CSCI567 Machine Learning (Spring 2021)

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Outline

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1. Clustering
   - Problem setup
   - K-means algorithm
   - Initialization and Convergence

Supervised learning v.s unsupervised learning

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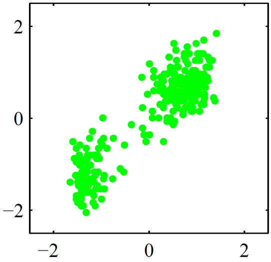
Today's focus: **clustering**, an important unsupervised learning problem

Clustering: informal definition

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



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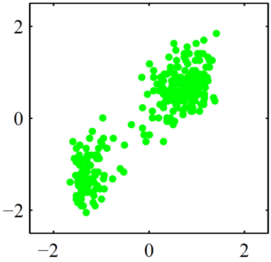

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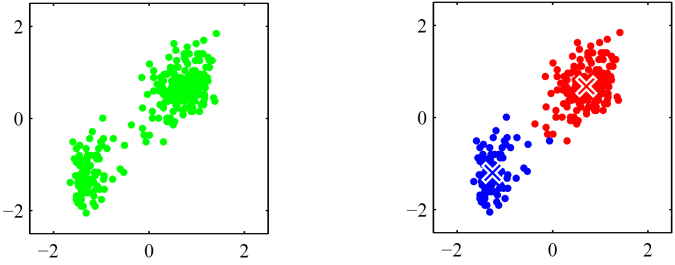
- assign each point to a specific cluster
- find the center (representative/prototype/...) of each cluster



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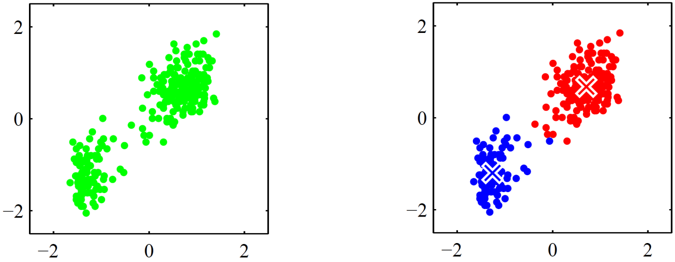

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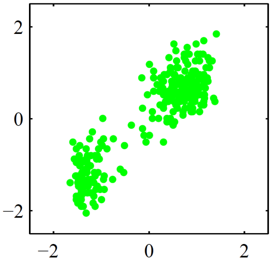

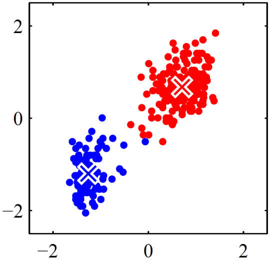

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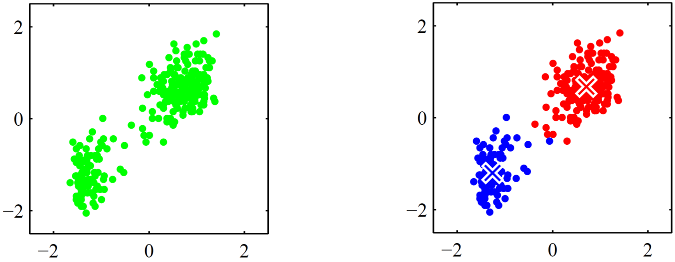
Output: group the data into K clusters, which means

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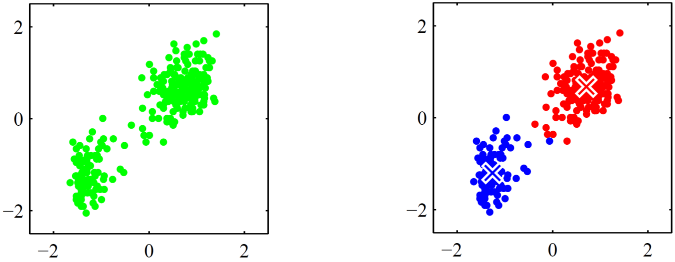
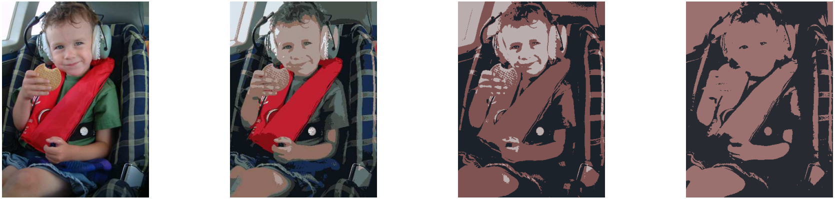
- find the cluster centers $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K \in \mathbb{R}^{\mathsf{D}}$



Many applications

One example: **image compression** (vector quantization)

- 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 x_n to the closest $\boldsymbol{\mu}_k$**, i.e.

