Curse of Dimensionality
&
Clustering

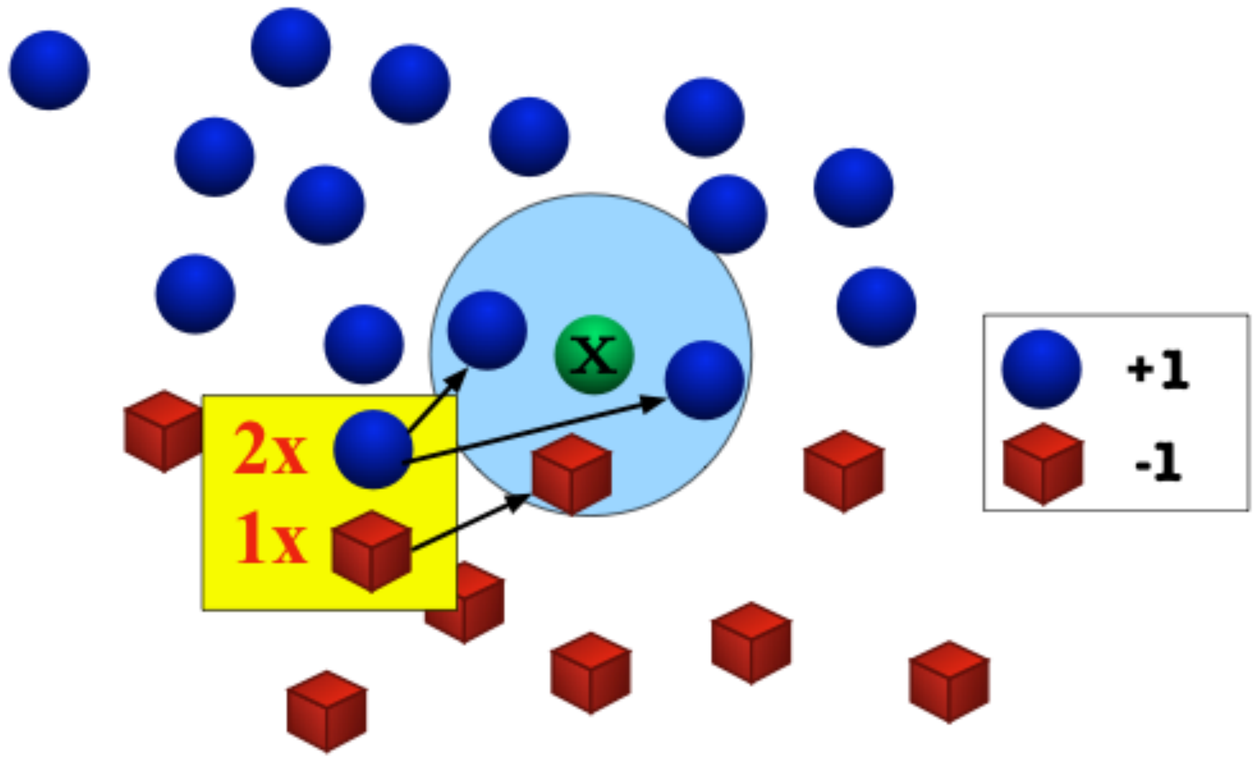
Announcement:

1. P1 will be out today

2. Office hour today 2-3 pm

Recap

The K-NN algorithm



Example: 3-NN with Euclidean distance on a binary classification data

Recap

Bayes optimal Predictor: $y_b = h_{opt}(x) = \arg \max_{y \in \{-1,1\}} P(y \mid x)$

Assume $x \in [-1,1]^2$, $P(x)$ has support everywhere $P(x) > 0, \forall x \in [-1,1]^2$, $n \to \infty$

$$\forall x \in [-1,1]^2 : \ \mathbb{P}(y \neq \text{1NN}(x)) \leq 2\mathbb{P}(y \neq h_{opt}(x))$$

Key point: K-NN can work well when $\frac{n}{d}$ is very large.

Outline for Today

1. Curse of dimensionality

2. Unsupervised Learning: Clustering and the K-means algorithm

3. Convergence of K-means

Finite sample error rate of 1-NN in high-dimension setting

(Informal result and no proof)

Fix $n \in \mathbb{N}^+$, assume $x \in [0,1]^d$, assume $P(y \mid x)$ is Lipschitz continuous with respect to x, i.e., $|P(y \mid x) - P(y \mid x')| \leq d(x, x')$

Then, we have:

$$\mathbb{E}_{x,y\sim P}\left[\mathbf{1}(y \neq \text{1NN}(x))\right] \leq 2\mathbb{E}_{x,y\sim P}\left[\mathbf{1}(y \neq h_{opt}(x))\right] + O\left(\left(\frac{1}{n}\right)^{1/d}\right)$$

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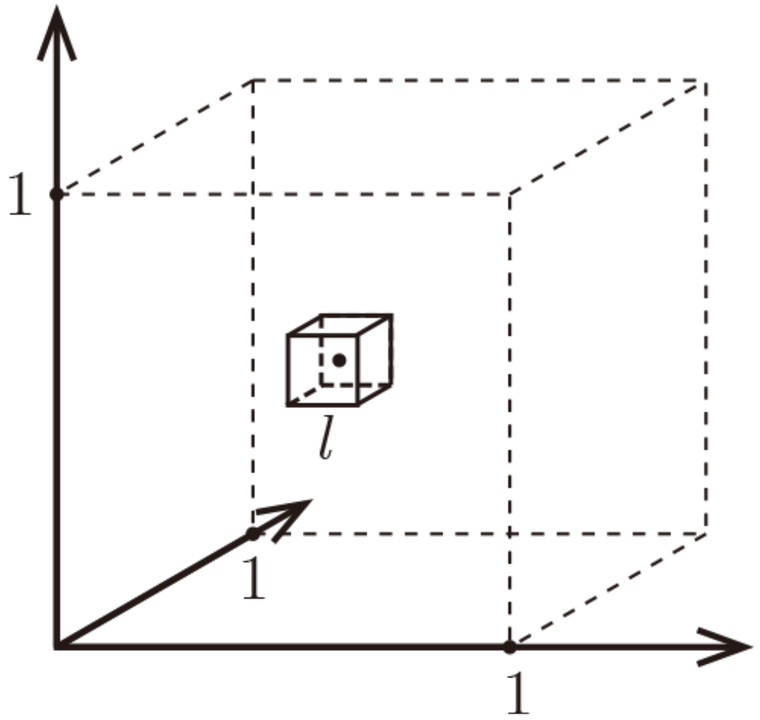
$$(1/n)^{1/d} = 0.1 \Rightarrow n = (10)^d$$

