

CSCI567 Machine Learning (Fall 2023)

Prof. Dani Yogatama
Slide Deck from Prof. Haipeng Luo

University of Southern California

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Outline

- 1 Clustering
- 2 Gaussian mixture models

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 - Problem setup
 - K-means algorithm
 - Initialization and Convergence
- 2 Gaussian mixture models

Supervised learning v.s unsupervised learning

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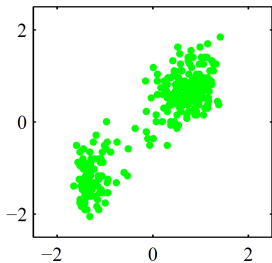
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Today's focus: **clustering**, an important unsupervised learning problem

Clustering: informal definition

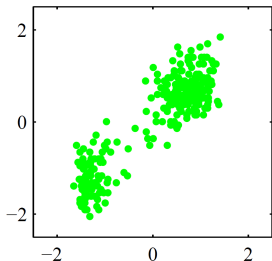
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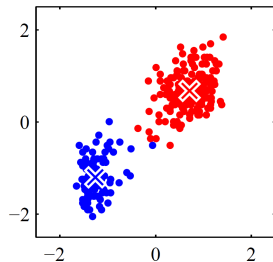
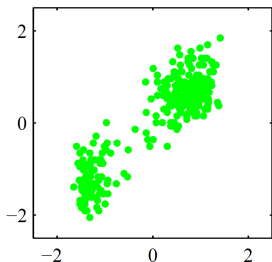


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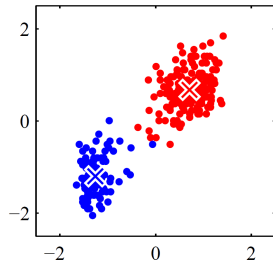
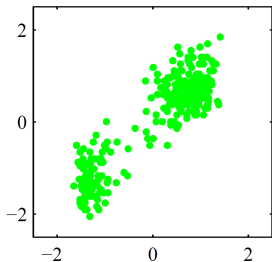
Output: group the data into some clusters, which means

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



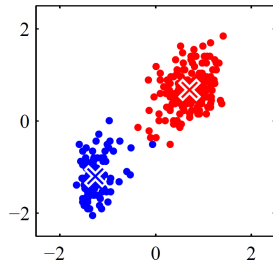
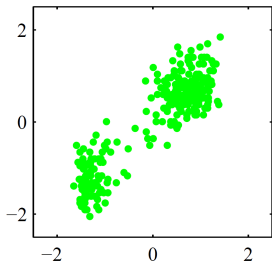
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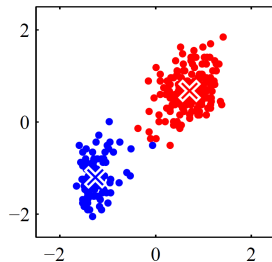
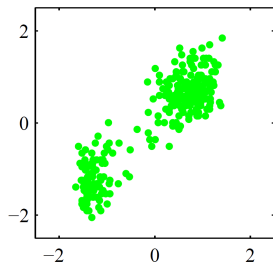


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s.t. $\sum_{k \in [K]} \gamma_{nk} = 1$ for any fixed n

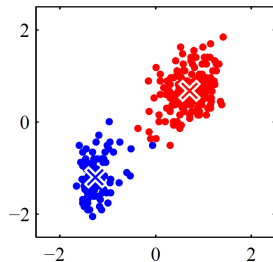
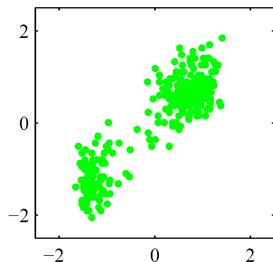


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- find the cluster **centers** $\boldsymbol{\mu}_1, \dots, \boldsymbol{\mu}_K \in \mathbb{R}^D$



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 \rightarrow Small K

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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 μ_k to minimize

$$F(\{\gamma_{nk}\}, \{\mu_k\}) = \sum_{n=1}^N \sum_{k=1}^K \gamma_{nk} \|\mathbf{x}_n - \mu_k\|_2^2$$

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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.

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

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)

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

for each $k \in [K]$.