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

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

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

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

for each $k \in [K]$.

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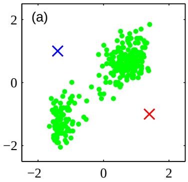
Step 3 Return to Step 1 if not converged

An example



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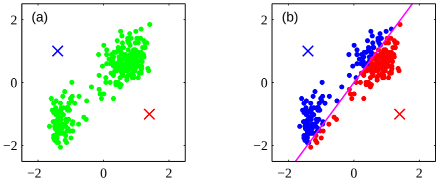

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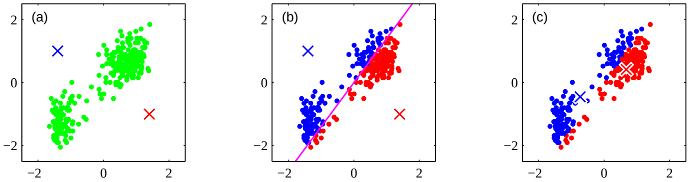

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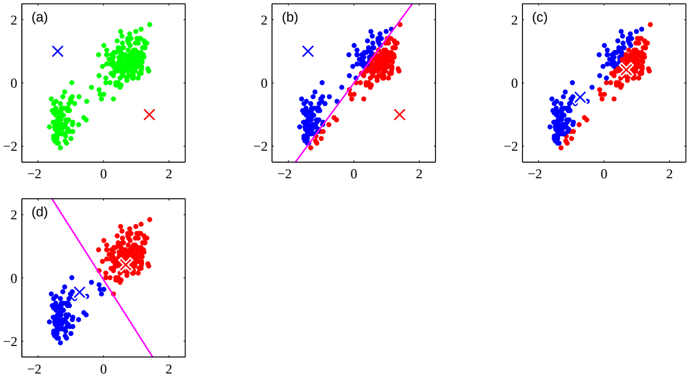

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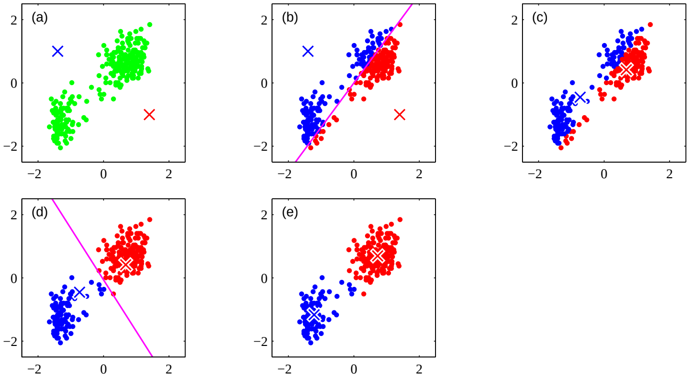

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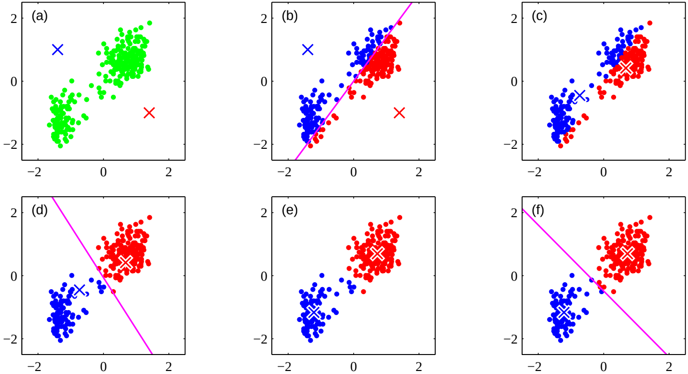

