CSCI567 Machine Learning (Fall 2025)

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Administration

Exam 1 grading still ongoing.

HW3 will be available after today's lecture.

Outline

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Unsupervised learning

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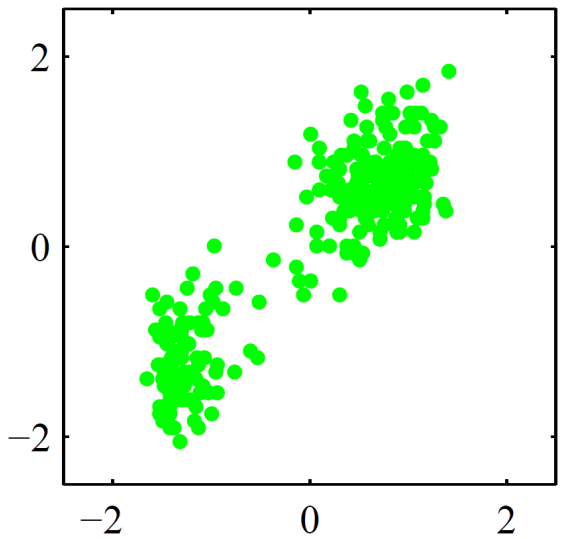
Today's focus: **clustering**, a canonical unsupervised learning problem

Clustering: informal definition

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



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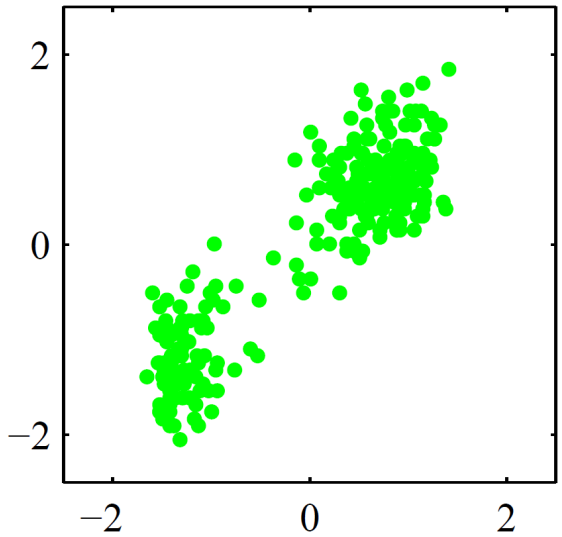

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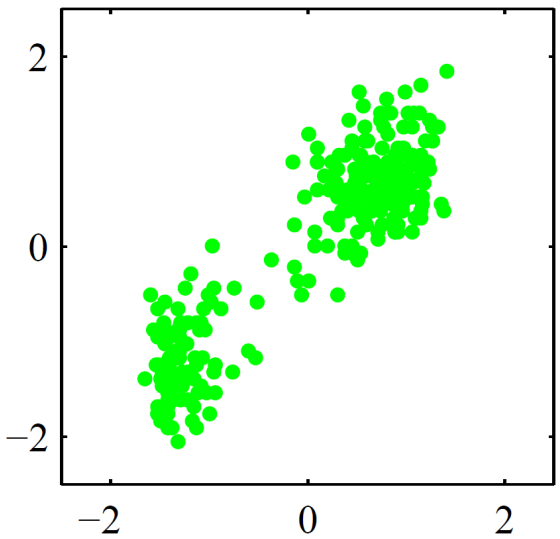
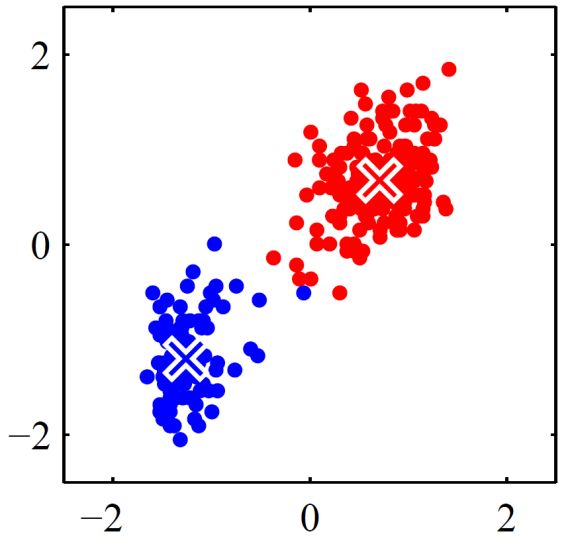
- assign each point to a specific cluster
- find the center (representative/prototype/...) of each cluster





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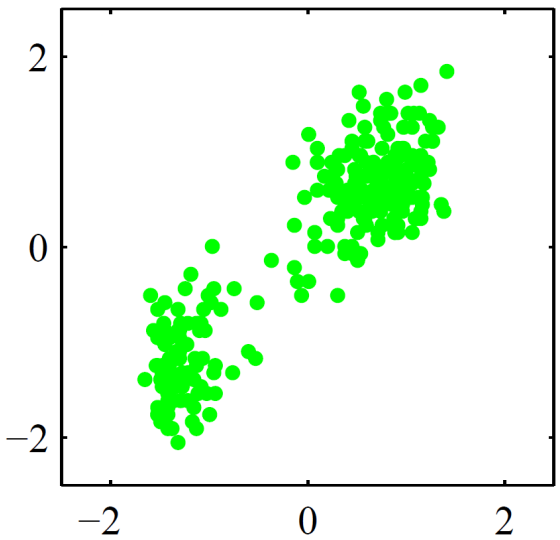
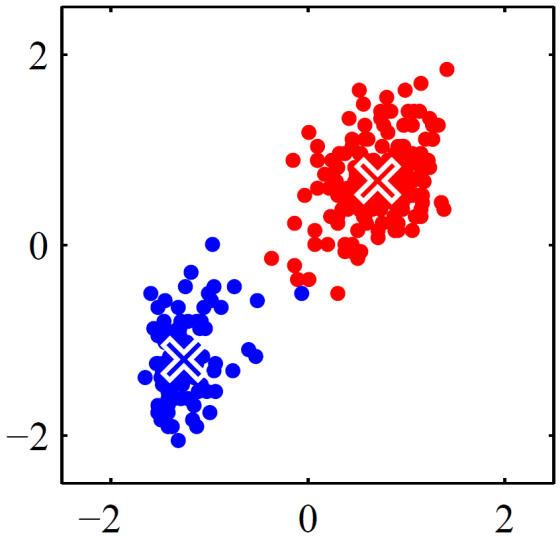
Given: data points $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N \in \mathbb{R}^{\mathsf{D}}$





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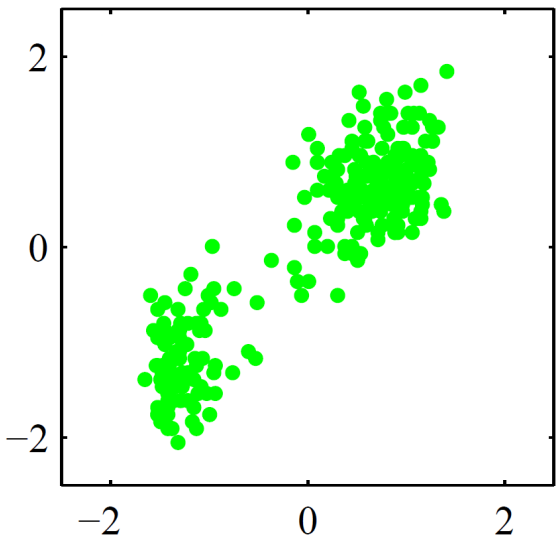

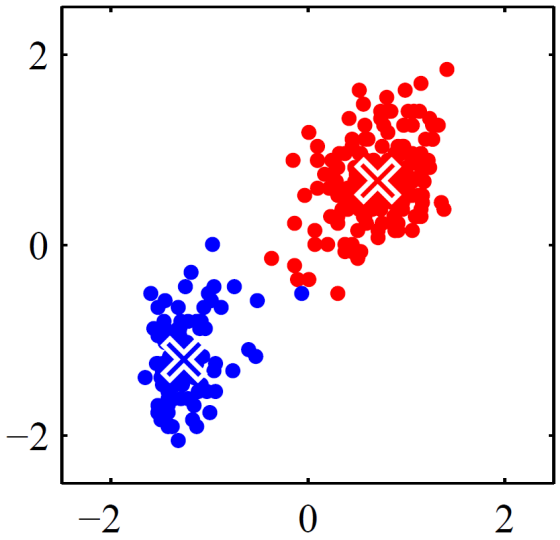

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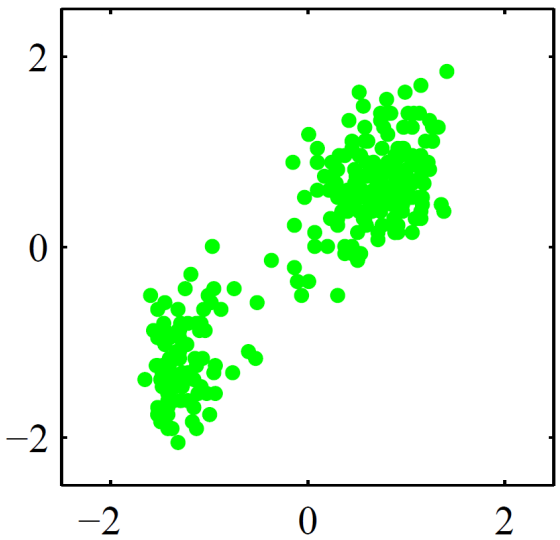
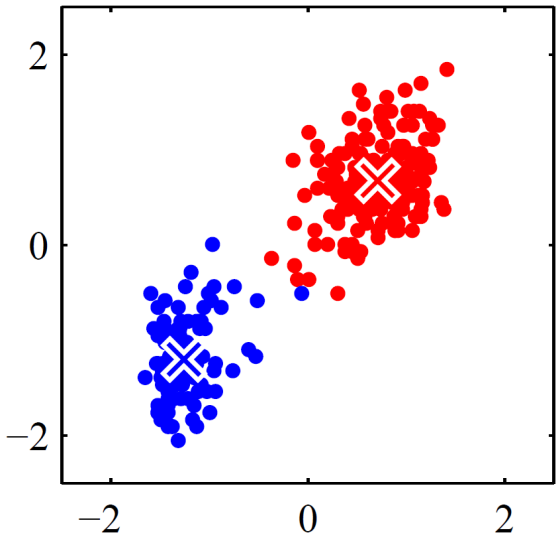
- find assignment $\gamma_{nk} \in \{0, 1\}$ for each data point $n \in [N]$ and $k \in [K]$ s.t. $\sum_{k \in [K]} \gamma_{nk} = 1$ for any fixed n





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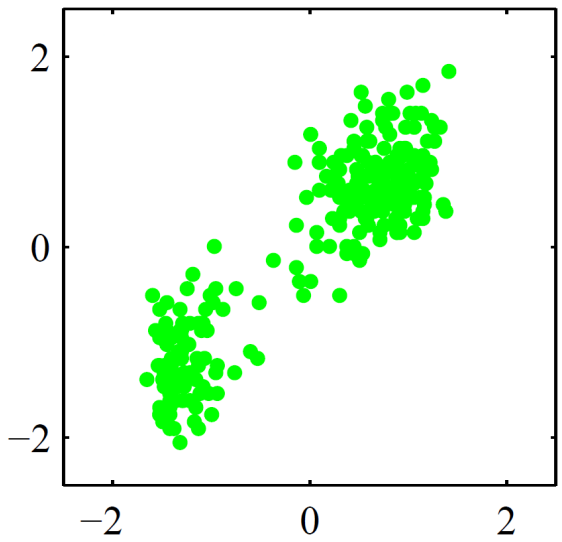
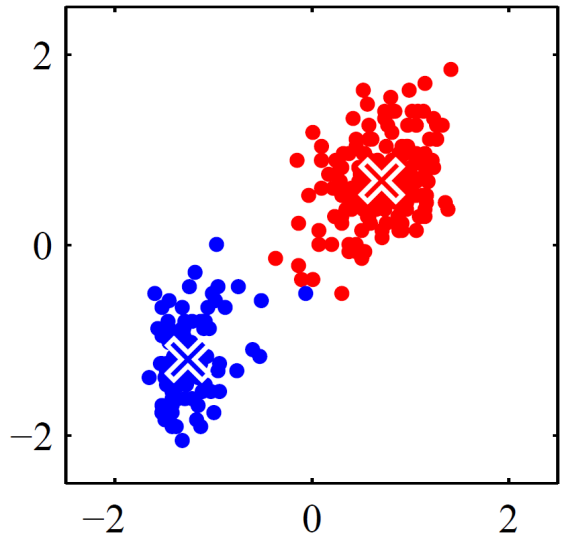
- find the cluster centers $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K \in \mathbb{R}^{\mathsf{D}}$





Many applications

- recognize communities in a social network
- group similar customers in market research
- grouping documents into different topics
- image segmentation
- identifying groups of genes with similar expression patterns
- 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 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

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

$$\gamma_{nk} = \begin{cases} 1, & \text{if } k = \operatorname{argmin}_c \|\boldsymbol{x}_n - \boldsymbol{\mu}_c\|_2^2 \\ 0, & \text{else} \end{cases}$$

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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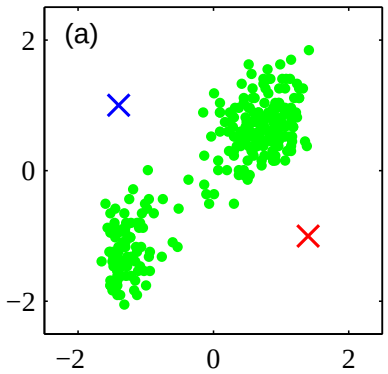

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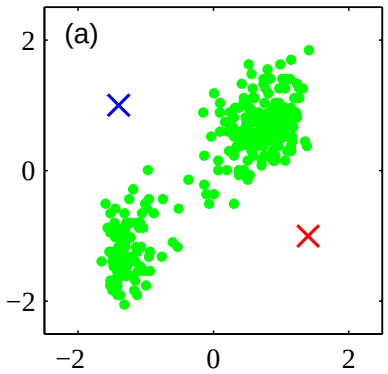

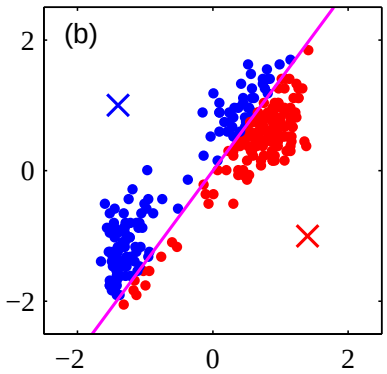

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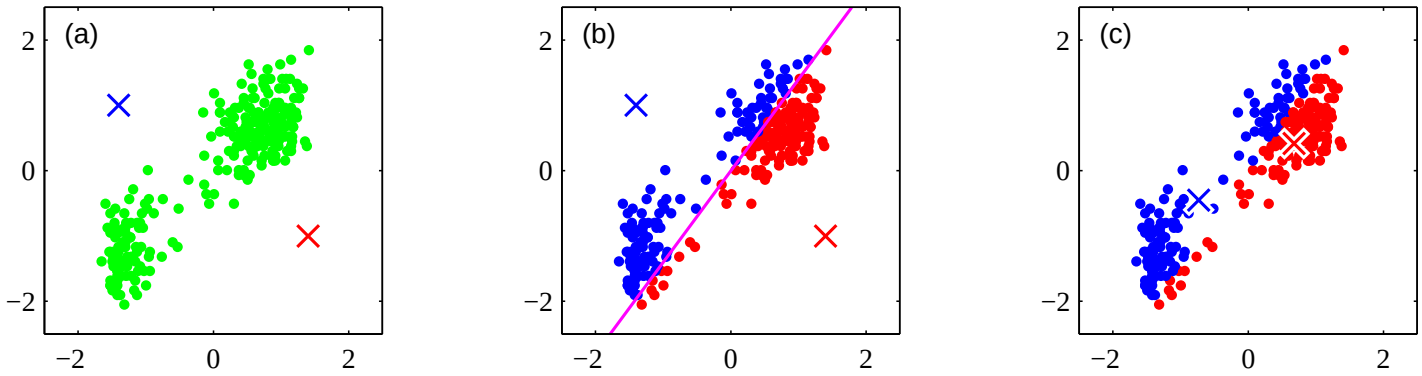