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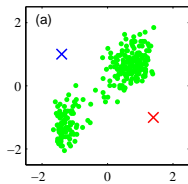
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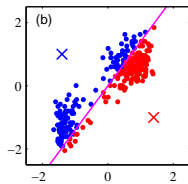
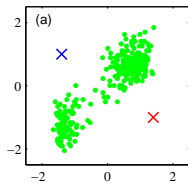
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Step 3 Return to Step 1 if not converged

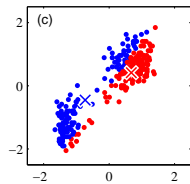
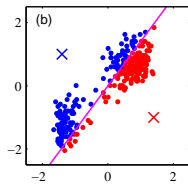
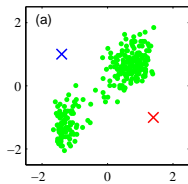
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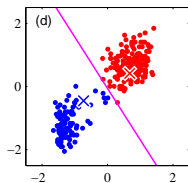
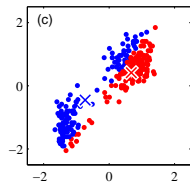
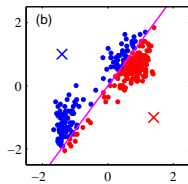
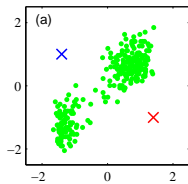
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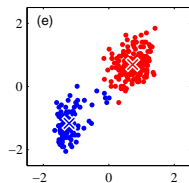
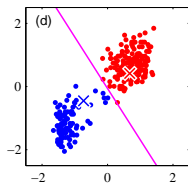
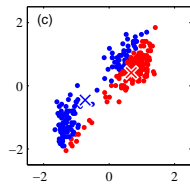
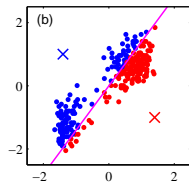
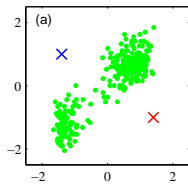
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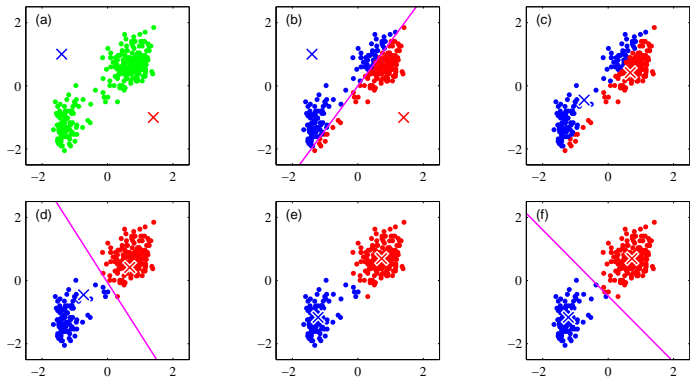
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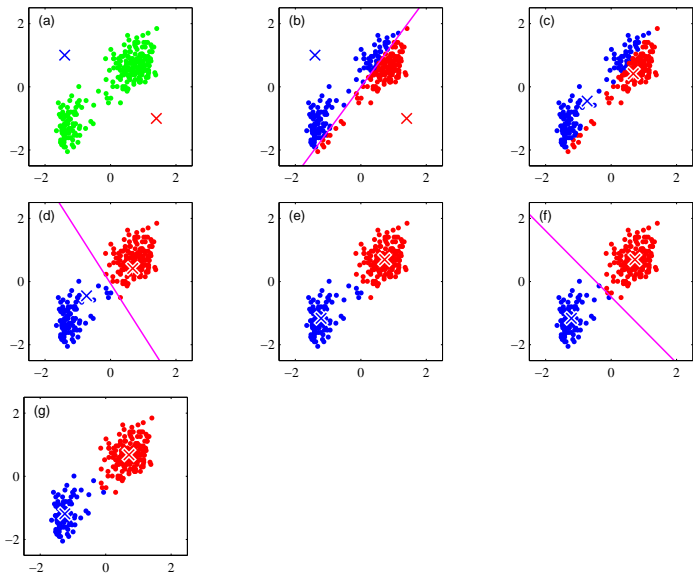
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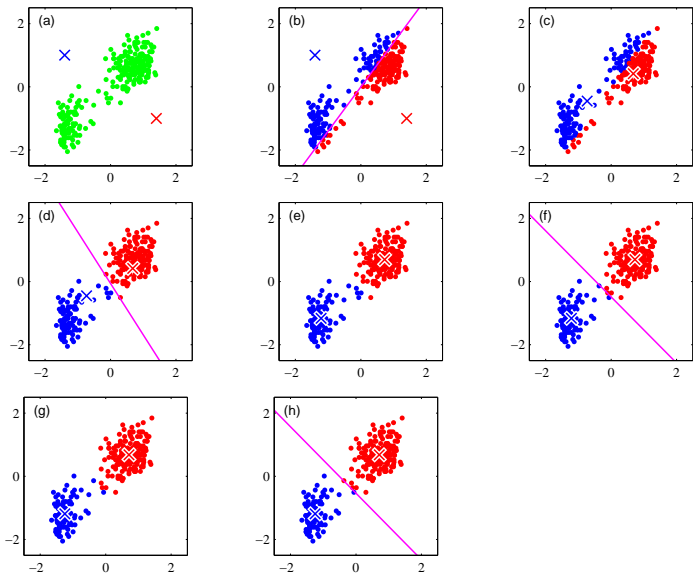
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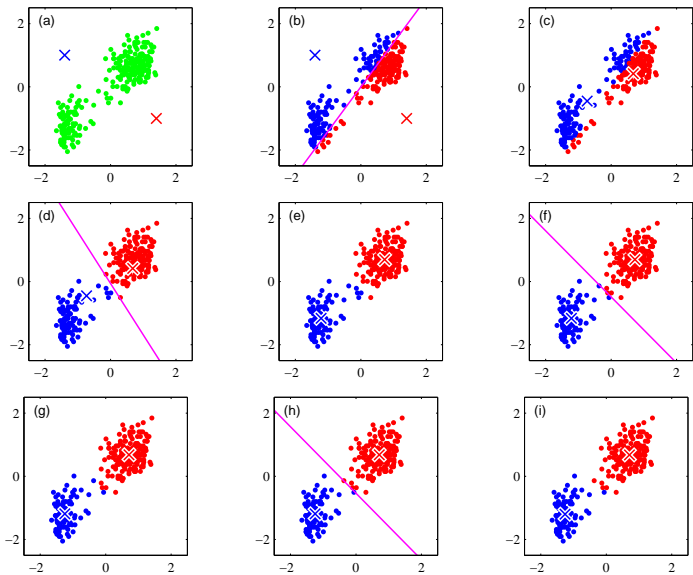
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Initialization matters for **convergence**.