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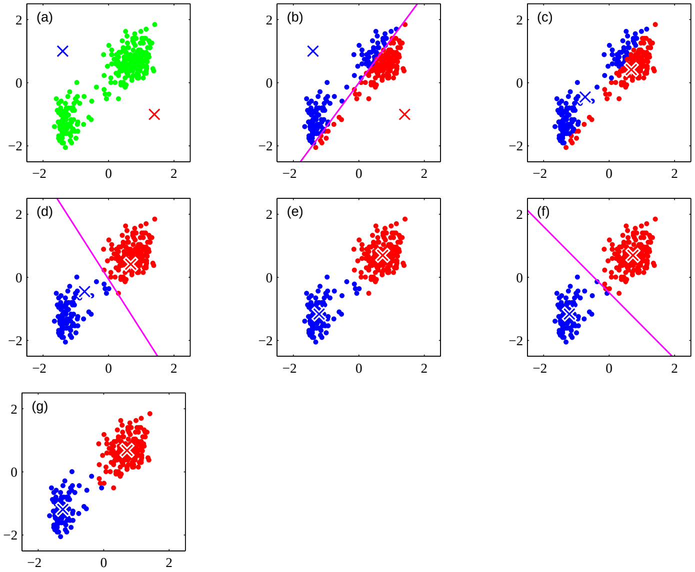

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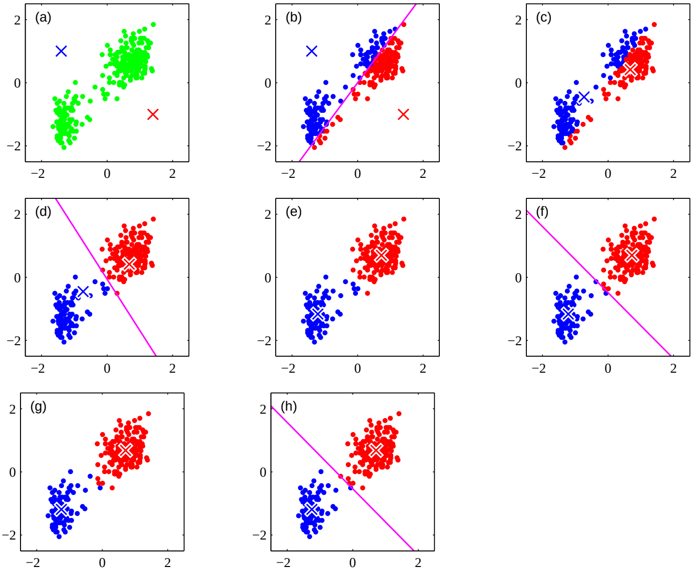

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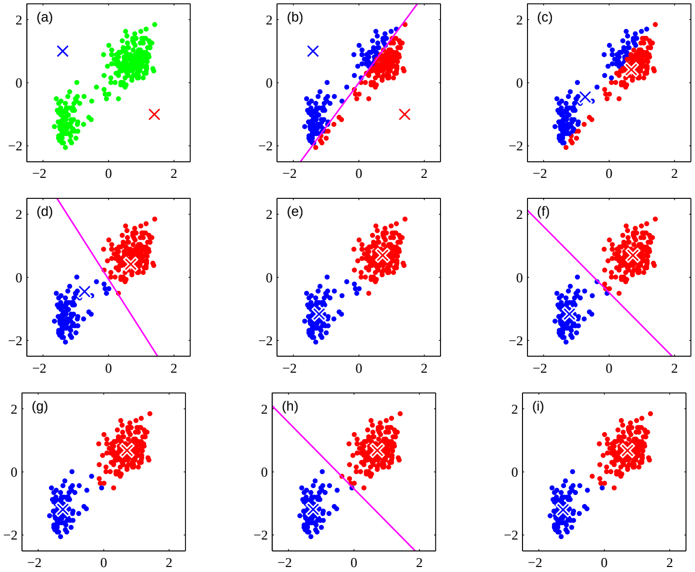

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Initialization matters for **convergence**.