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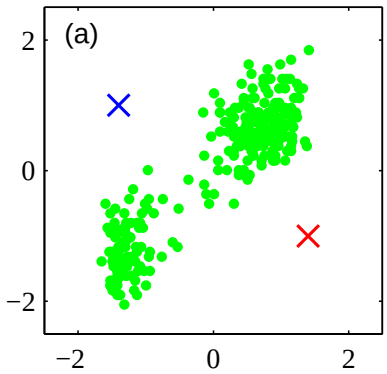

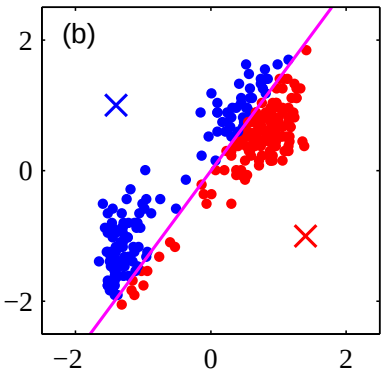

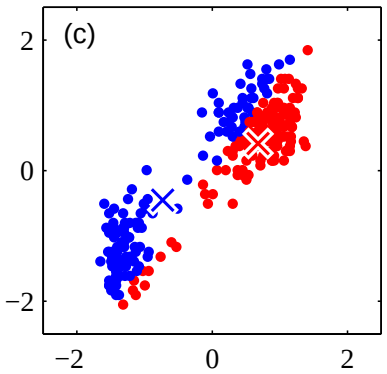

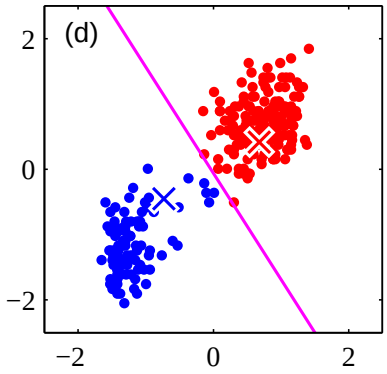

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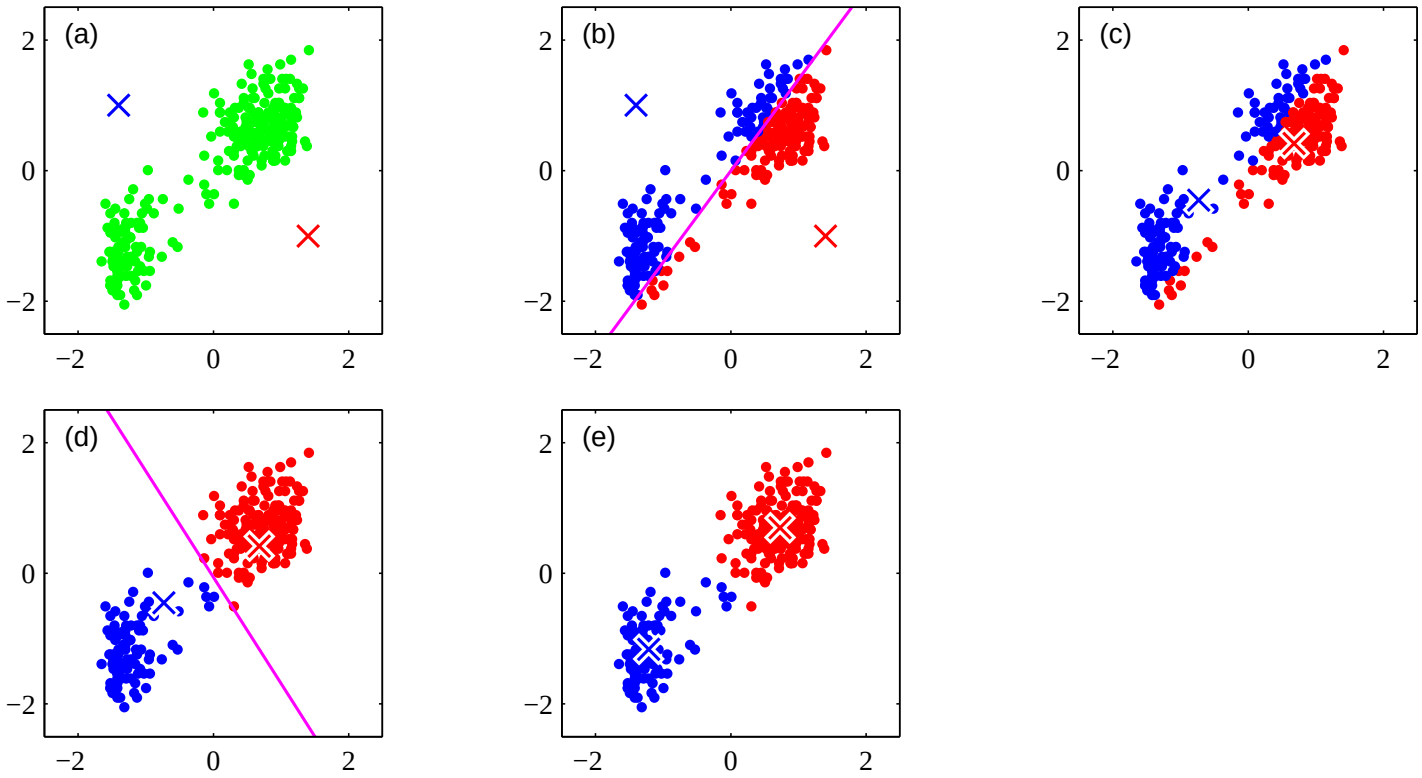

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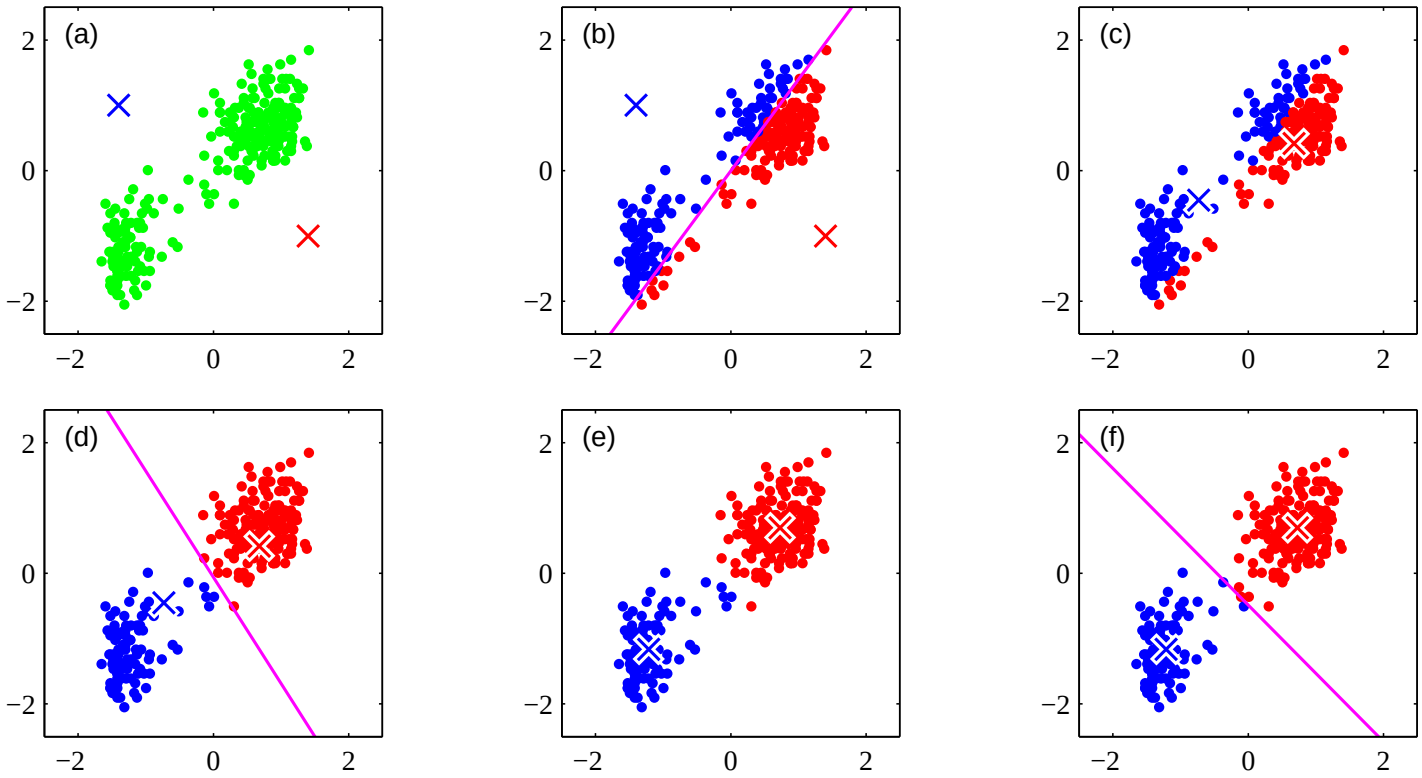

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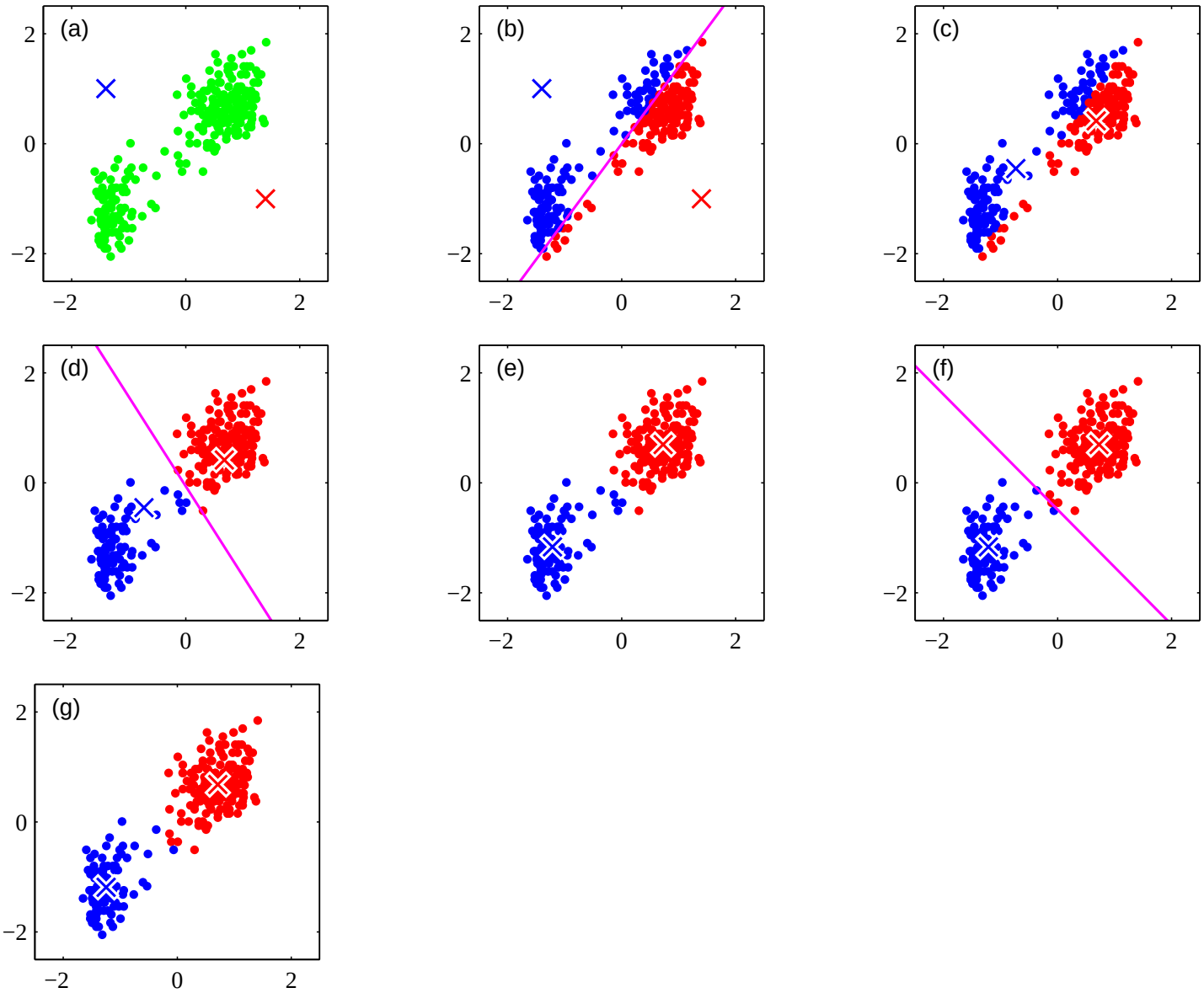

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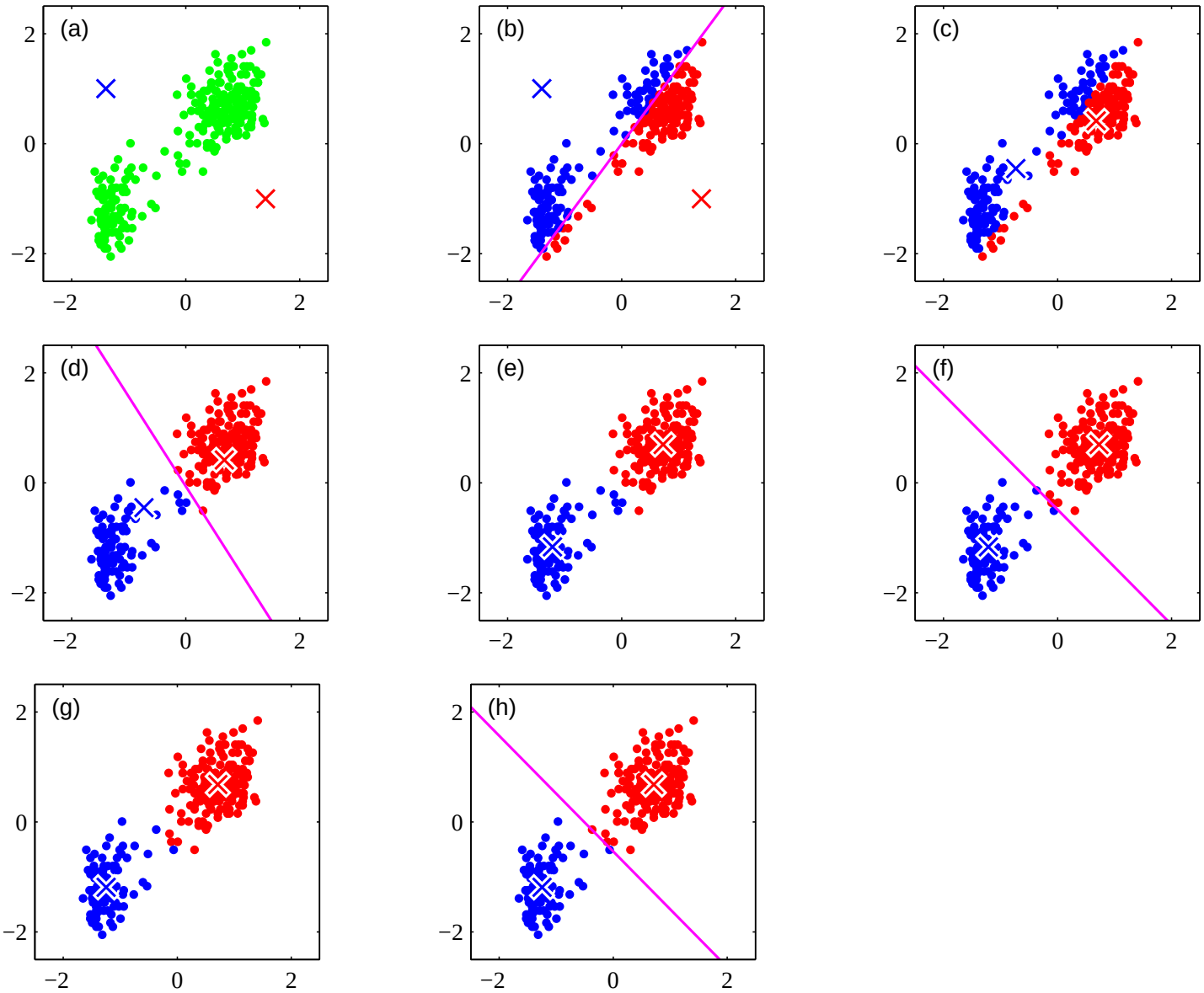