Convergence

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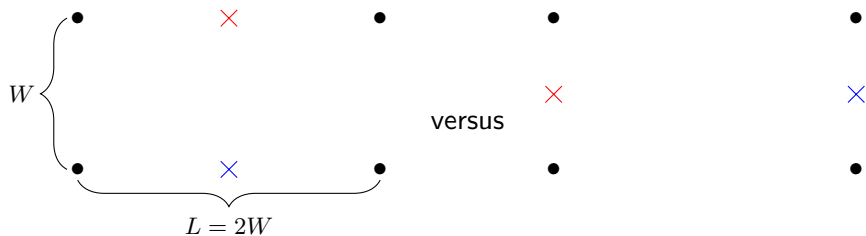
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- and it *might not converge to the global minimum* of the K-means objective

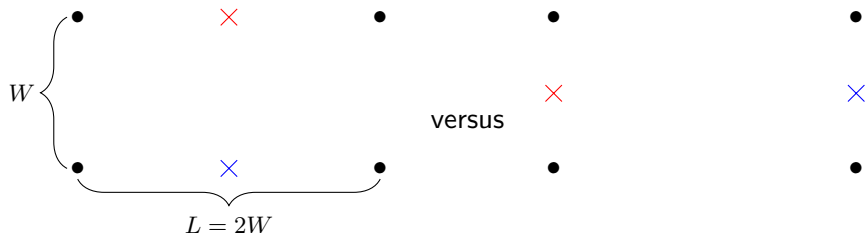
Local minimum v.s global minimum

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



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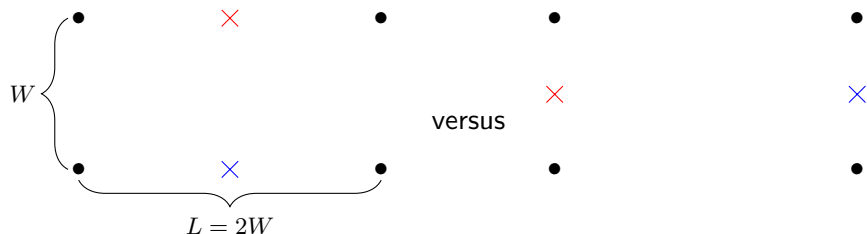
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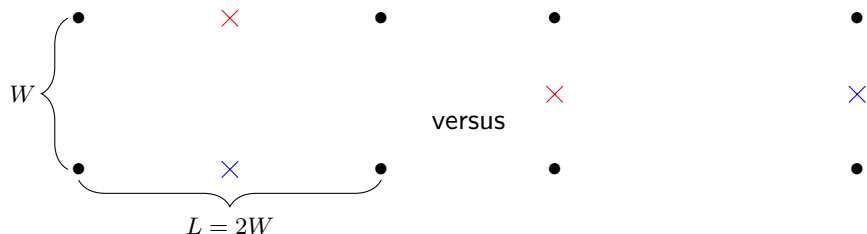