Curse of Dimensionality Intuitive Explanation

Key problem: in high dimensional space, points that are draw from a distribution tends to be far away from each other!



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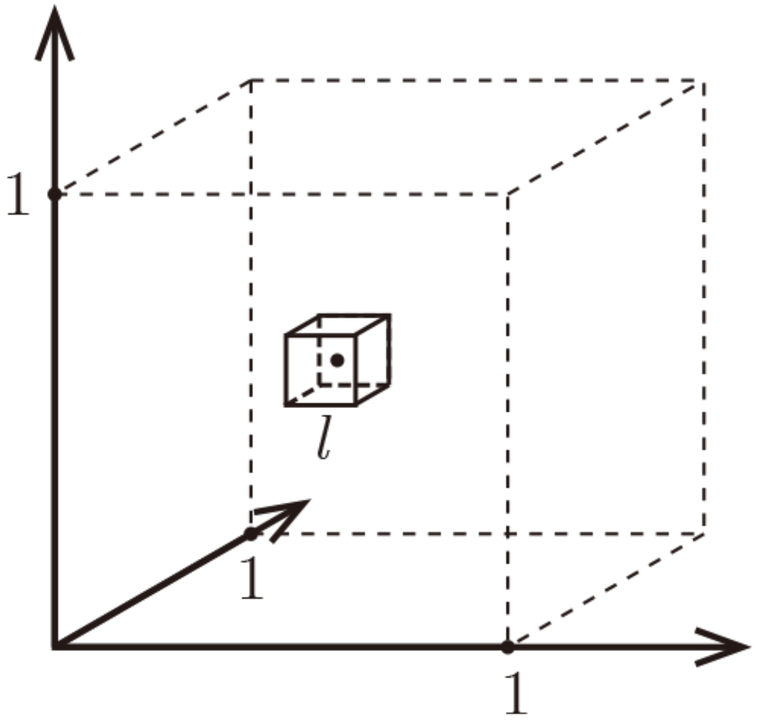

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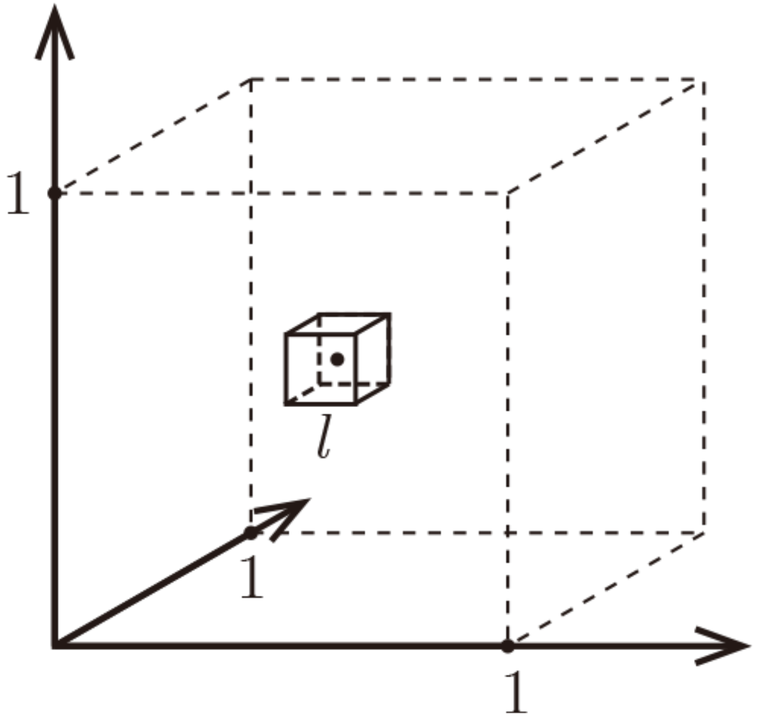

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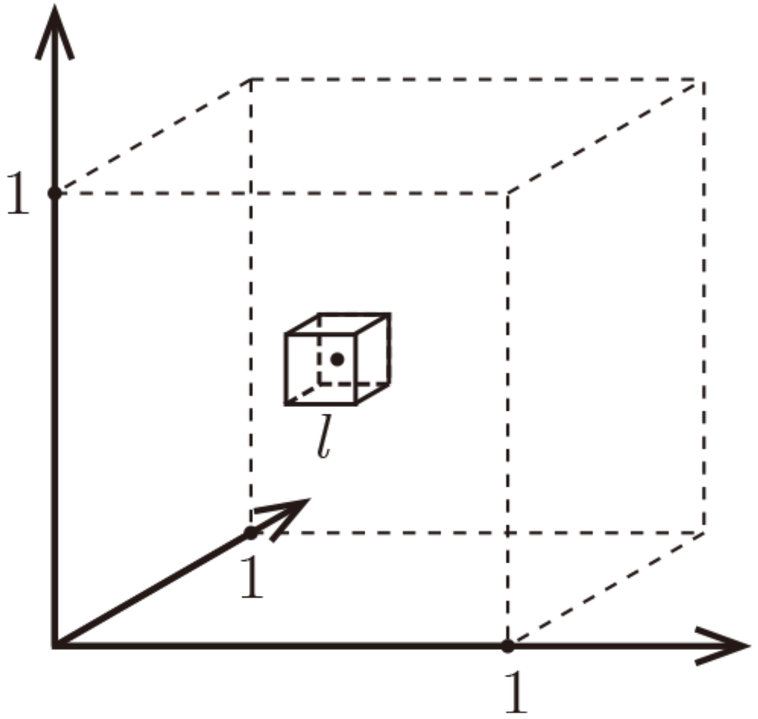