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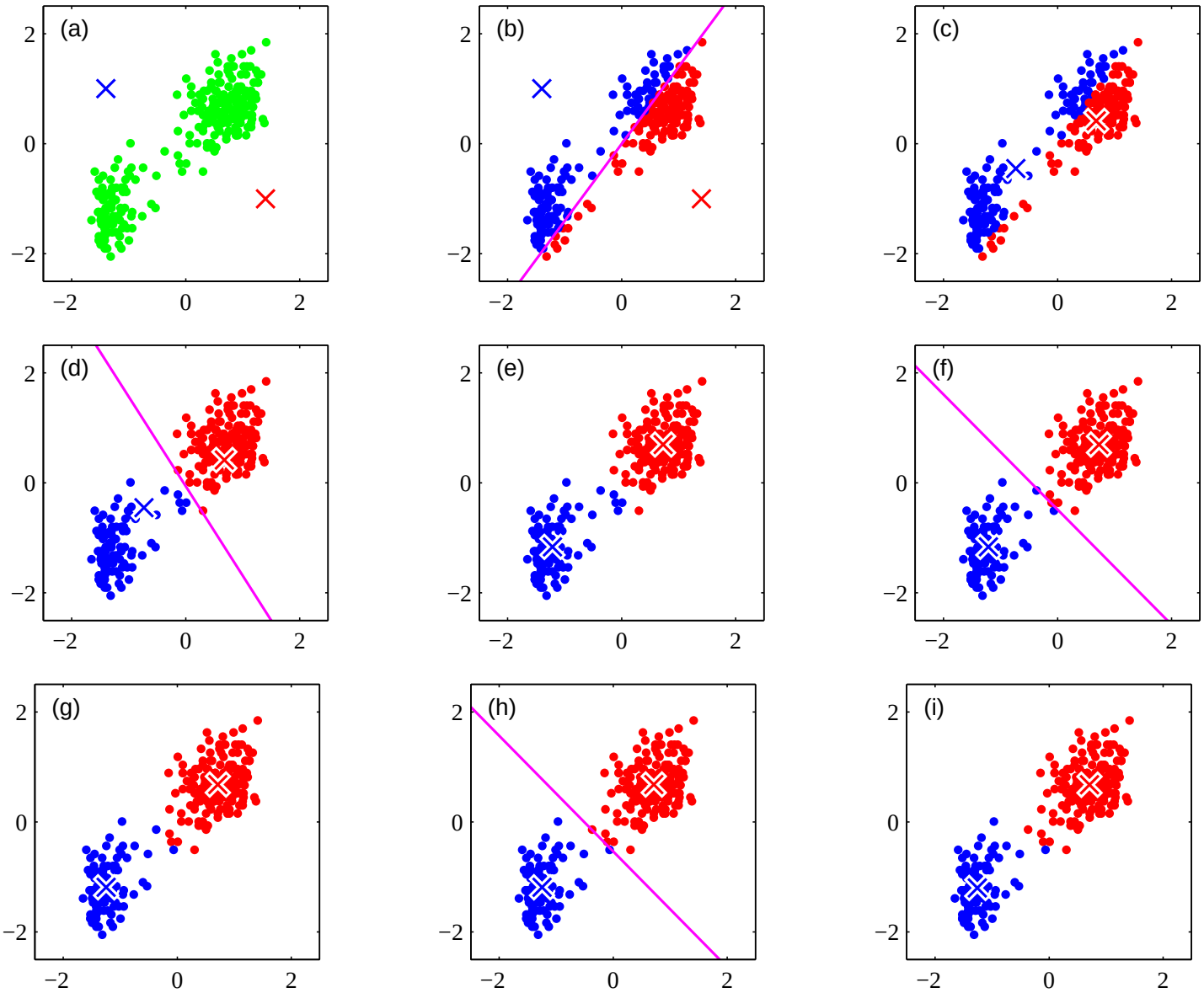

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Initialization matters for **convergence**.

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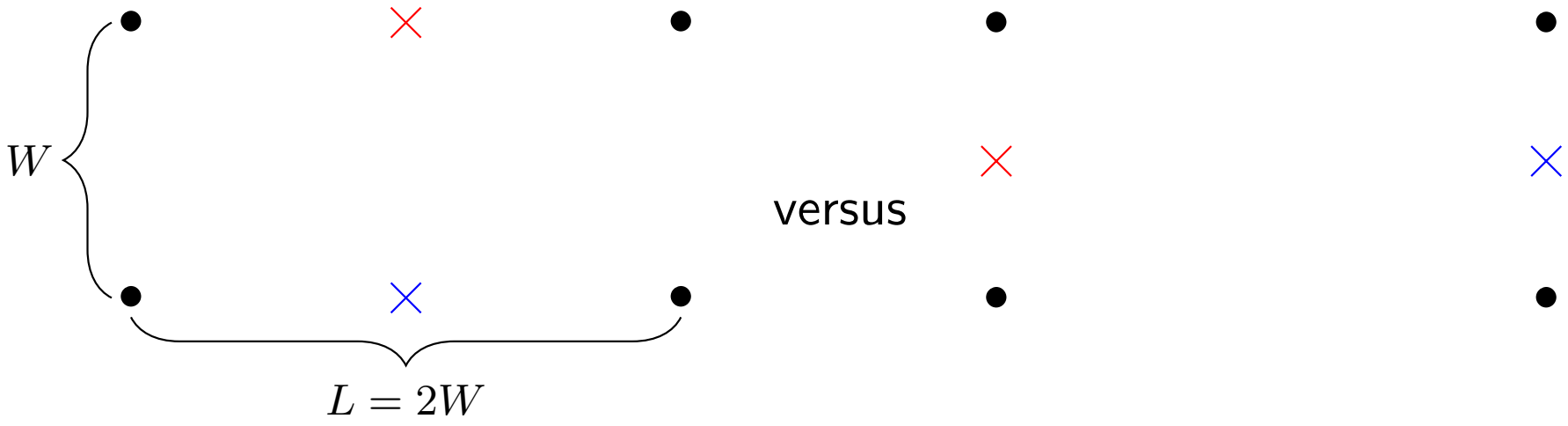
- and it *might not converge to the global minimum* of the K-means objective

Local minimum v.s global minimum

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



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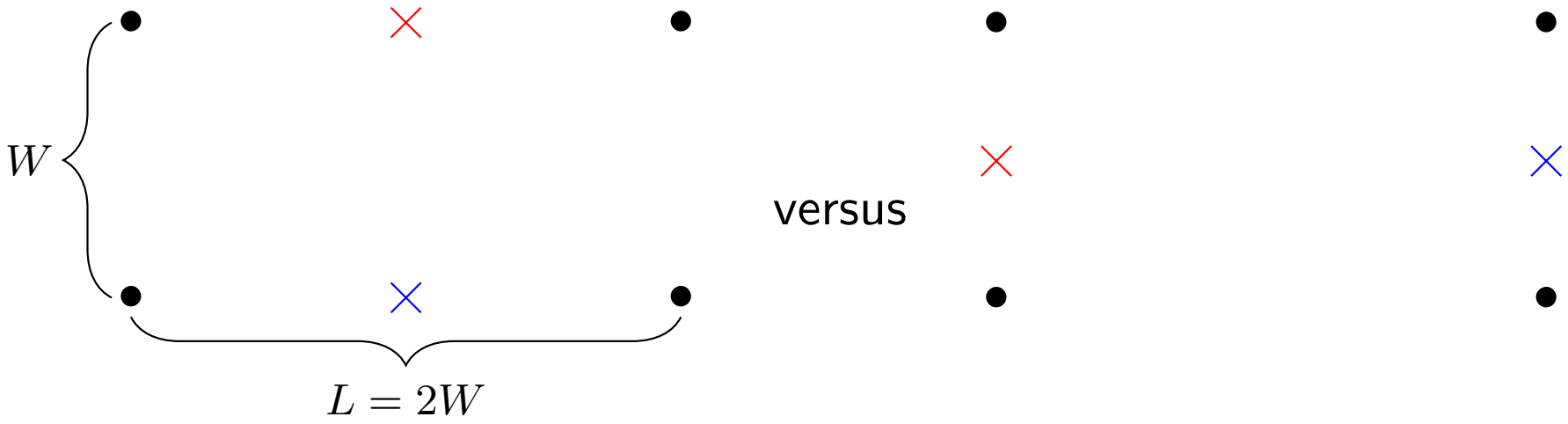

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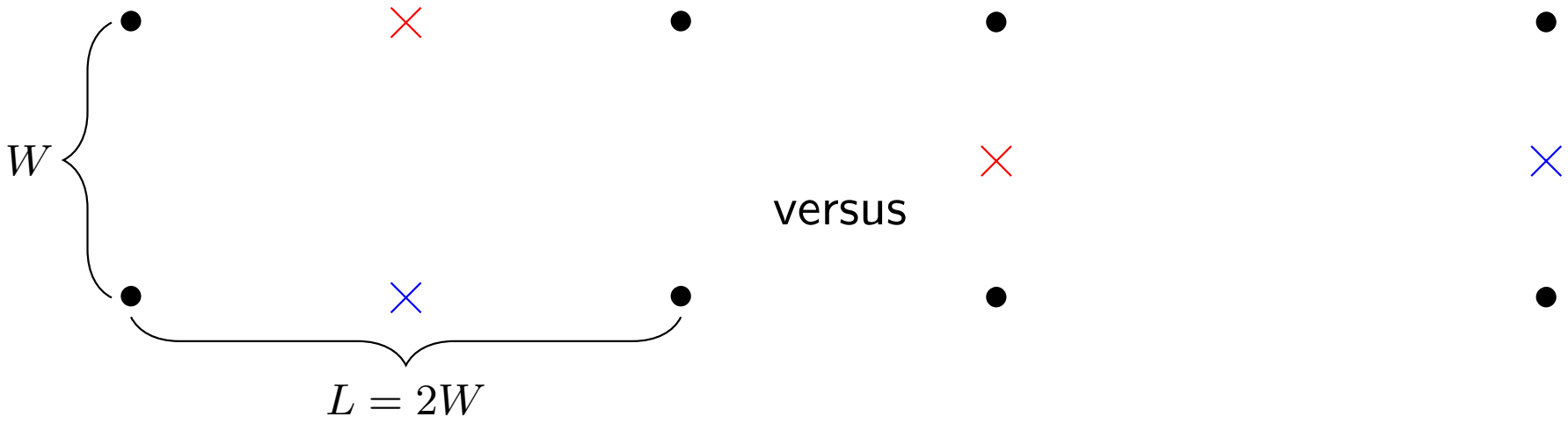

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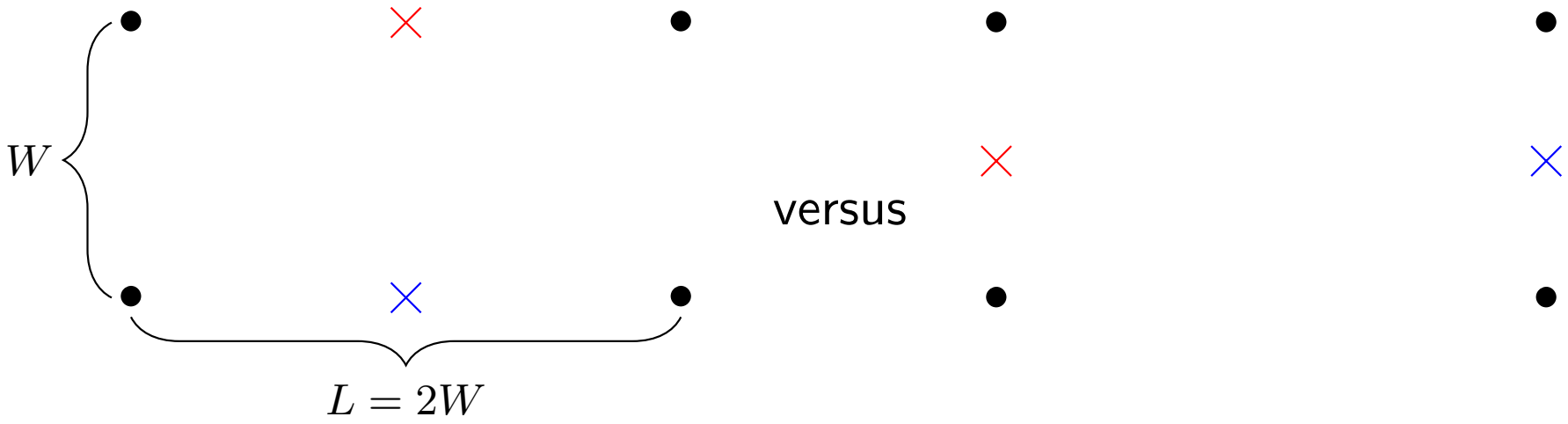

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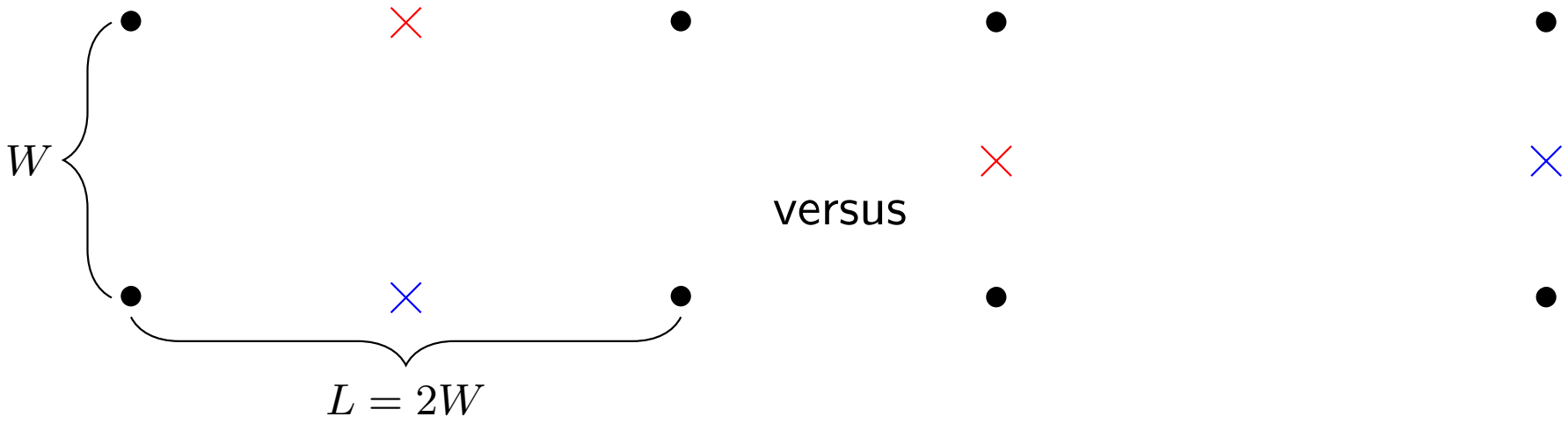

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- in fact, left is **local minimum**, and right is **global minimum**.