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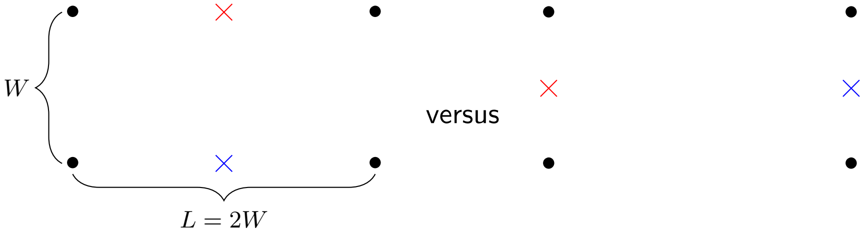
- and it *might not converge to the global minimum* of the K-means objective

Local minimum v.s global minimum

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



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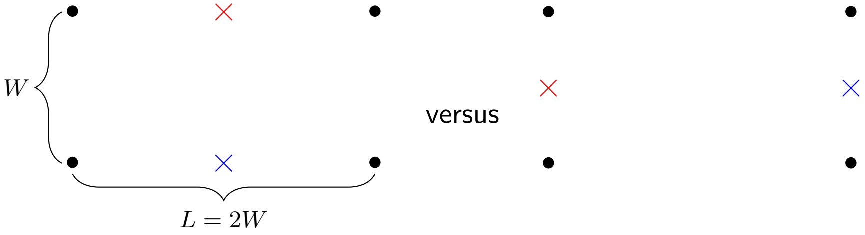

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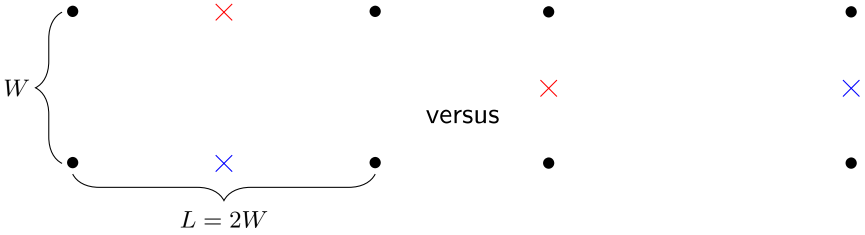

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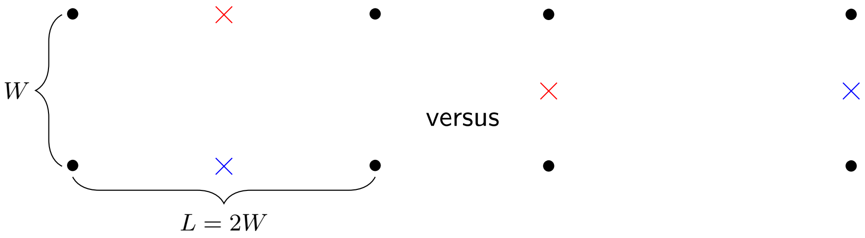

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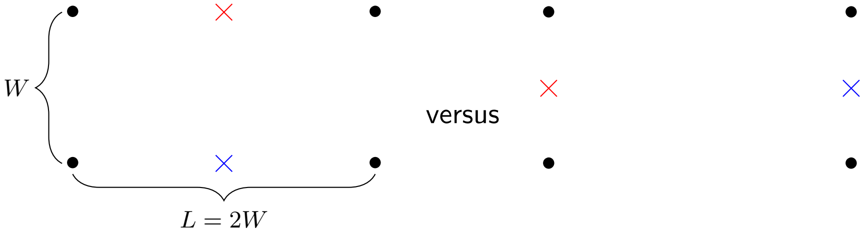

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- left has K-means objective $L^2 = 4W^2$
- right has K-means objective W^2, *4 times better than left!*
- in fact, left is **local minimum**, and right is **global minimum**.

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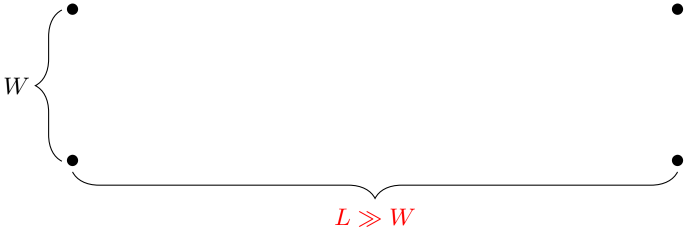

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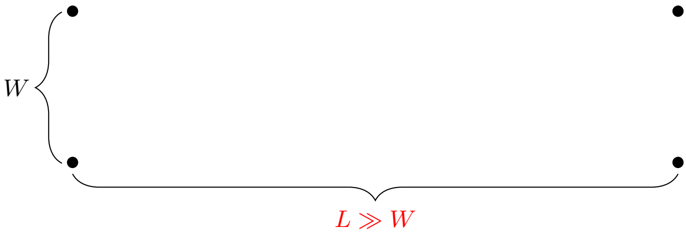