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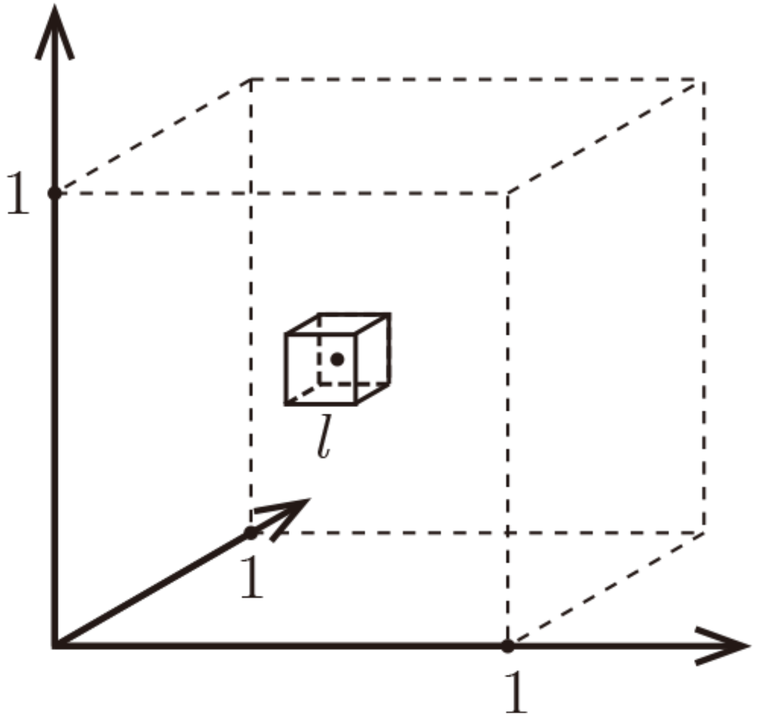

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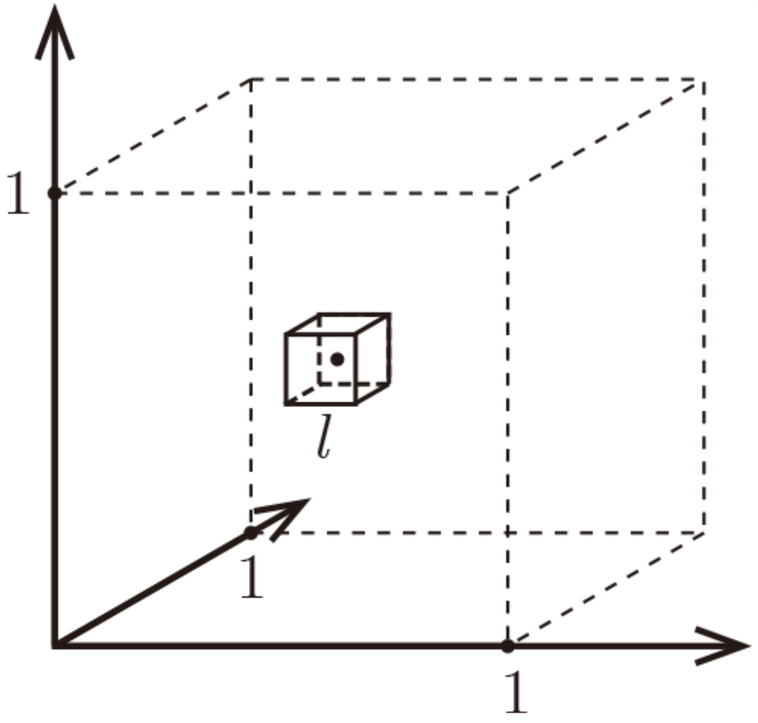

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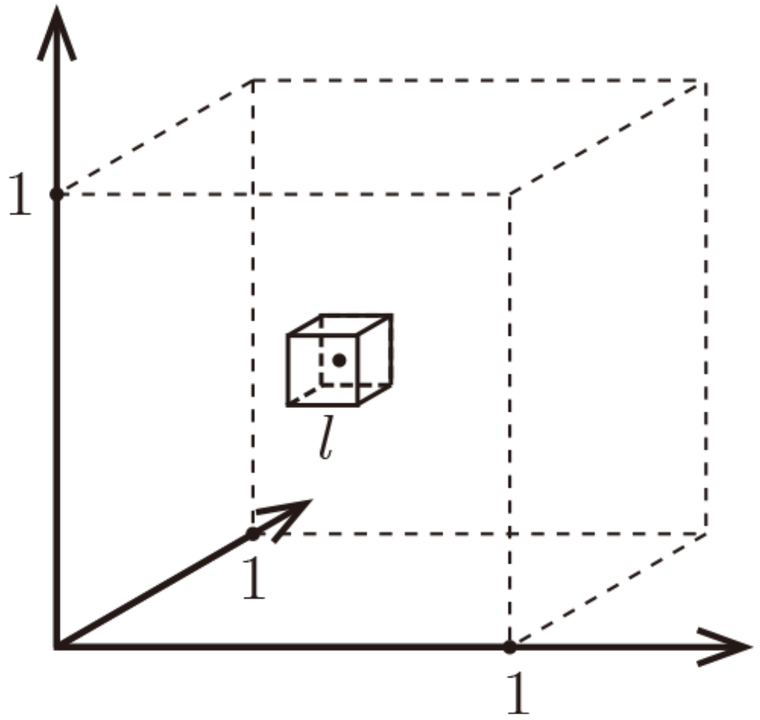