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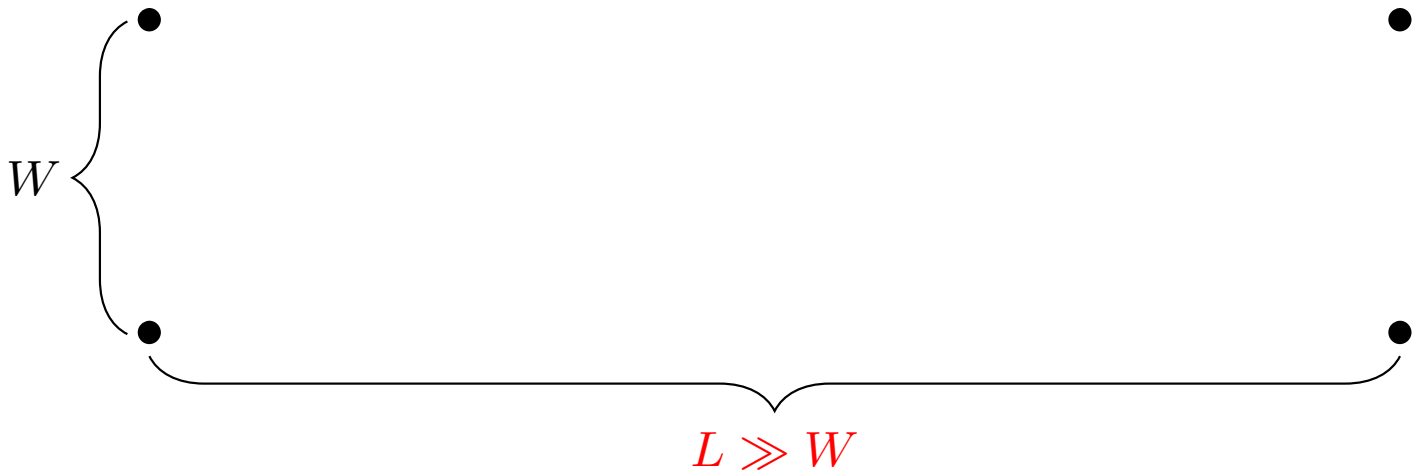

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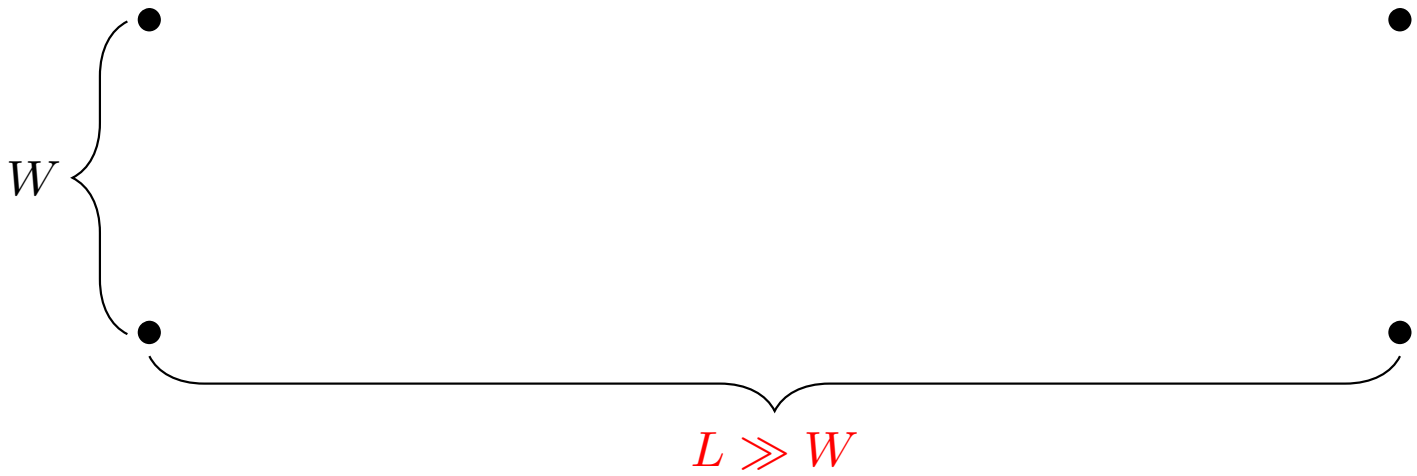

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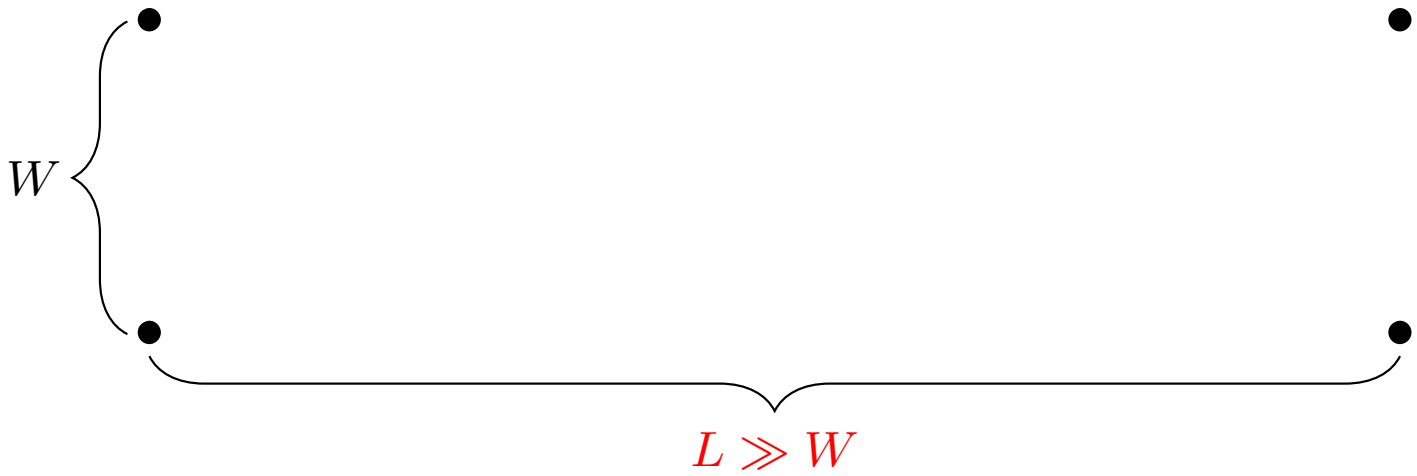
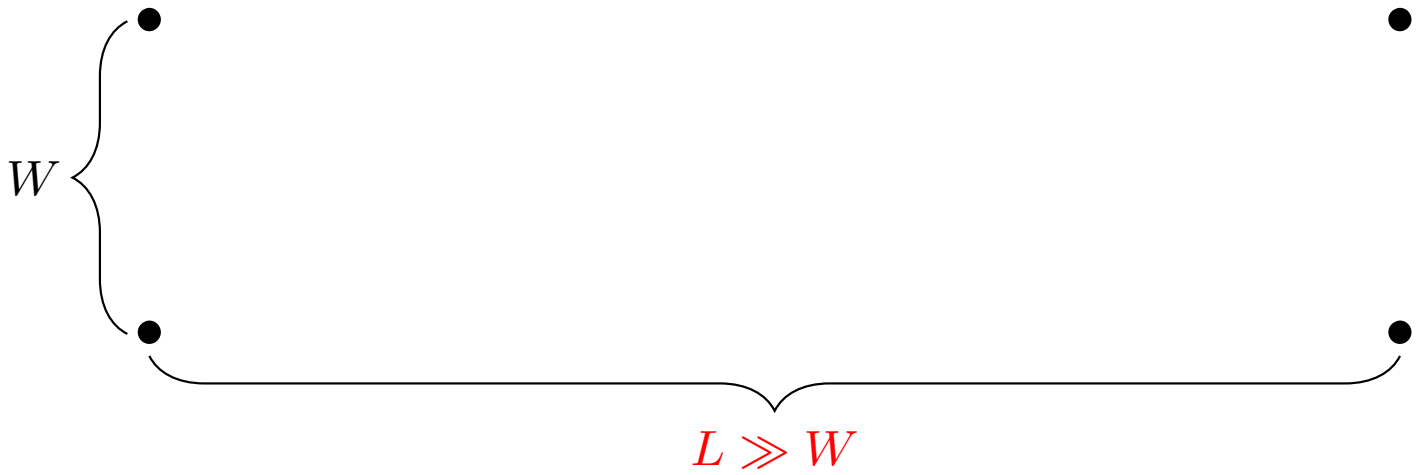


- moreover, local minimum can be *arbitrarily worse* if we increase L
- so *initialization matters a lot* for K-means

How common initialization methods perform?



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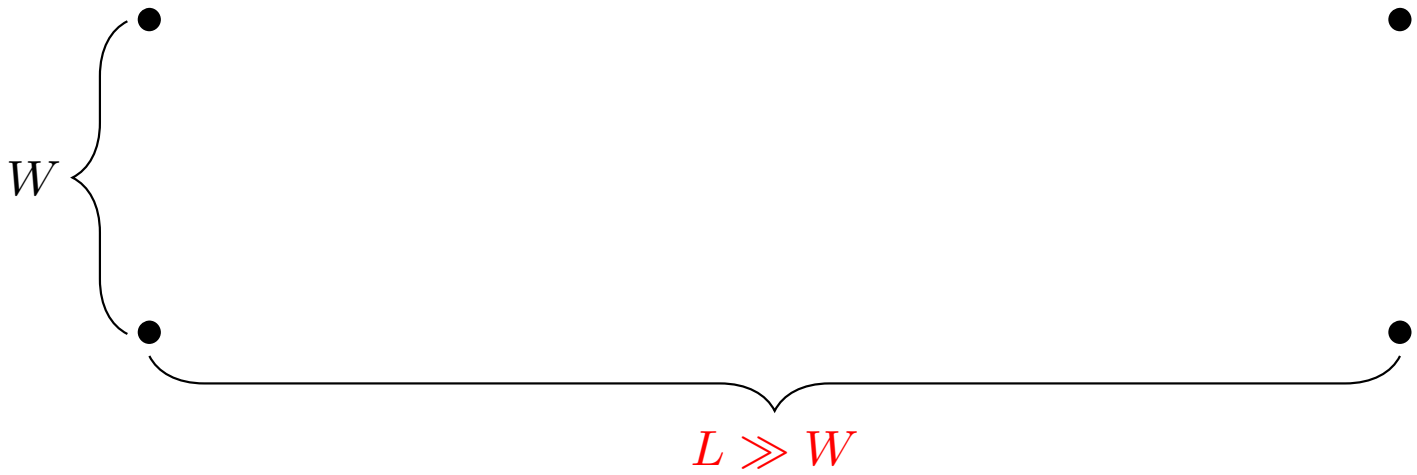

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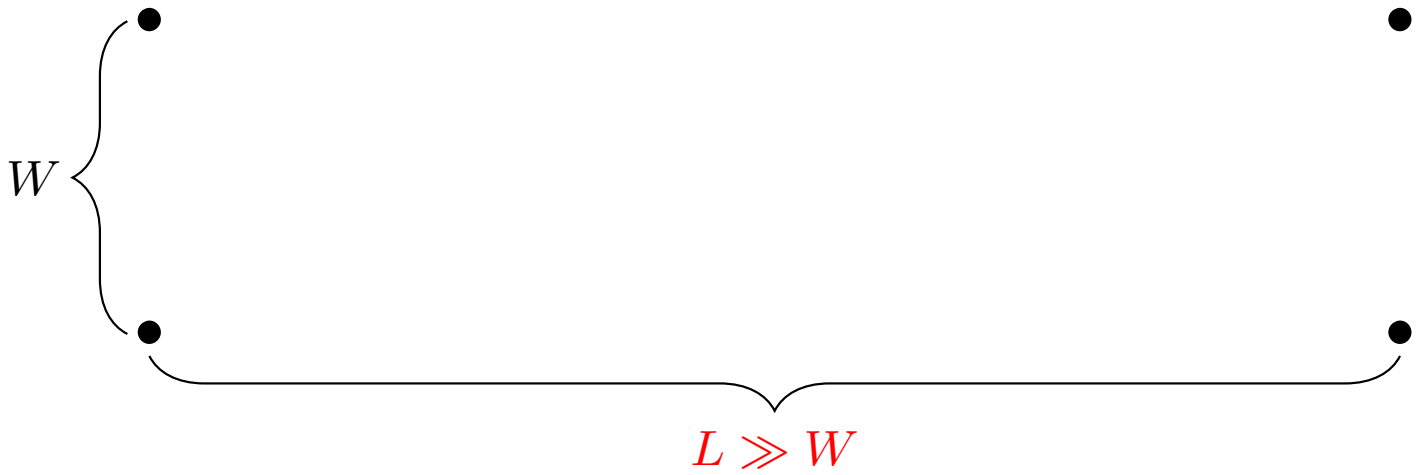

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An Intuitive and Greedy Approach

Idea: *spread out the initial centers*

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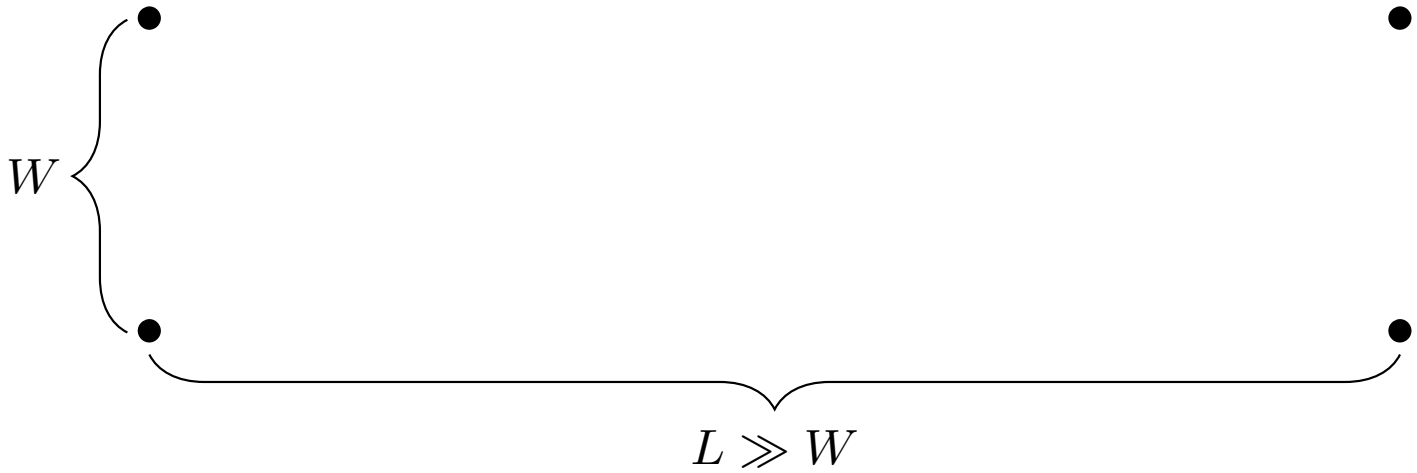
Start with a random data point as the first center $\boldsymbol{\mu}_1$