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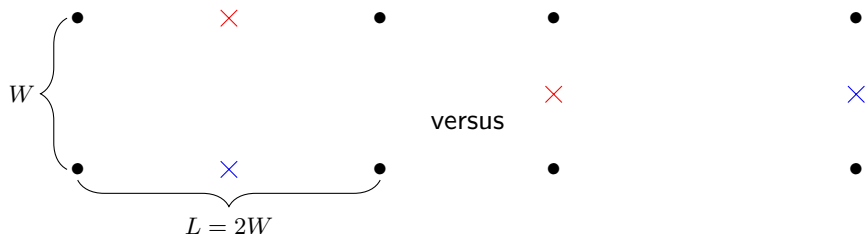


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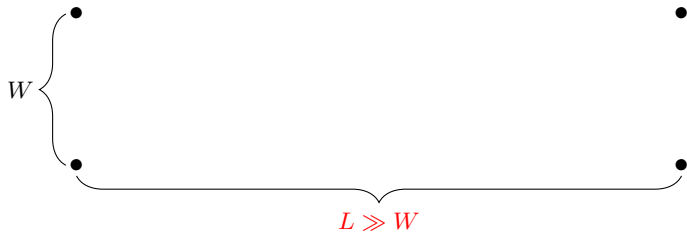
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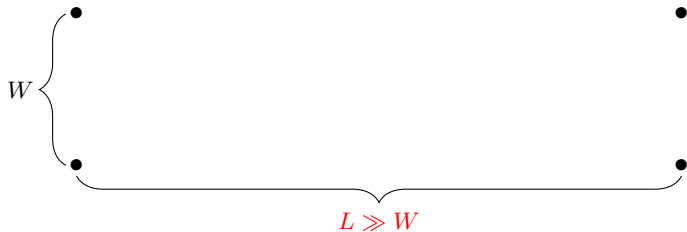
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- left has K-means objective $L^2 = 4W^2$
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- in fact, left is **local minimum**, and right is **global minimum**.

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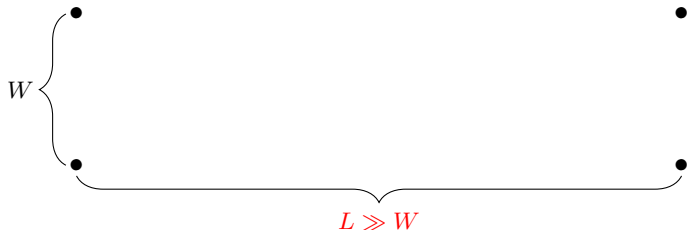


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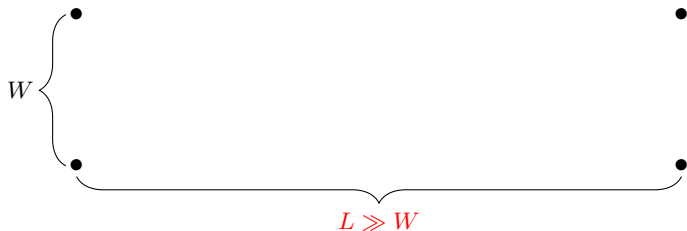
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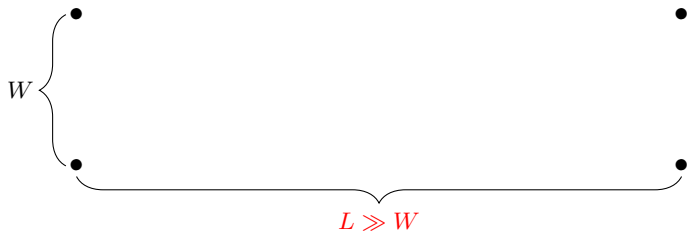
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- so *initialization matters a lot* for K-means

How common initialization methods perform?