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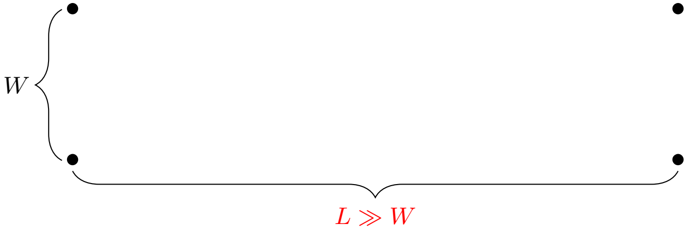
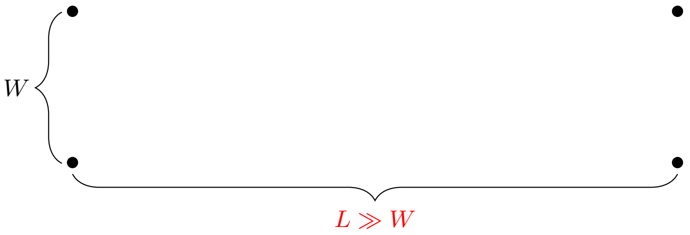


- moreover, local minimum can be *arbitrarily worse* if we increase L
- so *initialization matters a lot* for K-means

How do common initialization methods perform?



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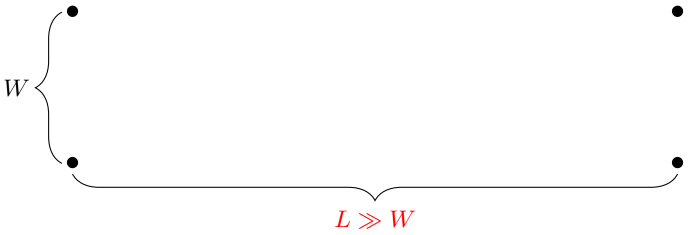

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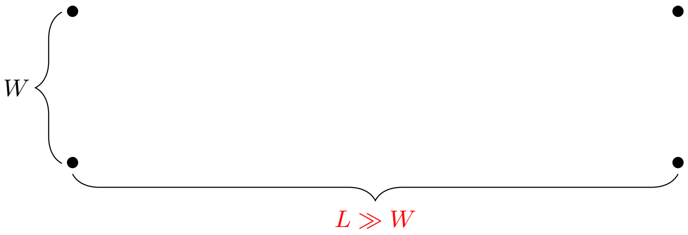

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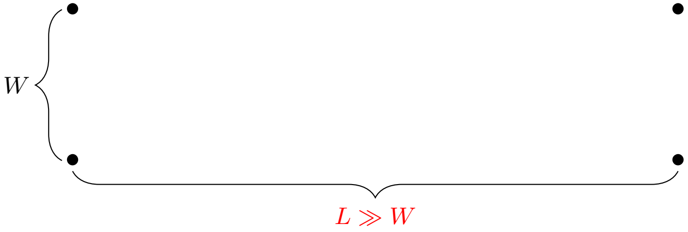

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- or randomly assign each point to a cluster, then average: similarly fail with a constant probability
- or more sophisticated approaches: **K-means++** *guarantees* to find a solution that in expectation is at most $O(\log K)$ times of the optimal

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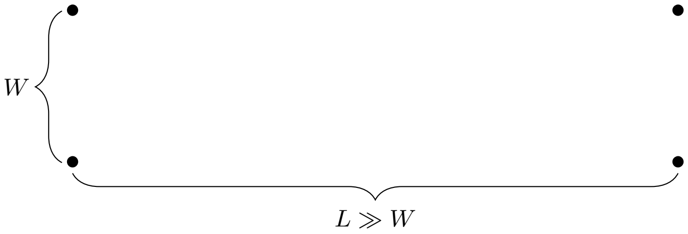
Intuitively this *spreads out the initial centers*.