For $k = 2, \ldots, K$

- let the k-th center $\boldsymbol{\mu}_k$ be the farthest from the chosen centers:

$$\boldsymbol{\mu}_k = \underset{\boldsymbol{x} \in \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\}}{\operatorname{argmax}} \min_{j=1,\ldots,k-1} \|\boldsymbol{x} - \boldsymbol{\mu}_j\|_2^2$$

Greedy initialization on the same example



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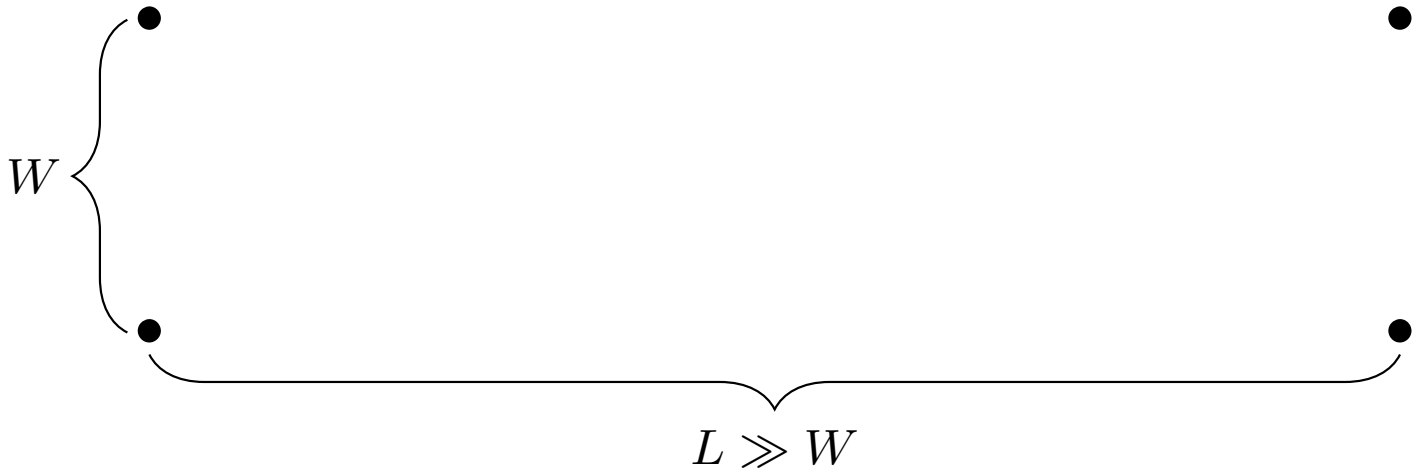

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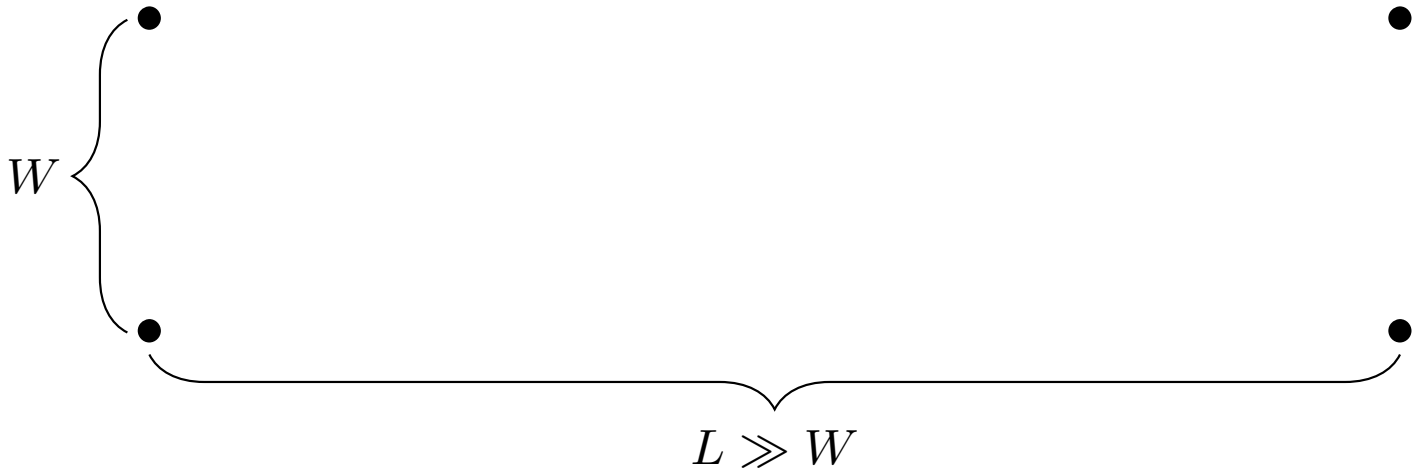

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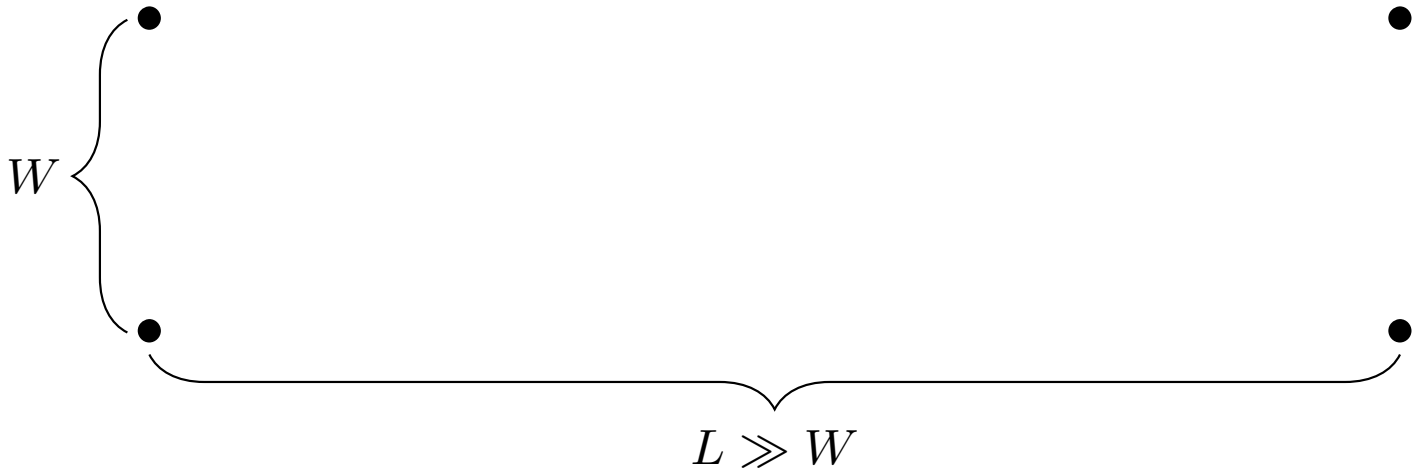

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See demo at `https://www.naftaliharris.com/blog/visualizing-k-means-clustering/`.

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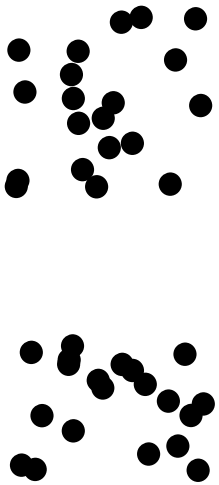

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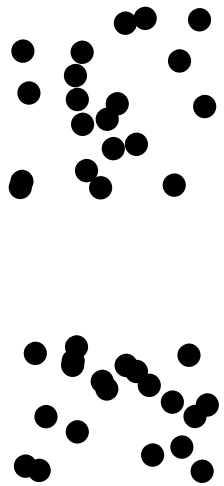

• outlier

In HW3, you will verify that greedy initialization can also lead to *arbitrarily bad* local minimums.

Solution: K-means++

K-means++: robustify the greedy approach via **randomness**

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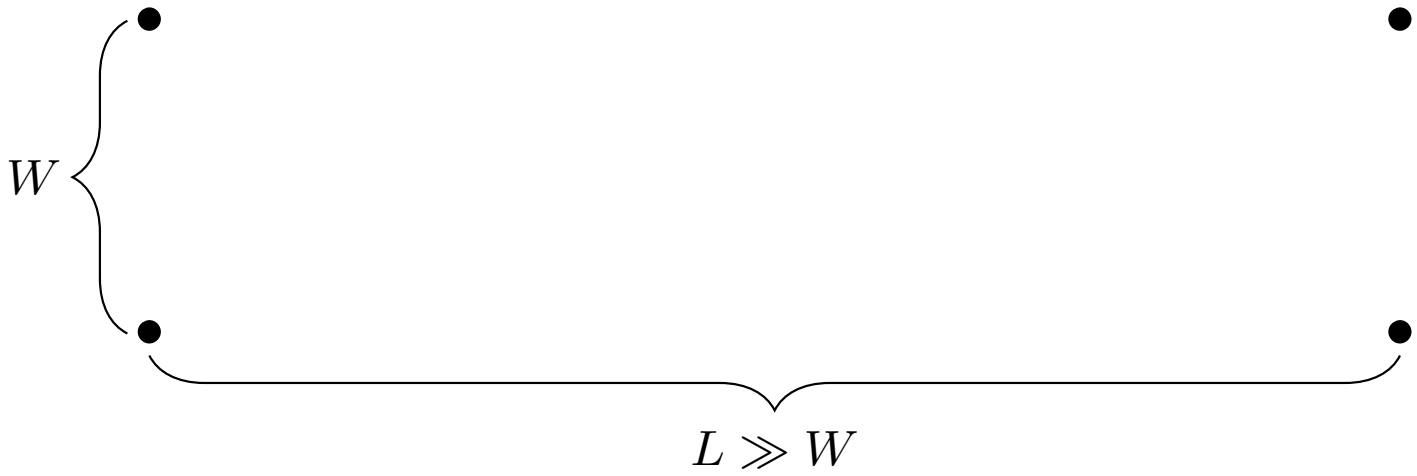
K-means++ *guarantees* to find a solution that in expectation is at most $O(\log K)$ times of the global optimal.

K-means++ on the same example



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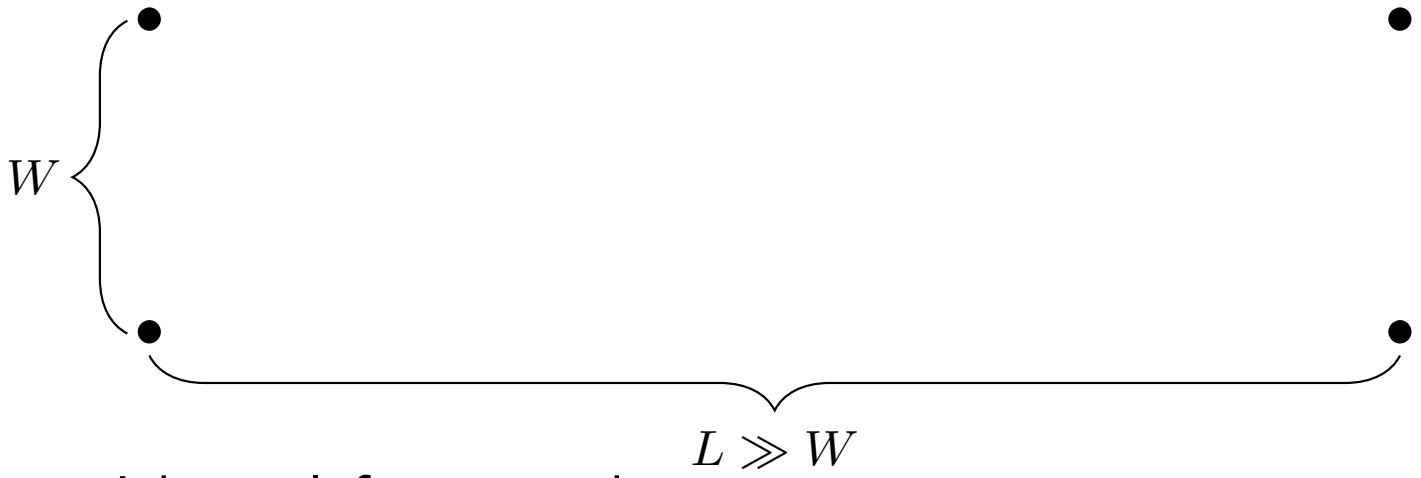

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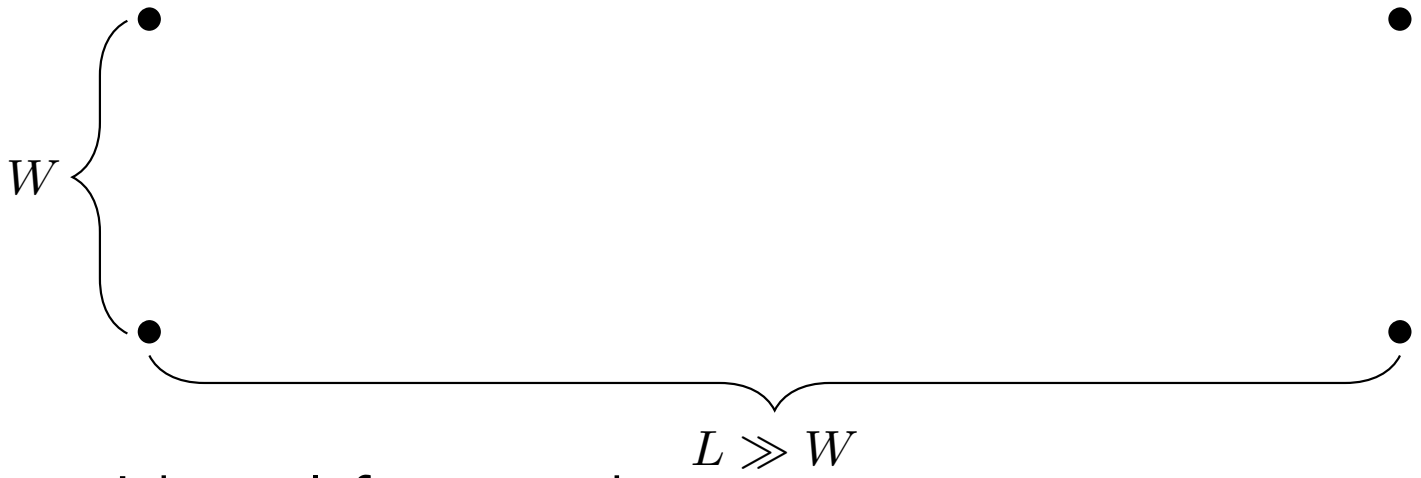