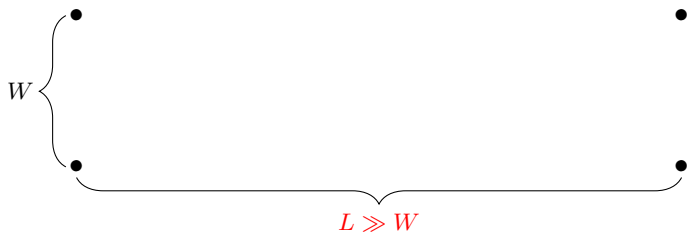
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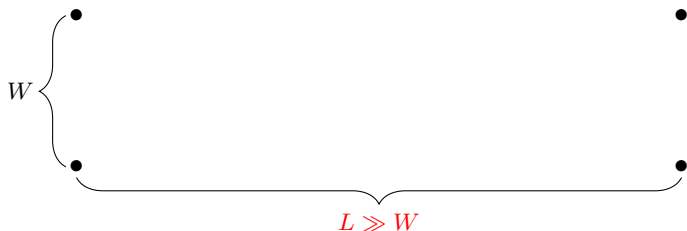
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- randomly pick K points as initial centers: fails with $1/3$ probability
- or randomly assign each point to a cluster, then average: similarly fail with a constant probability
- or more sophisticated approaches: **K-means++** *guarantees* to find a solution that in expectation is at most $O(\log K)$ times of the optimal

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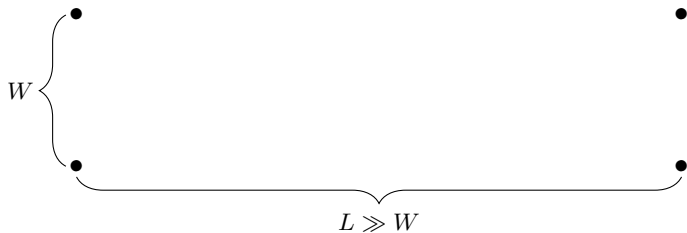
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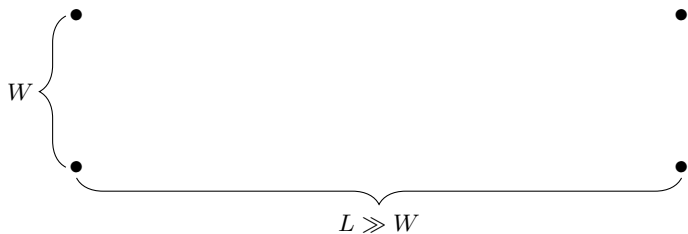
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Intuitively this *spreads out the initial centers*.

K-means++ on the same example

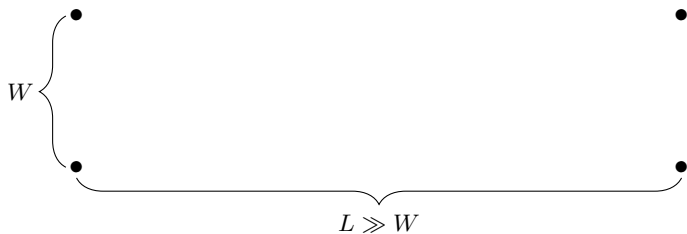


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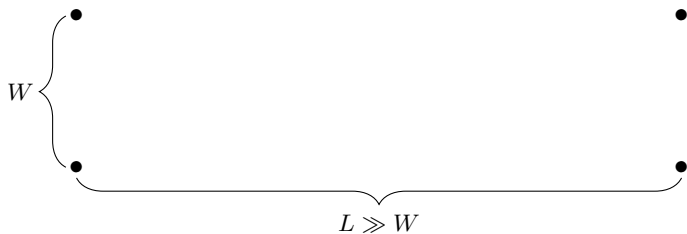
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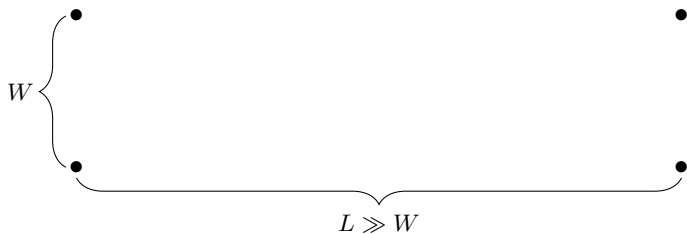
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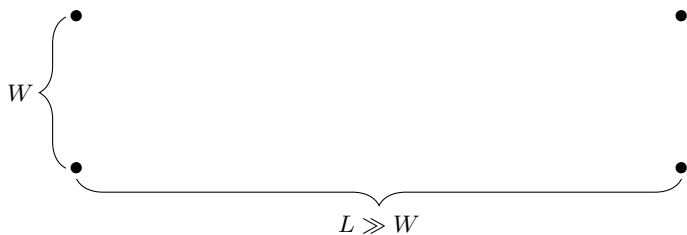
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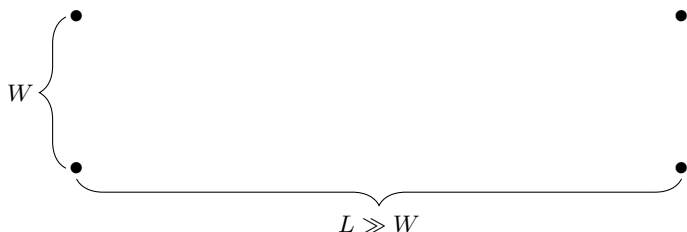
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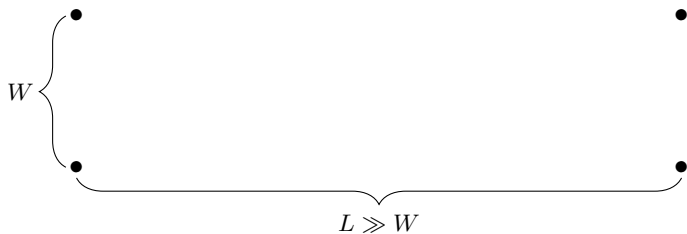
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that is, *at most 1.5 times of the optimal.*