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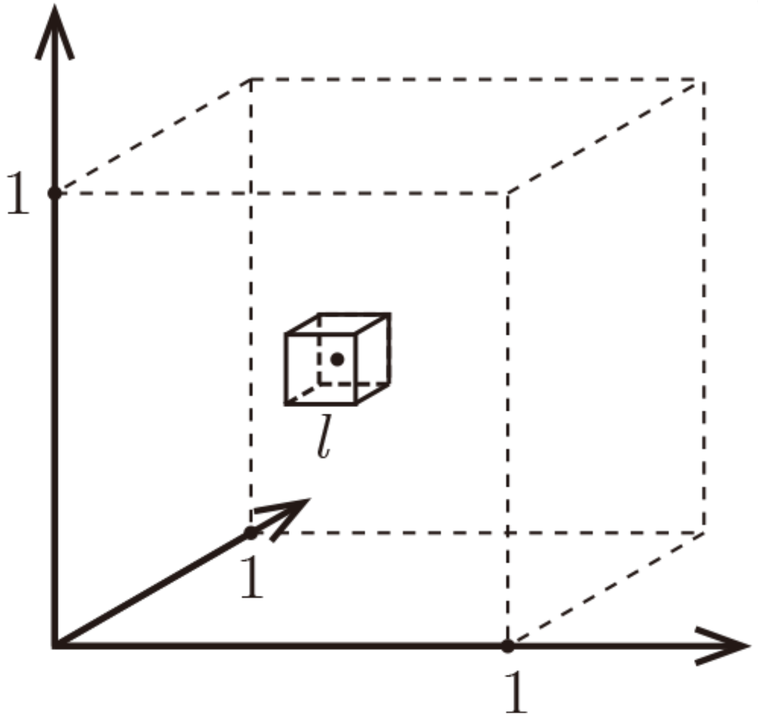

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Thus, we have $l^d \approx \frac{K}{n}$

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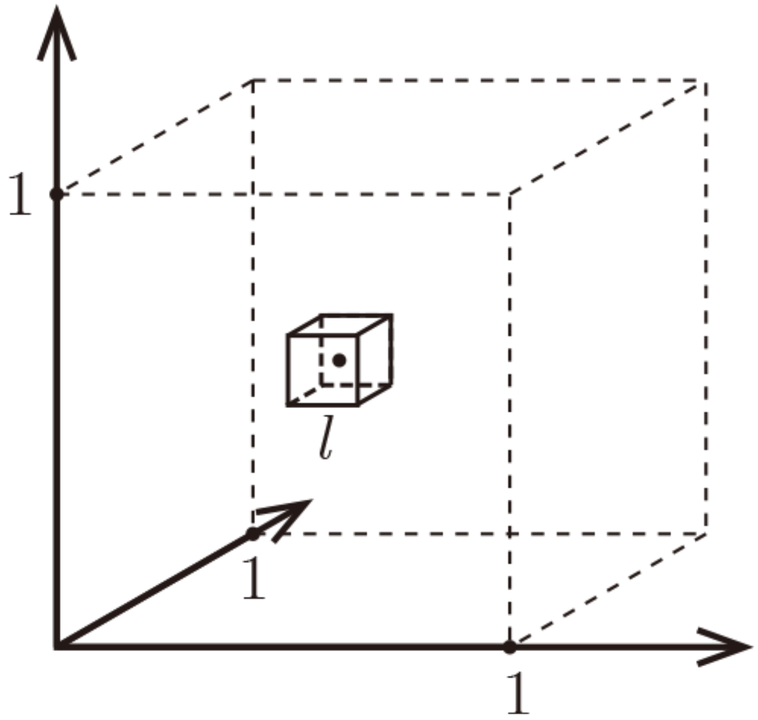

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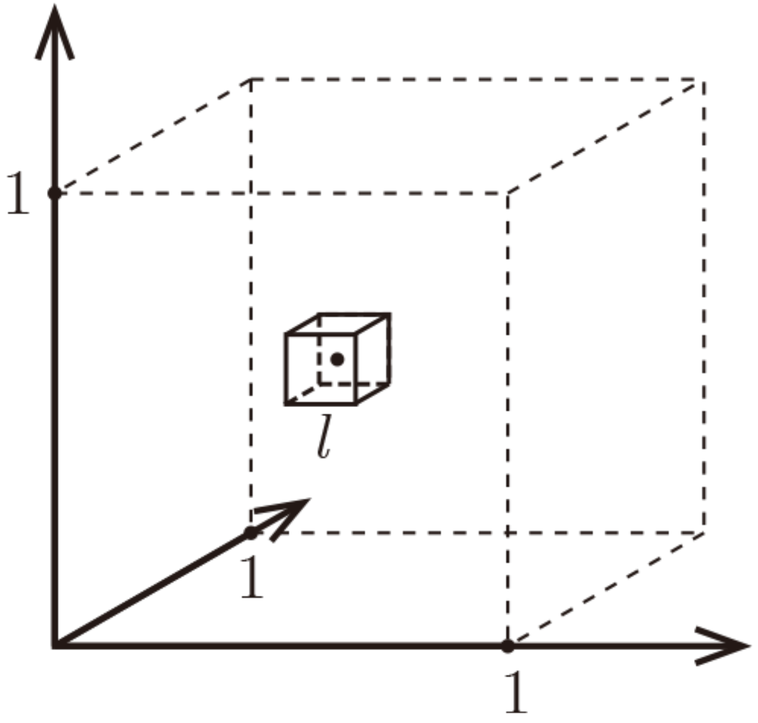

Q: how large we should set l, s.t., we will have K examples (out of n) fall inside the small cube?