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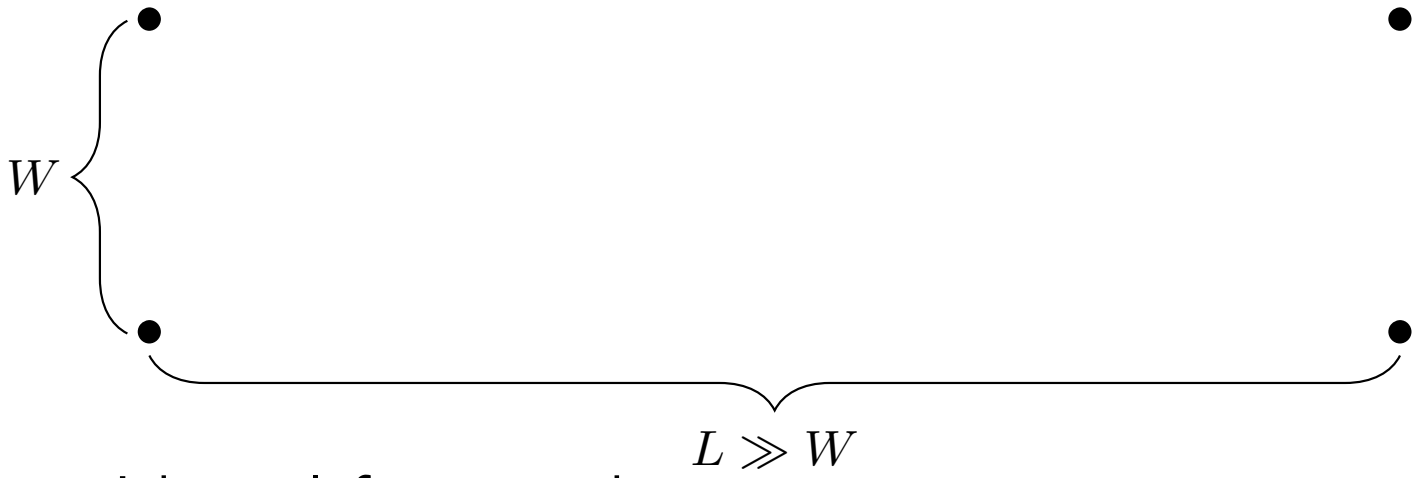

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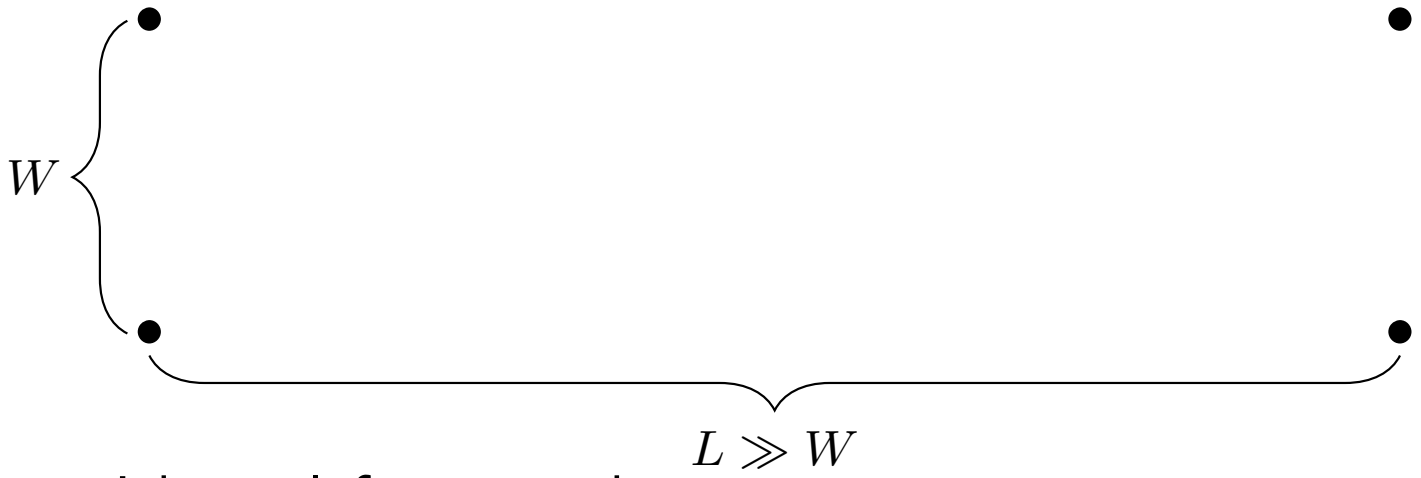

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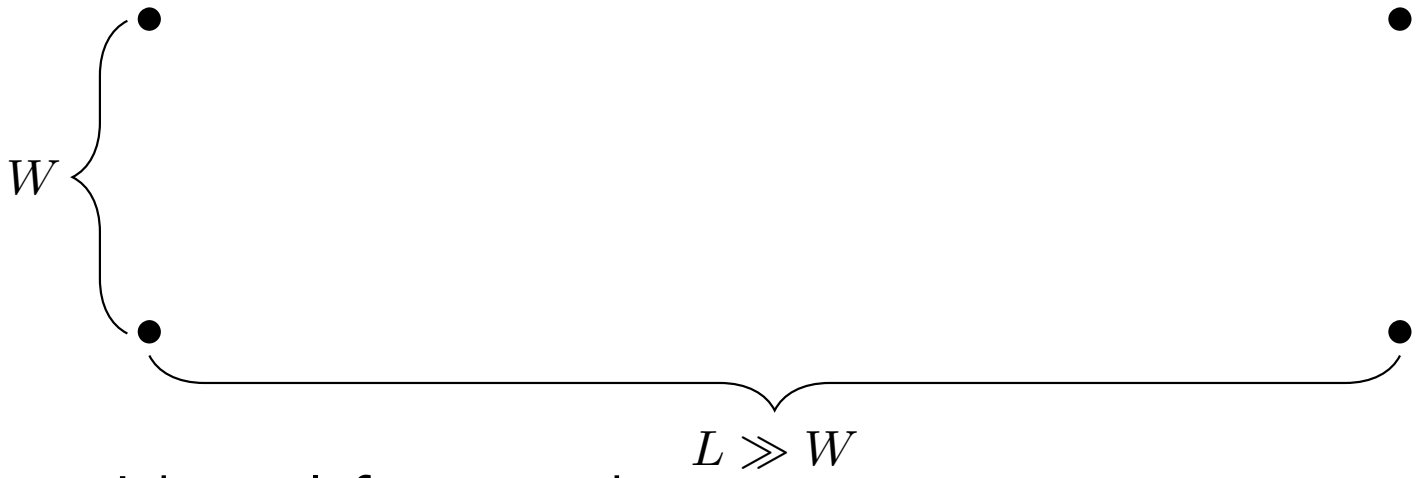

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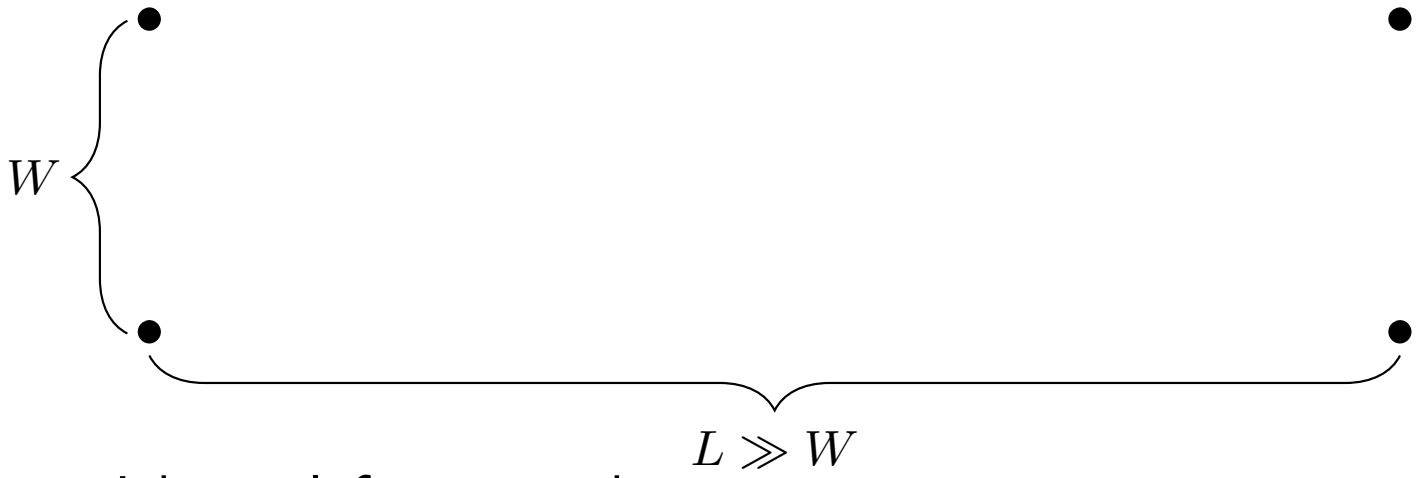

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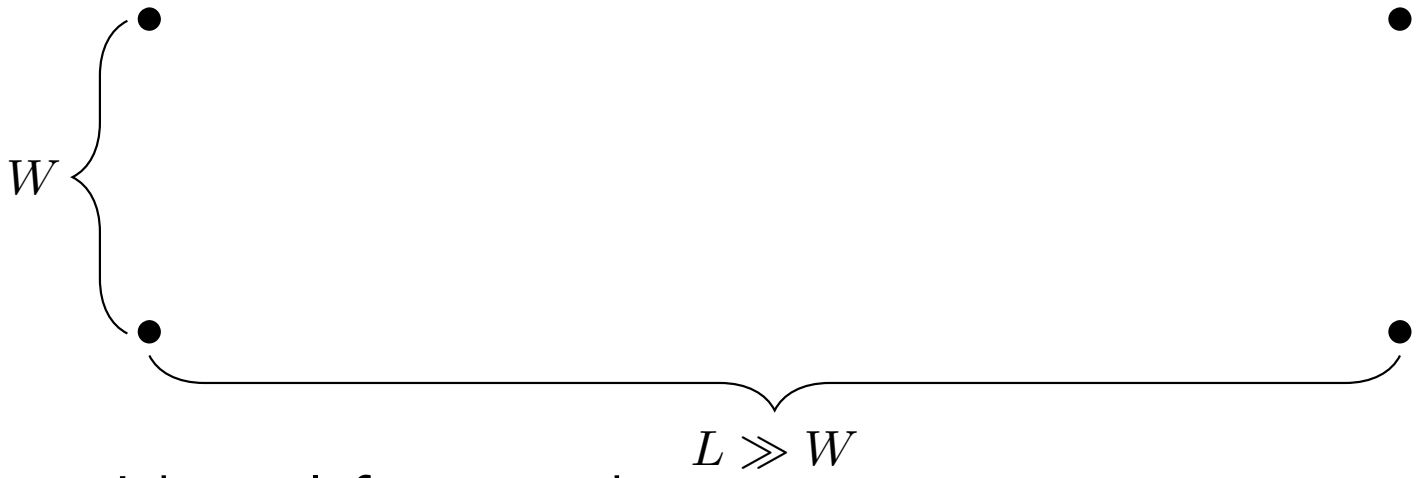

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that is, *at most 1.5 times of the optimal*.

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

Gaussian mixture models (GMM) is a probabilistic approach for clustering

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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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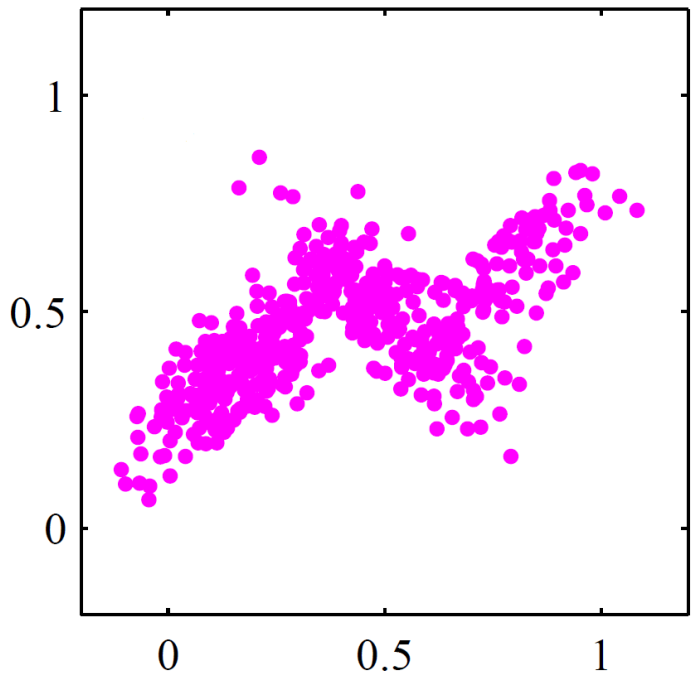

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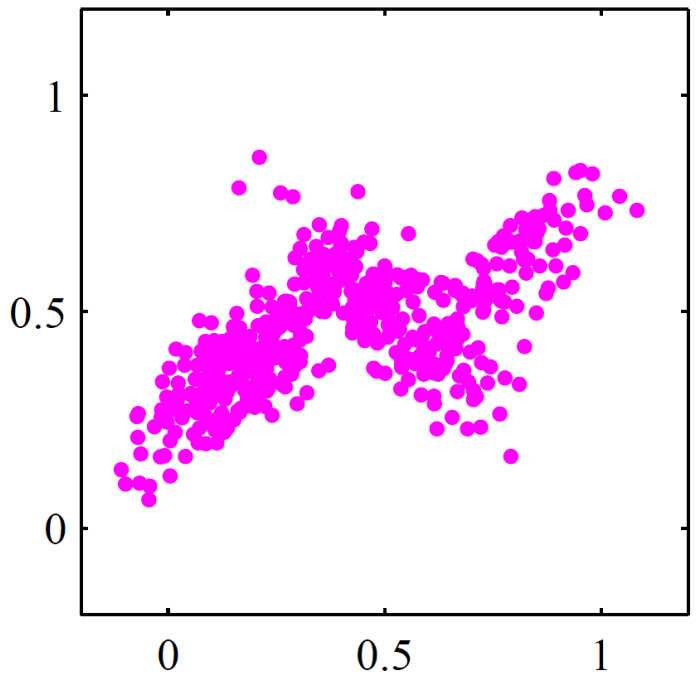
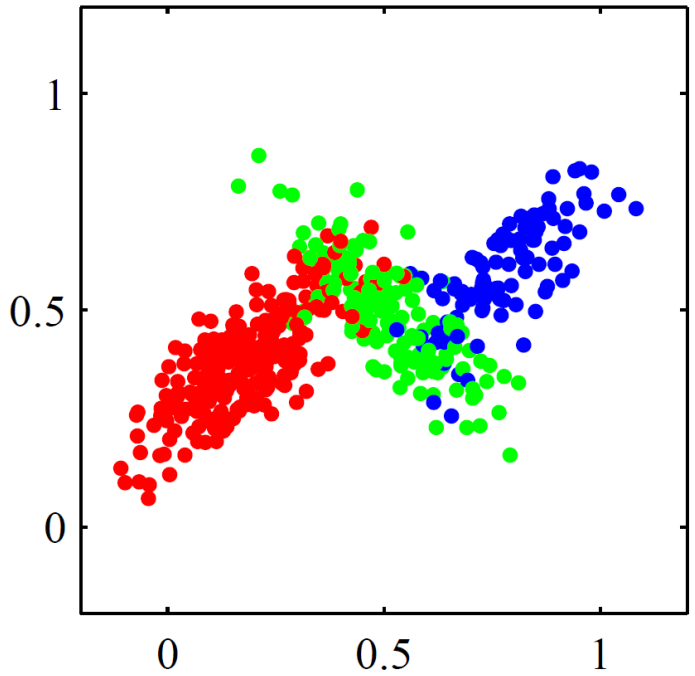
What probabilistic model generates data like this?



GMM: intuition

GMM is a natural model to explain such data

Assume there are 3 ground-truth Gaussian models.