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

- 1 Clustering
- 2 Gaussian mixture models
 - Motivation and Model
 - EM algorithm
 - EM applied to GMMs

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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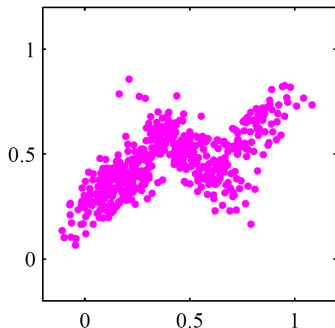
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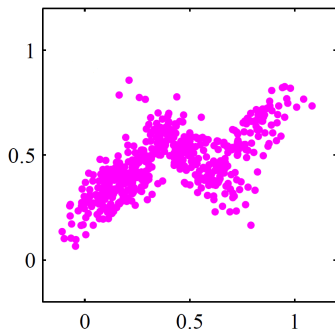
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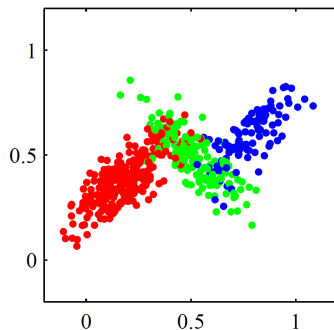
What probabilistic model generates data like this?



GMM: intuition

GMM is a natural model to explain such data

Assume there are 3 ground-truth
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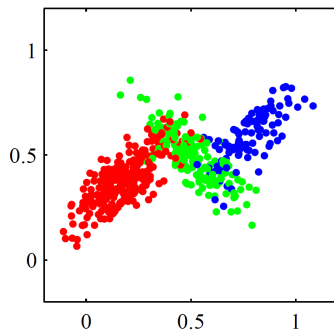


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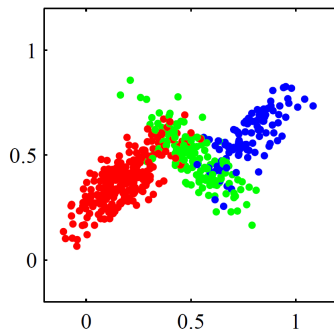


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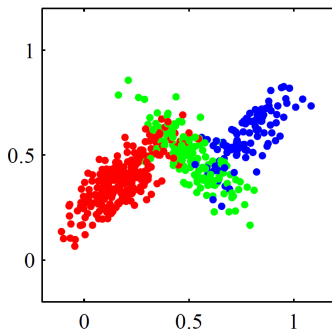


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Hence the name “**Gaussian mixture model**”.

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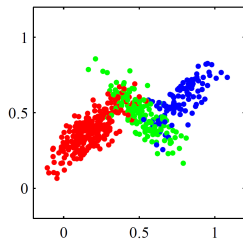
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\mathbf{x} and z are both random variables drawn from the model

- \mathbf{x} is **observed**
- z is **unobserved/latent**

An example



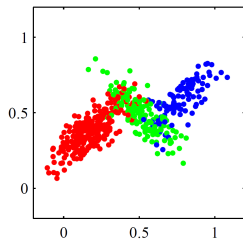
The conditional distributions are

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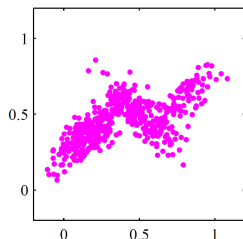