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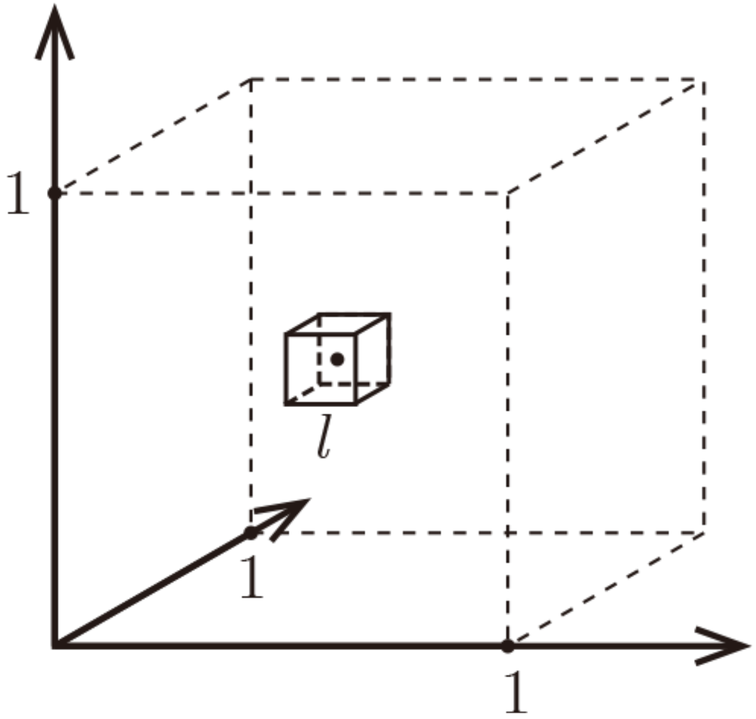

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$$l \approx (K/n)^{1/d}$$

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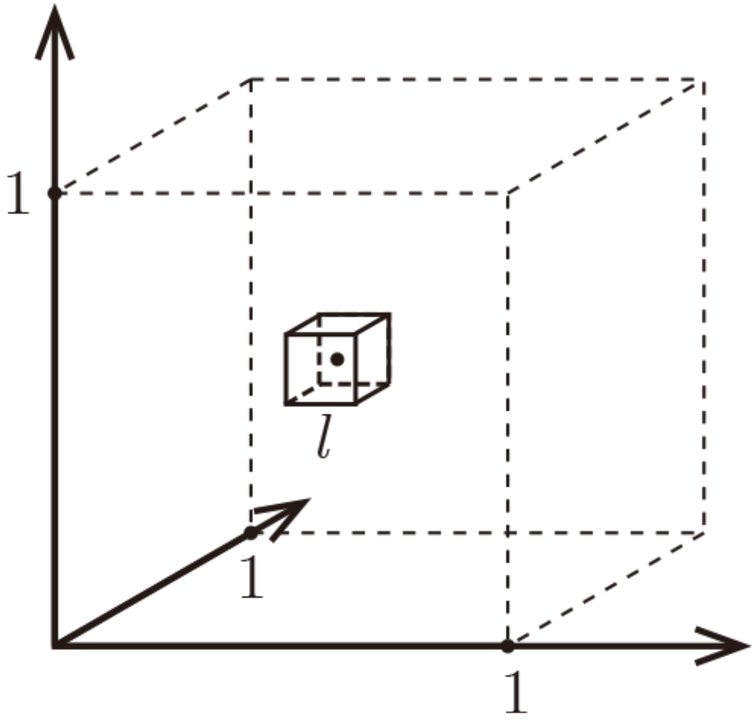

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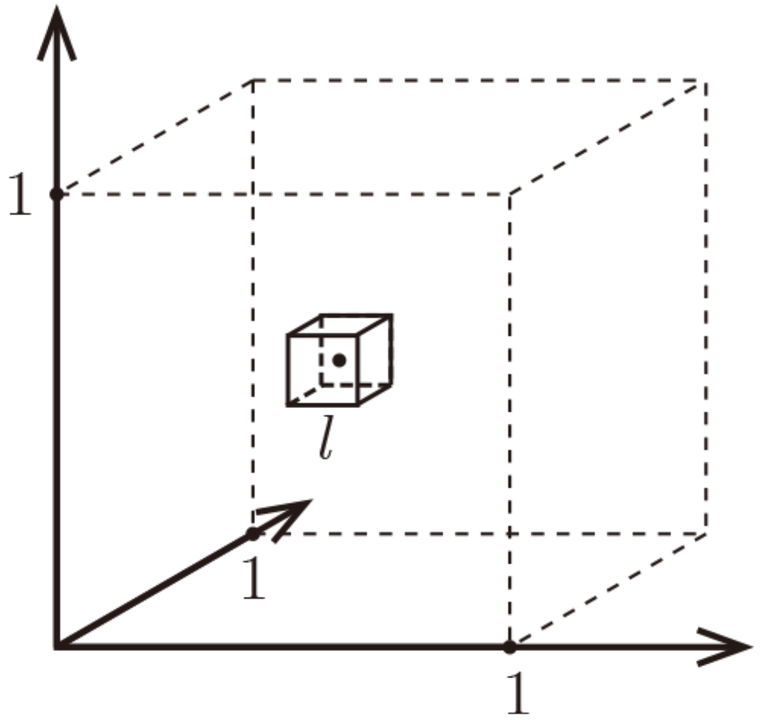

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Bad news: when $d \rightarrow \infty$, the K nearest neighbors will be all over the place!
(Cannot trust them, as they are not nearby points anymore!)