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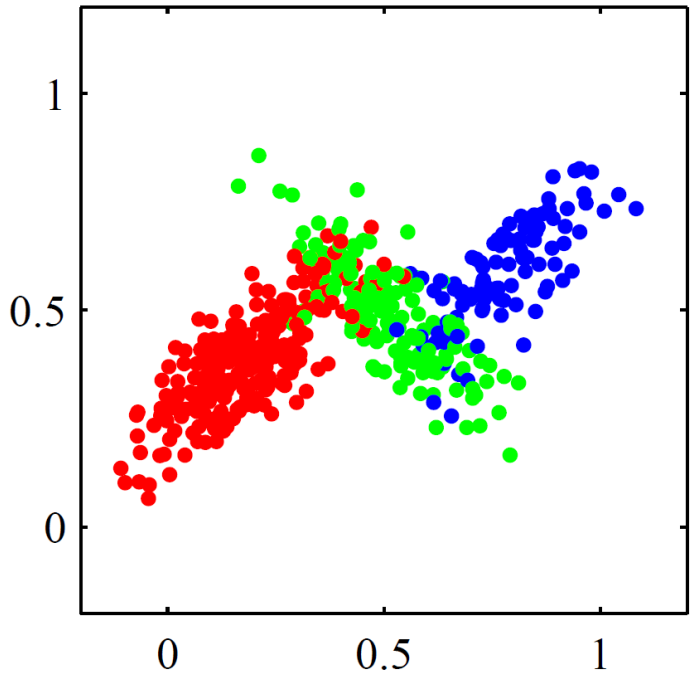

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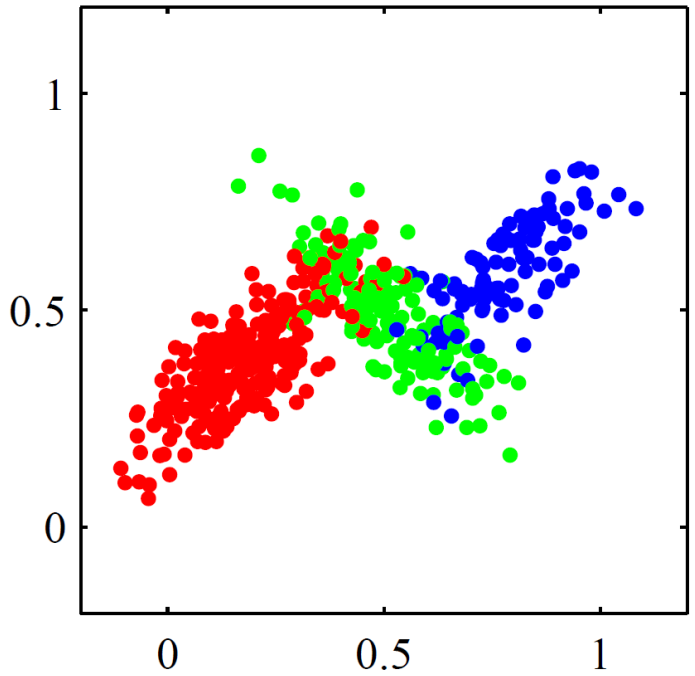

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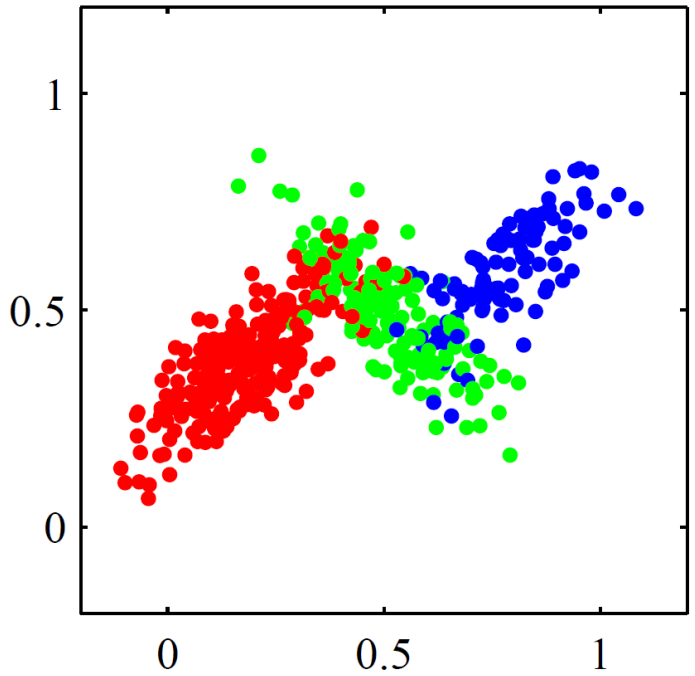

Hence the name "**Gaussian mixture model**".

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A GMM has the following density function:

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Another view

By introducing a **latent variable** $z \in [K]$, which indicates cluster membership, we can see p as a **marginal distribution**

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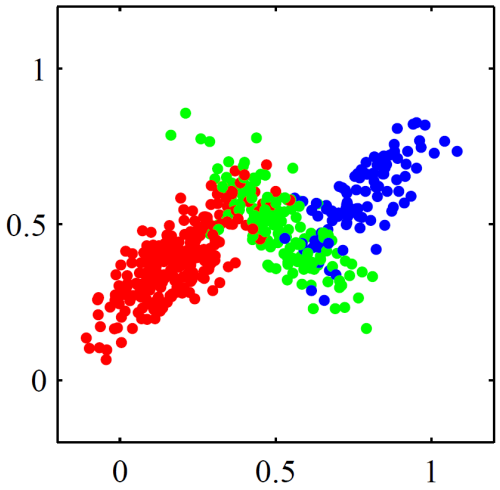
$\boldsymbol{x}$ and z are both random variables drawn from the model

- $\boldsymbol{x}$ 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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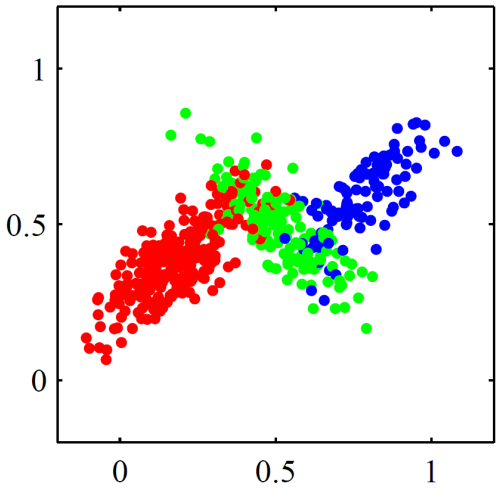

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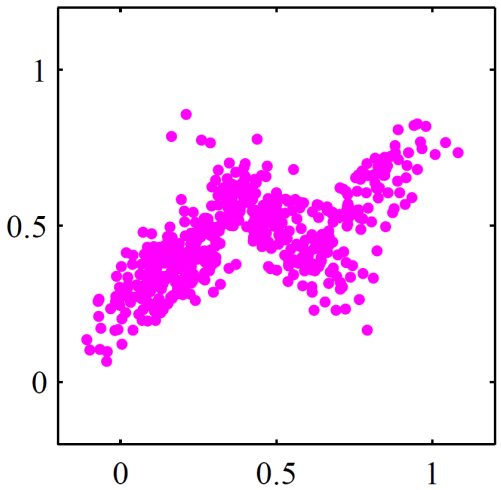

The marginal distribution is

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

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$$p(z_n = k \mid \boldsymbol{x}_n) \triangleq \gamma_{nk} \in [0, 1]$$

i.e. "soft assignment" of each point to each cluster, as opposed to "hard assignment" by K-means.

Learning GMMs

Learning a GMM means finding all the parameters $\boldsymbol{\theta} = \{\omega_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_{k=1}^K$.

In the process, we will learn the latent variable z_n as well:

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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

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

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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

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

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

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

Demo

Generate 50 data points from a mixture of 2 Gaussians with

- $\omega_1 = 0.3, \mu_1 = -0.8, \Sigma_1 = 0.52$
- $\omega_2 = 0.7, \mu_2 = 1.2, \Sigma_2 = 0.35$

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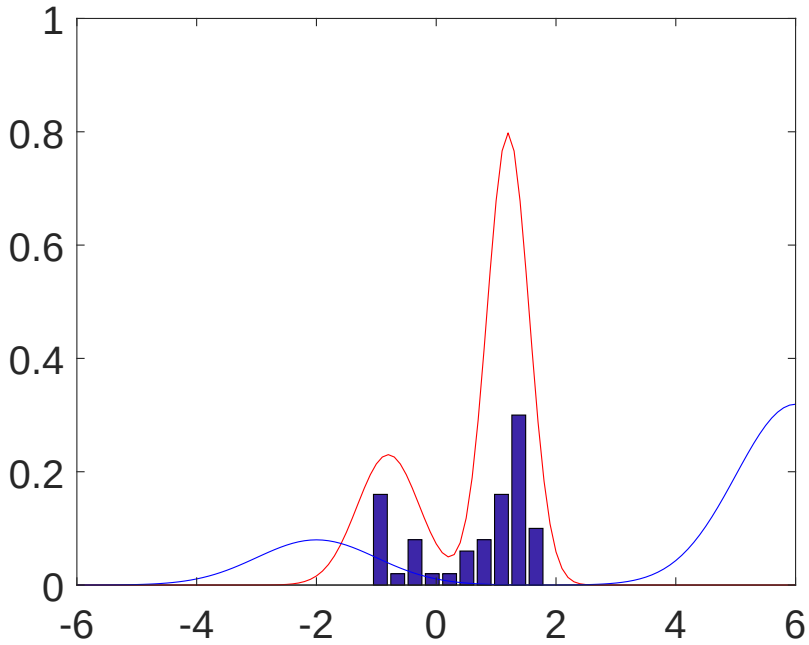

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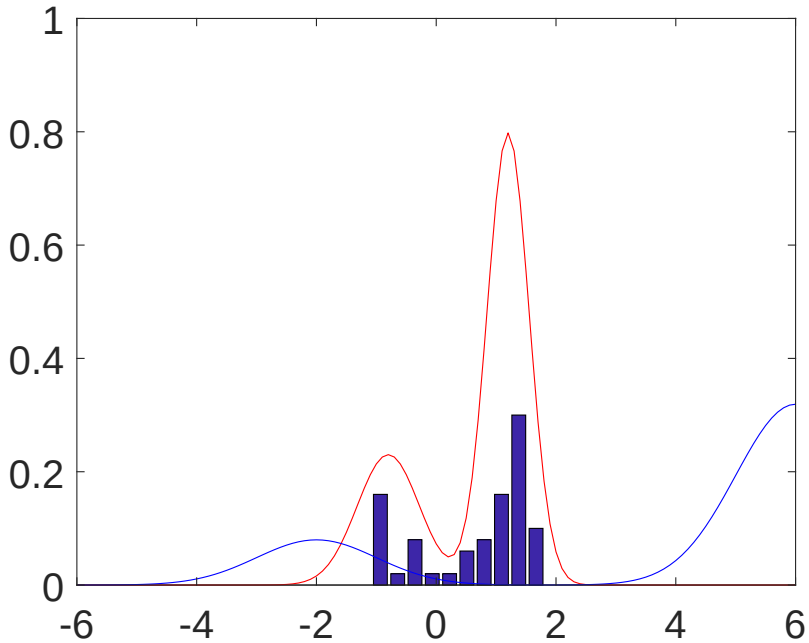

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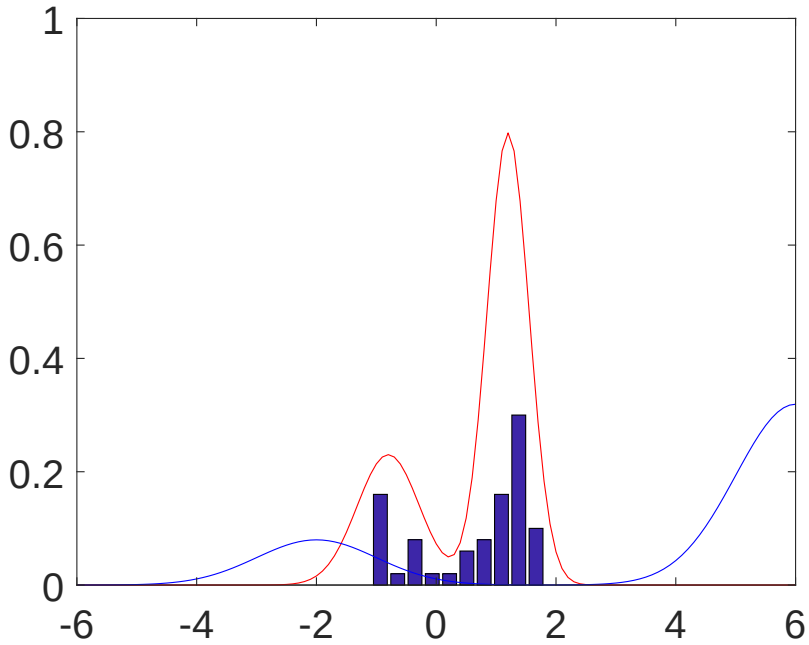

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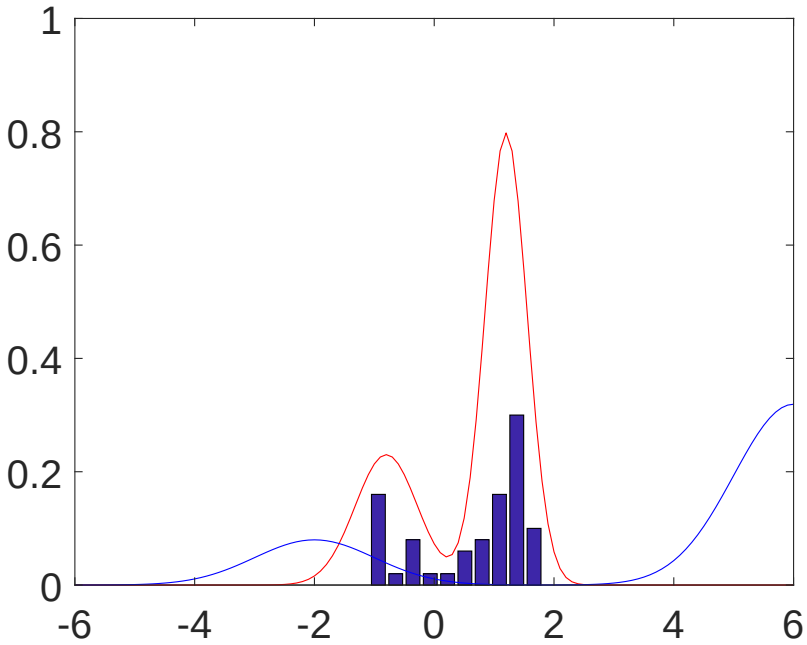

EM_demo_1D.pdf shows how the blue curve moves towards red curve quickly via EM

EM algorithm

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

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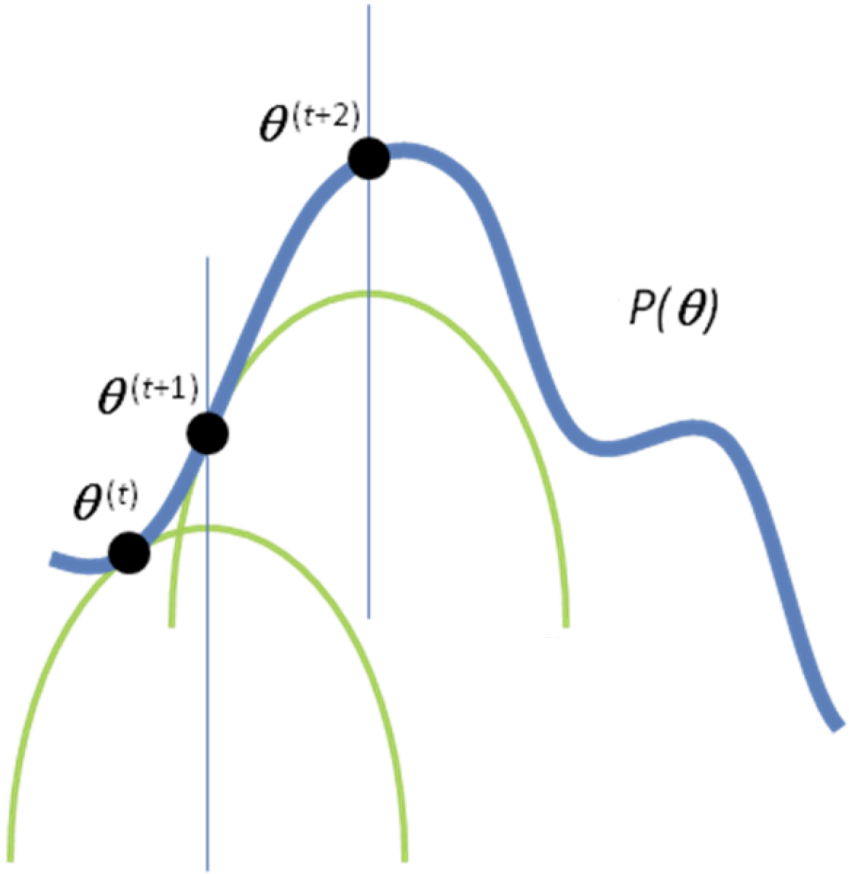
Again, directly solving the objective is intractable.