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$$p(\mathbf{x}) = p(\text{red})N(\mathbf{x} \mid \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1) + p(\text{blue})N(\mathbf{x} \mid \boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2) \\ + p(\text{green})N(\mathbf{x} \mid \boldsymbol{\mu}_3, \boldsymbol{\Sigma}_3)$$

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- both learn the cluster centers $\boldsymbol{\mu}_k$'s
- in addition, GMM learns cluster weight 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

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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

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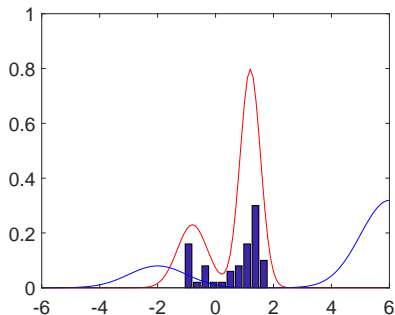
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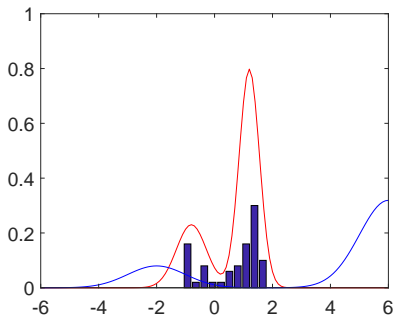
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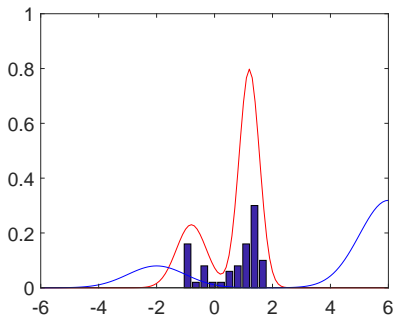
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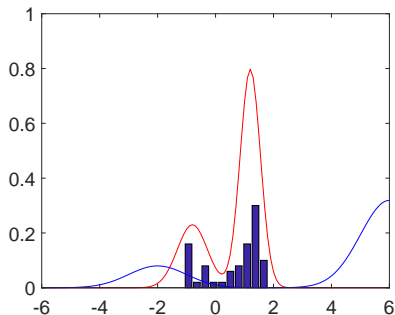
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EM_demo.pdf shows how the blue curve moves towards red curve quickly via EM

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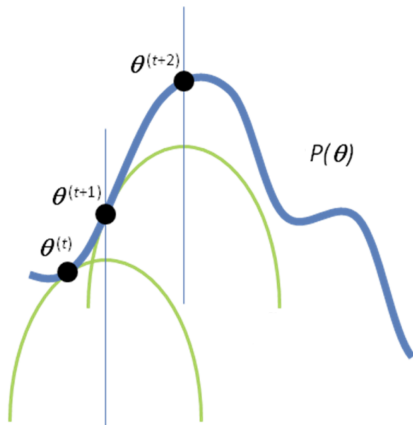
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Again, directly solving the objective is intractable.

High level idea

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



Derivation of EM

Finding the lower bound of P :

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

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

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 &\geq \mathbb{E}_{z \sim q} [\ln p(\mathbf{x}, z; \boldsymbol{\theta})] + H(q) - \ln \mathbb{E}_{z \sim q} \left[\frac{p(z|\mathbf{x}; \boldsymbol{\theta})}{q(z)} \right] && \text{(Jensen's inequality)}
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 &= \mathbb{E}_{z \sim q} [\ln p(\mathbf{x}, z; \boldsymbol{\theta})] + H(q)
 \end{aligned}$$

Alternatively maximize the lower bound

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

$$\begin{aligned} P(\boldsymbol{\theta}) &= \sum_{n=1}^N \ln p(\mathbf{x}_n ; \boldsymbol{\theta}) \\ &\geq \sum_{n=1}^N (\mathbb{E}_{z_n \sim q_n} [\ln p(\mathbf{x}_n, z_n ; \boldsymbol{\theta})] + H(q_n)) = F(\boldsymbol{\theta}, \{q_n\}) \end{aligned}$$

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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

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

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

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

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

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- $F(\boldsymbol{\theta}, \{q_n^{(t)}\}) \leq P(\boldsymbol{\theta})$ for all $\boldsymbol{\theta}$.