The distance between two sampled points increases as d grows

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$$d(x, x') = \|x - x'\|_2$$

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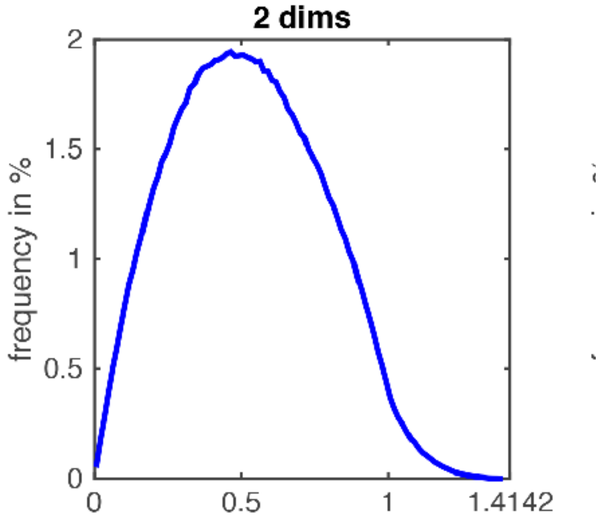

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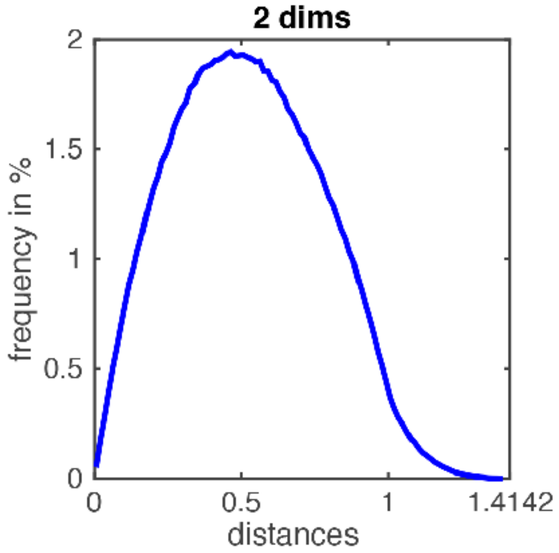