K-means++ on the same example



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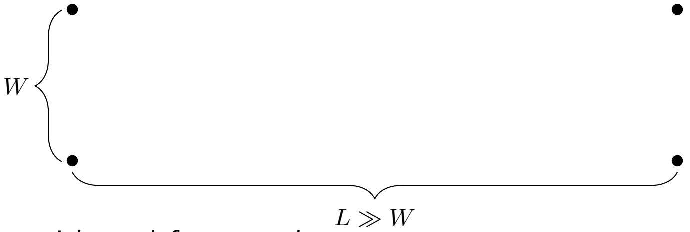

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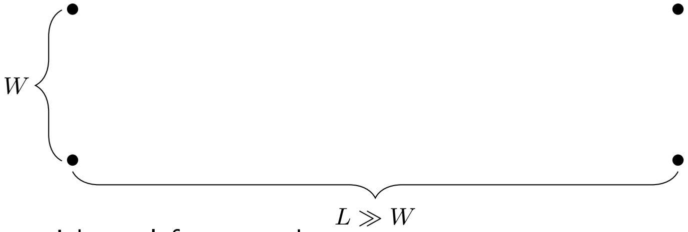

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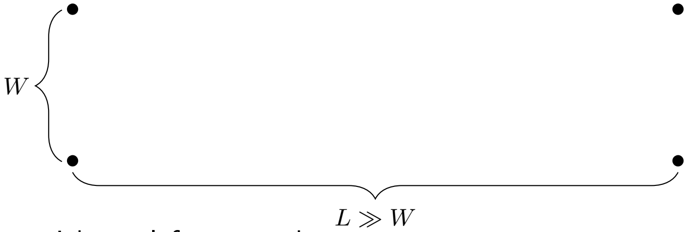

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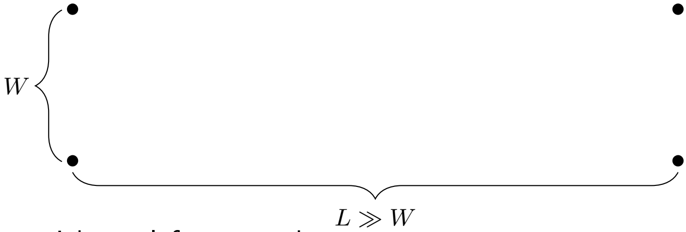
- $\Pr[\boldsymbol{\mu}_2 = \text{bottom left}] \propto W^2$, $\qquad \Pr[\boldsymbol{\mu}_2 = \text{top right}] \propto L^2$

K-means++ on the same example



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

- $\Pr[\boldsymbol{\mu}_2 = \text{bottom left}] \propto W^2$, $\Pr[\boldsymbol{\mu}_2 = \text{top right}] \propto L^2$
- $\Pr[\boldsymbol{\mu}_2 = \text{bottom right}] \propto W^2 + L^2$

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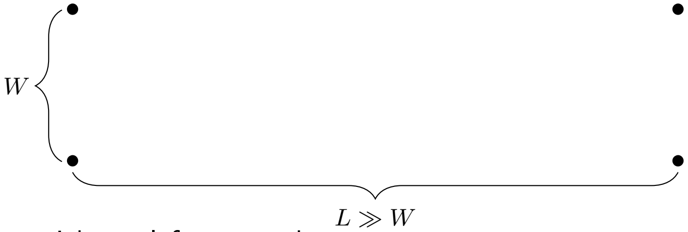

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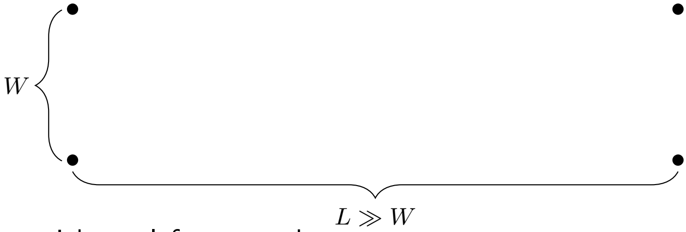
So the **expected K-means objective** is

$$\frac{W^2}{2(W^2+L^2)} \cdot L^2 + \left(\frac{L^2}{2(W^2+L^2)} + \frac{1}{2}\right) \cdot W^2$$

K-means++ on the same example



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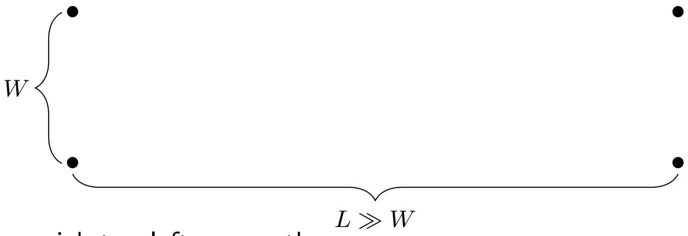

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that is, *at most 1.5 times of the optimal*.

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.