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

General EM algorithm

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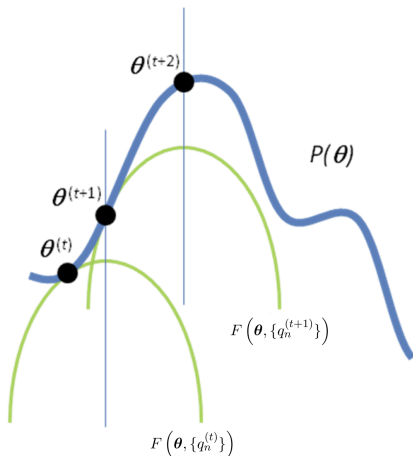
Step 2 (M-Step) update the model parameter via **Maximization**

$$\theta^{(t+1)} \leftarrow \underset{\theta}{\operatorname{argmax}} Q(\theta ; \theta^{(t)})$$

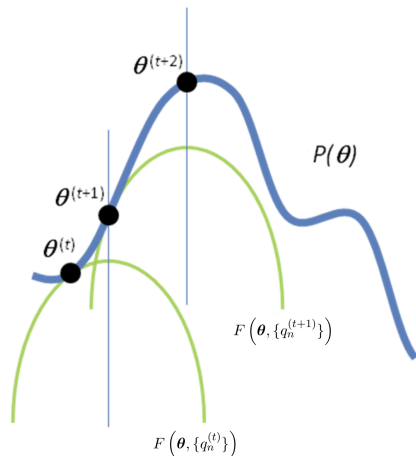
Step 3 $t \leftarrow t + 1$ and return to Step 1 if not converged

Pictorial explanation

$P(\theta)$ is non-concave, but $Q(\theta; \theta^{(t)})$ often is concave and easy to maximize.



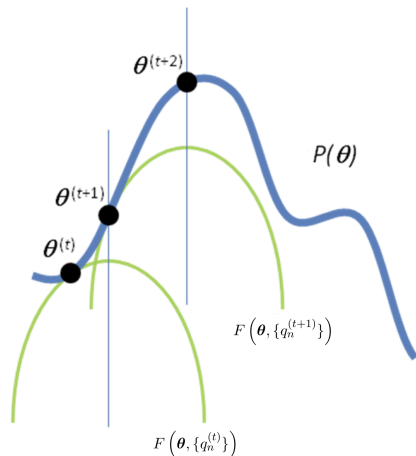
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$$P(\theta^{(t+1)}) \geq F(\theta^{(t+1)}; \{q_n^{(t)}\})$$

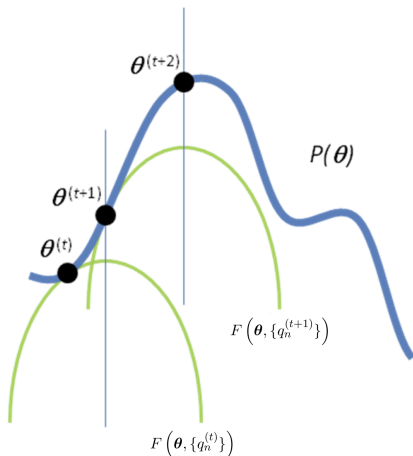
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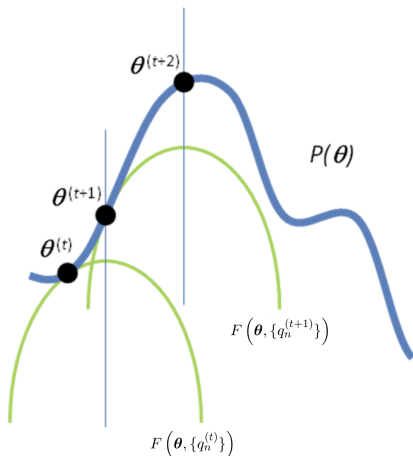
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 &\geq F\left(\theta^{(t)}; \{q_n^{(t)}\}\right) \\
 &= P(\theta^{(t)})
 \end{aligned}$$

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:

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

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This computes the “soft assignment” $\gamma_{nk} = q_n^{(t)}(z_n = k)$, i.e. conditional probability of \mathbf{x}_n belonging to cluster k .

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M-Step:

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

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 &= \operatorname{argmax}_{\{\omega_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}} \sum_{n=1}^N \sum_{k=1}^K \gamma_{nk} (\ln \omega_k + \ln N(\mathbf{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k))
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To find $\omega_1, \dots, \omega_K$, solve

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To find $\omega_1, \dots, \omega_K$, 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

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

M-Step (continued)

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

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

i.e. (weighted) fraction of examples belonging to cluster k

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You will verify some of these in HW4.

Putting it together

EM for learning GMMs:

Step 0 Initialize $\omega_k, \mu_k, \Sigma_k$ for each $k \in [K]$

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

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

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

Putting it together

EM for learning GMMs:

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

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

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

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

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

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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.