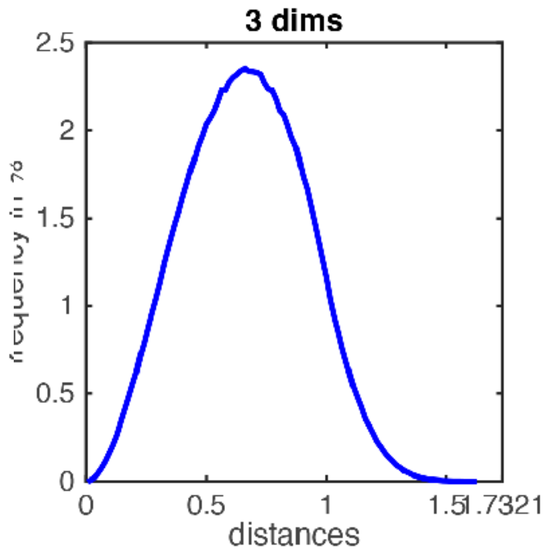

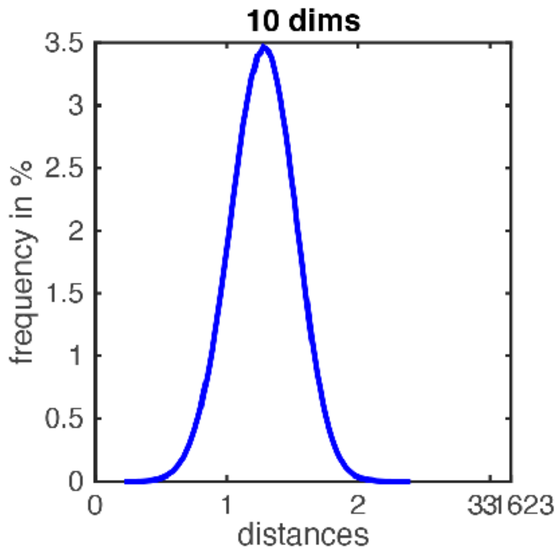

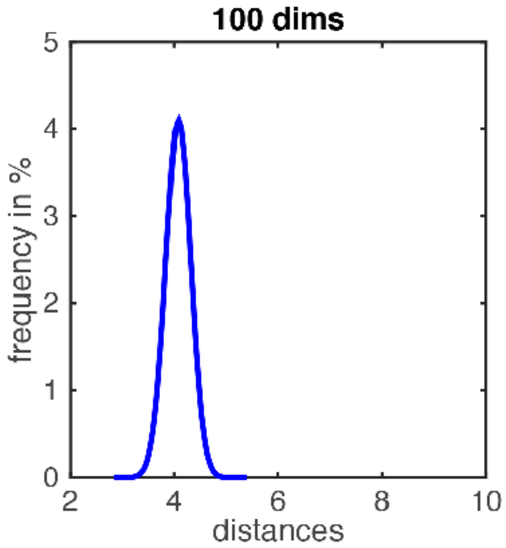

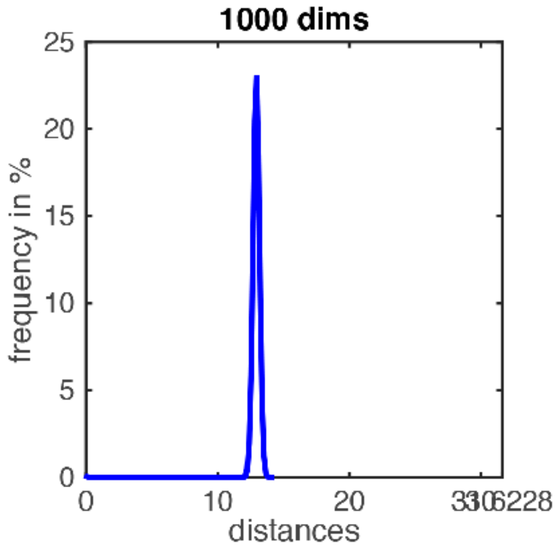

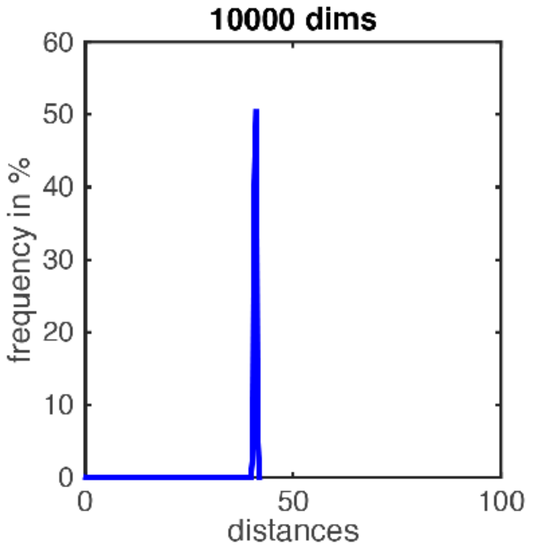

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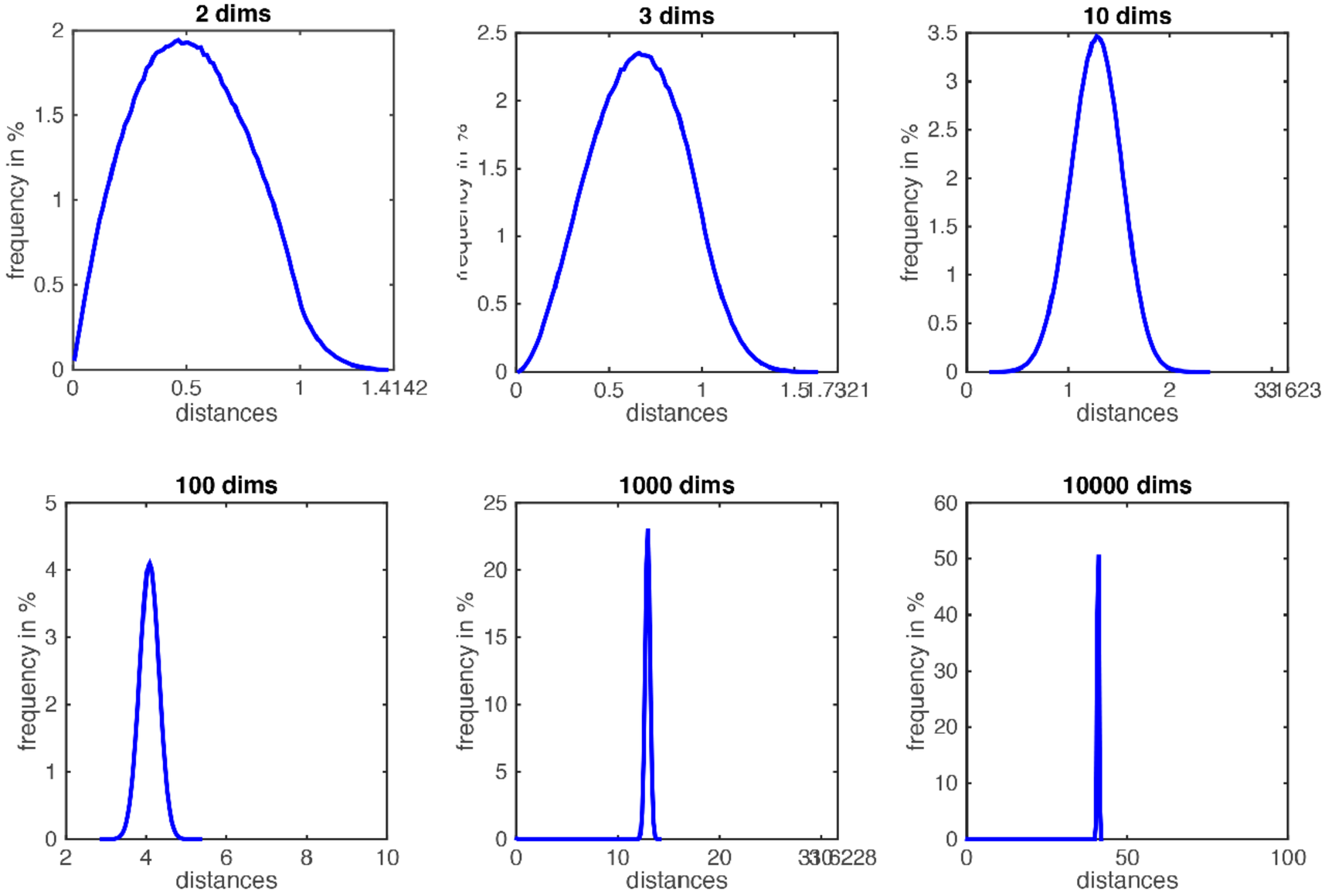
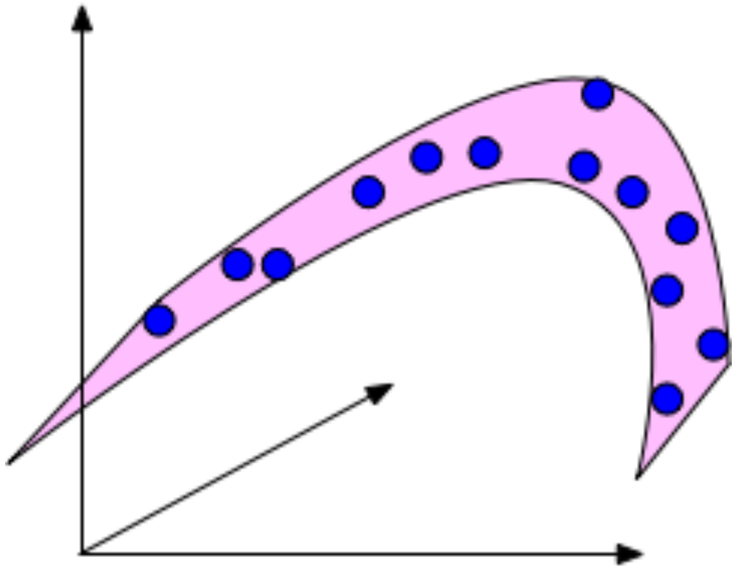


