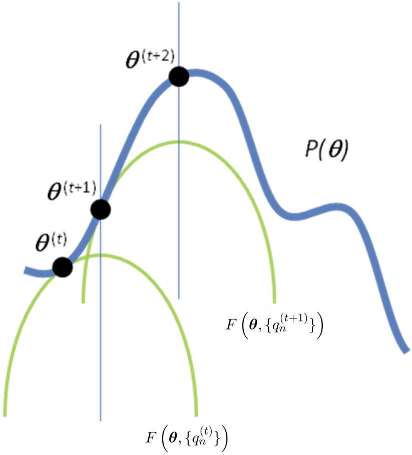

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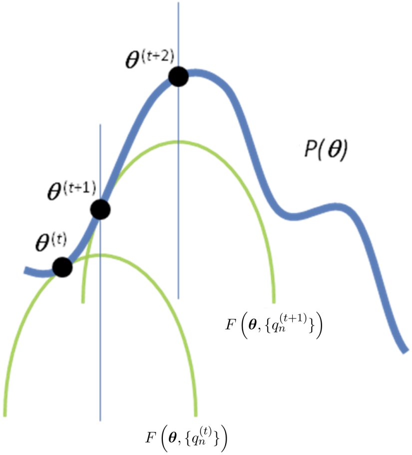

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$$

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:

$$\begin{aligned} q_n^{(t)}(z_n = k) &= p\left(z_n = k \mid \boldsymbol{x}_n \,; \boldsymbol{\theta}^{(t)}\right) \\ &\propto p\left(\boldsymbol{x}_n, z_n = k \,; \boldsymbol{\theta}^{(t)}\right) \end{aligned}$$

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\end{aligned}
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&= \omega_k^{(t)} N\left(\boldsymbol{x}_n \mid \boldsymbol{\mu}_k^{(t)}, \boldsymbol{\Sigma}_k^{(t)}\right)
\end{aligned}
$$

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.

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

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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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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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M-Step:

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

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

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

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)

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You will verify some of these in HW4.

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EM for learning GMMs:

Step 0 Initialize $\omega_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k$ for each $k \in [K]$

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

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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.