High level idea

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



Derivation of EM (not required)

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

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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

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

turns out to be $q_n^{(t)}$ s.t.

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- $F\left(\boldsymbol{\theta}^{(t)}, \{q_n^{(t)}\}\right) = P(\boldsymbol{\theta}^{(t)})$ (can be verified through Slide 40)

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&= \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] \qquad (H(q_n^{(t)}) \text{ is independent of } \boldsymbol{\theta}) \\
&\triangleq \operatorname*{argmax}_{\boldsymbol{\theta}} \; Q(\boldsymbol{\theta} \,; \boldsymbol{\theta}^{(t)}) \qquad (\{q_n^{(t)}\} \text{ are computed via } \boldsymbol{\theta}^{(t)})
\end{aligned}$$

Q is the (expected) **complete likelihood** and is usually more tractable.

Maximizing over $\boldsymbol{\theta}$

Fix $\{q_n^{(t)}\}$, maximize over $\boldsymbol{\theta}$:

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

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and obtain **Expectation** of complete likelihood

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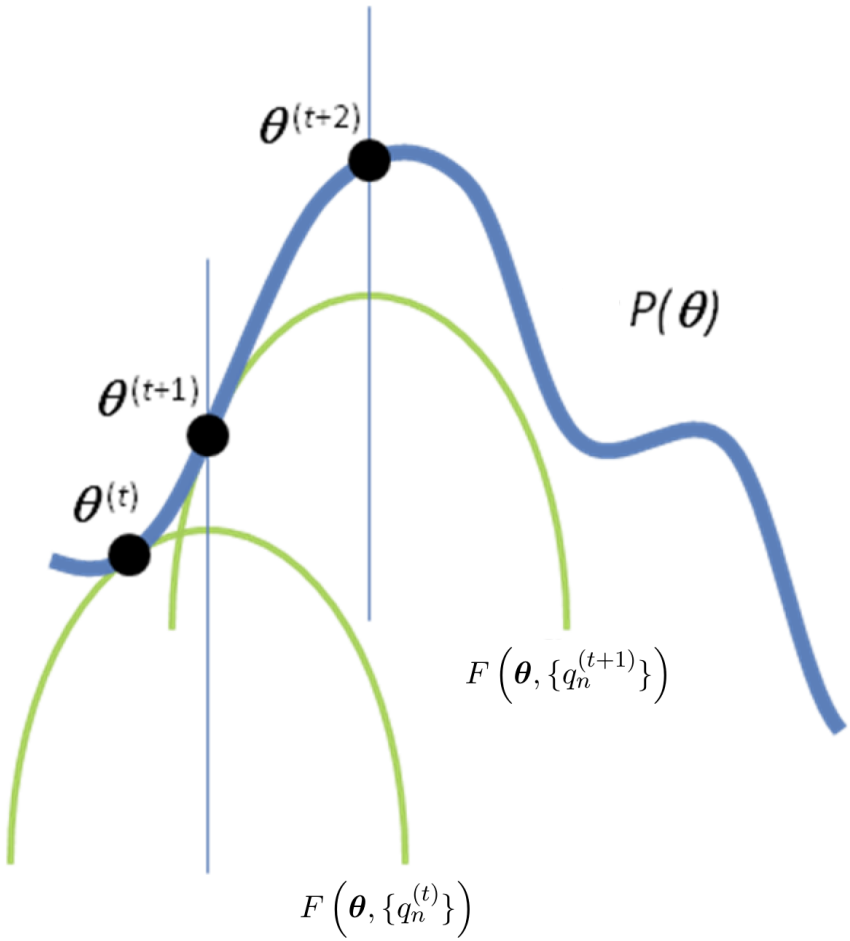
Step 2 (M-Step) **update the model parameter** via **Maximization**

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

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

Pictorial explanation



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

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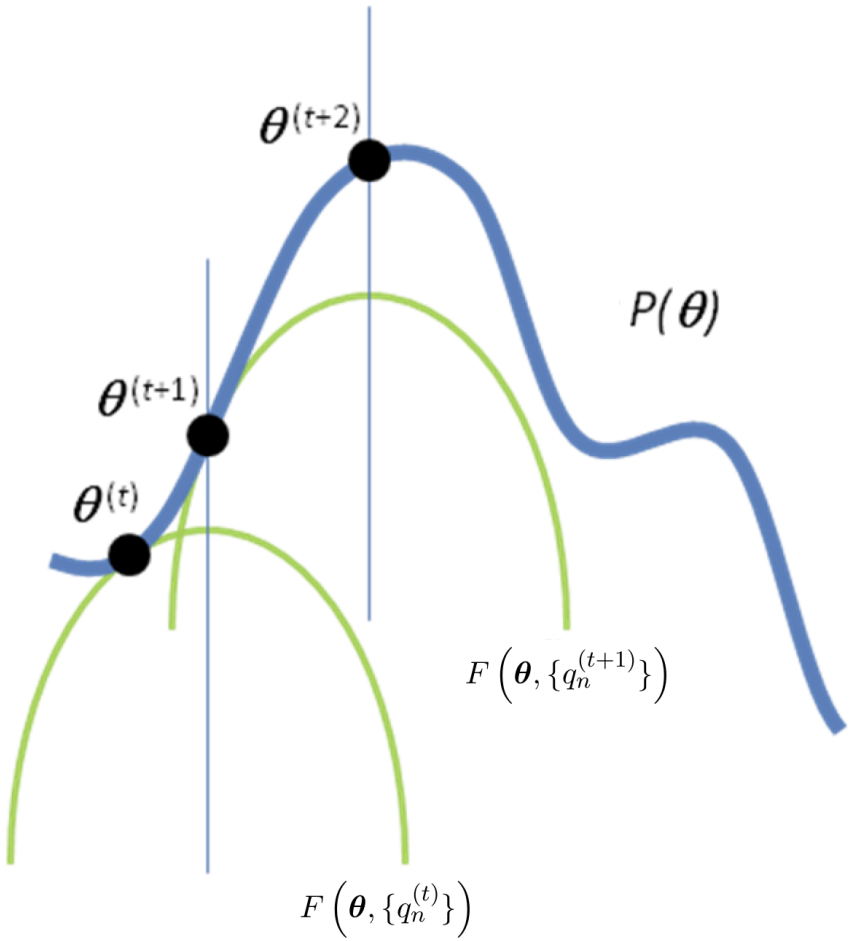

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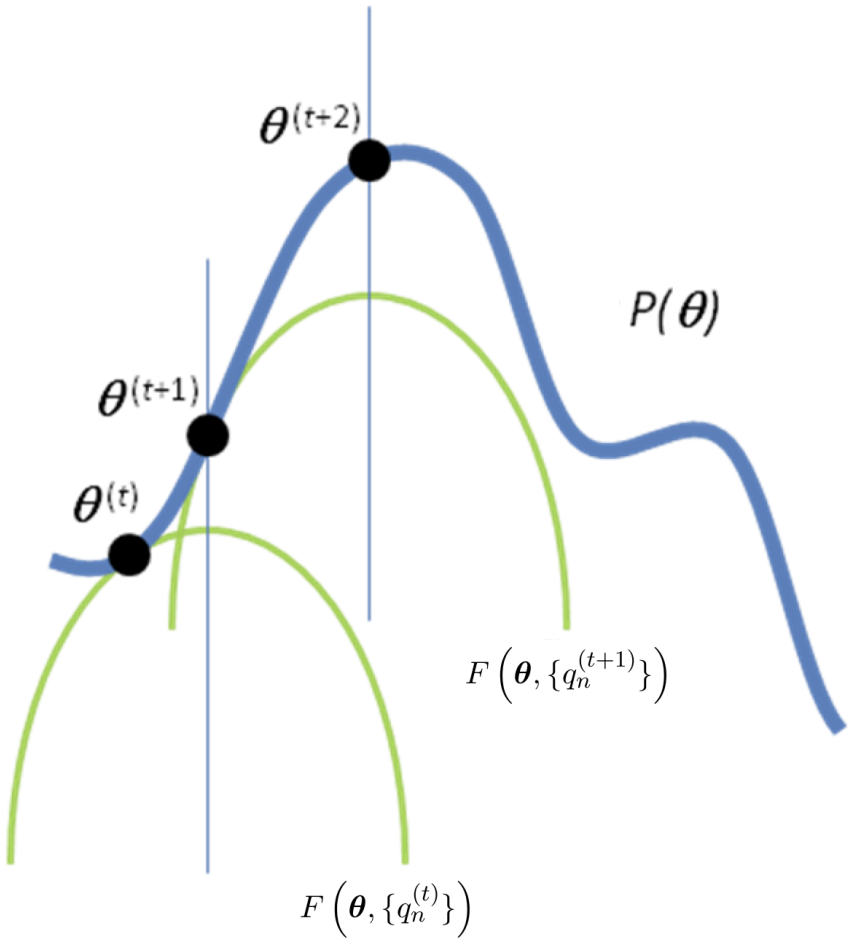

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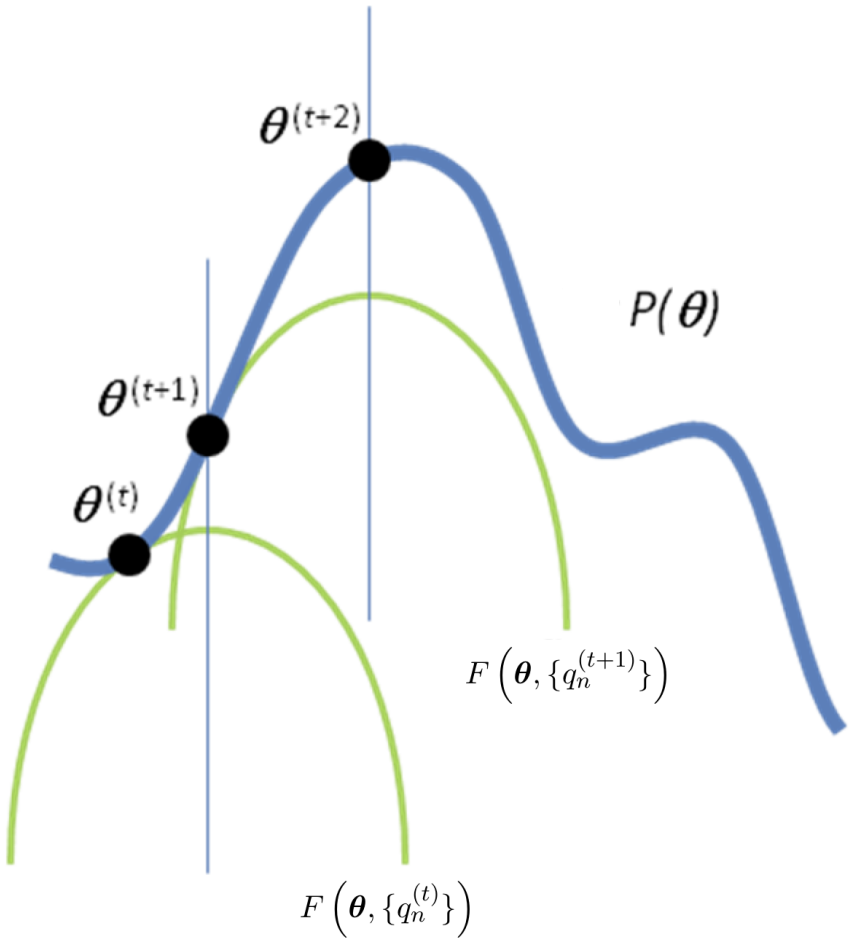

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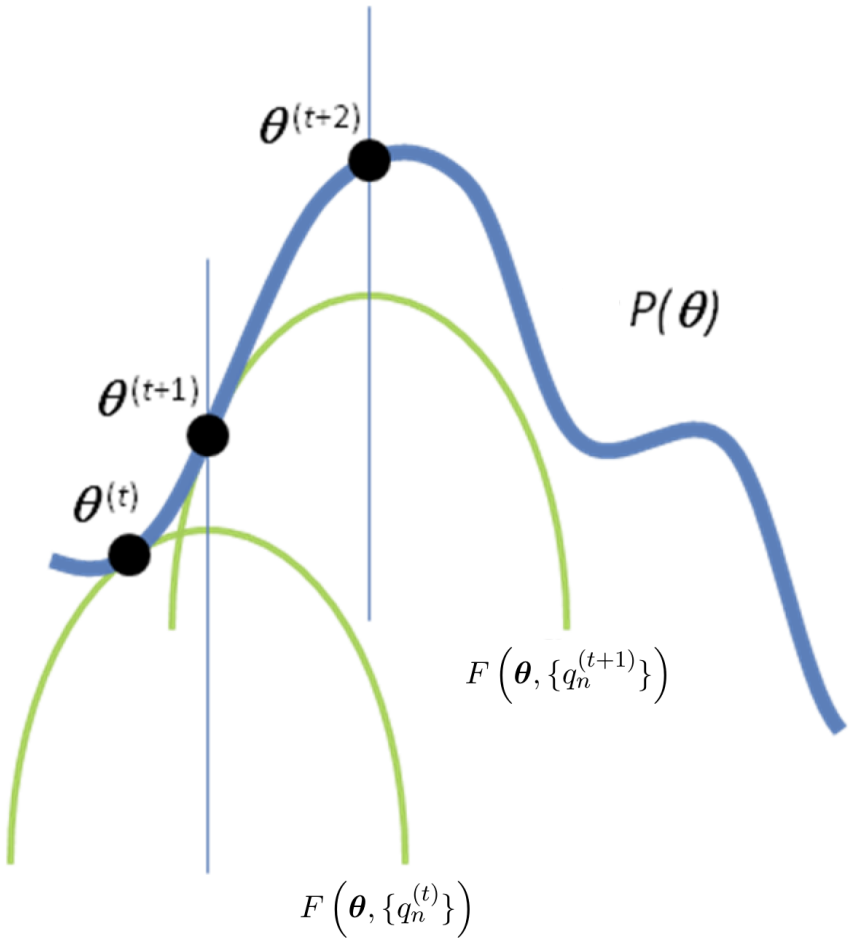

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So EM always increases the objective value and will converge to some local maximum (similar to K-means).

Apply EM to learn GMMs

E-Step:

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

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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.

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

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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

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

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

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(You can try to verify these for the 1D case.)

Putting it together

EM for learning GMMs:

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

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Putting it together

EM for learning GMMs: (see 2D demo)

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- when $\sigma \to 0$, EM becomes K-means

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.