Distance increases as $d \to \infty$

Luckily, real world data often has low-dimensional structure!



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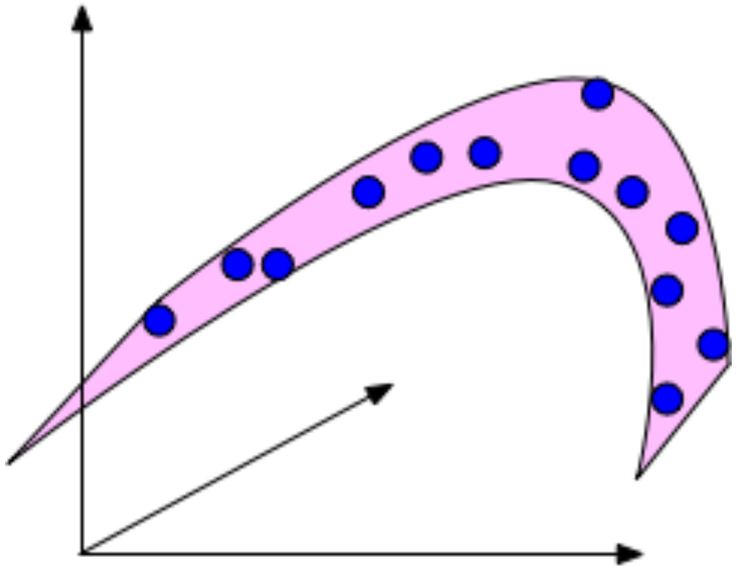

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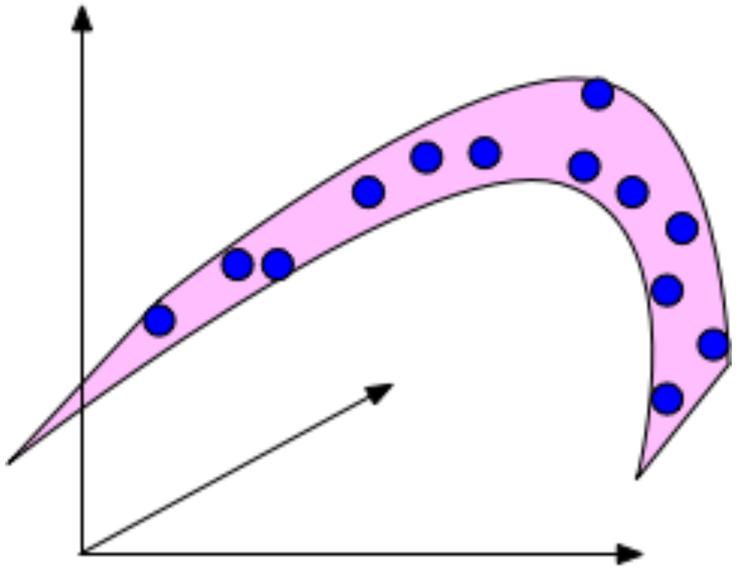

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Original image: $\mathbb{R}^{64^2}$

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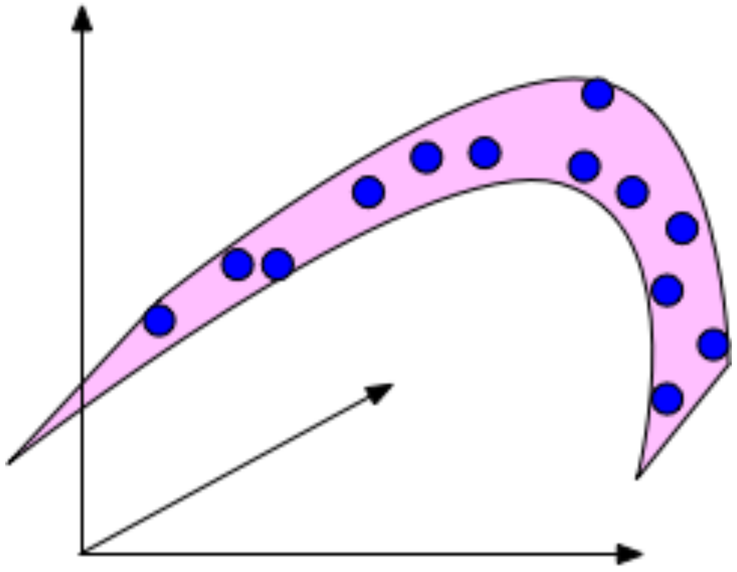

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Next week: we will see that these faces approximately live in 100-d space!

Outline for Today

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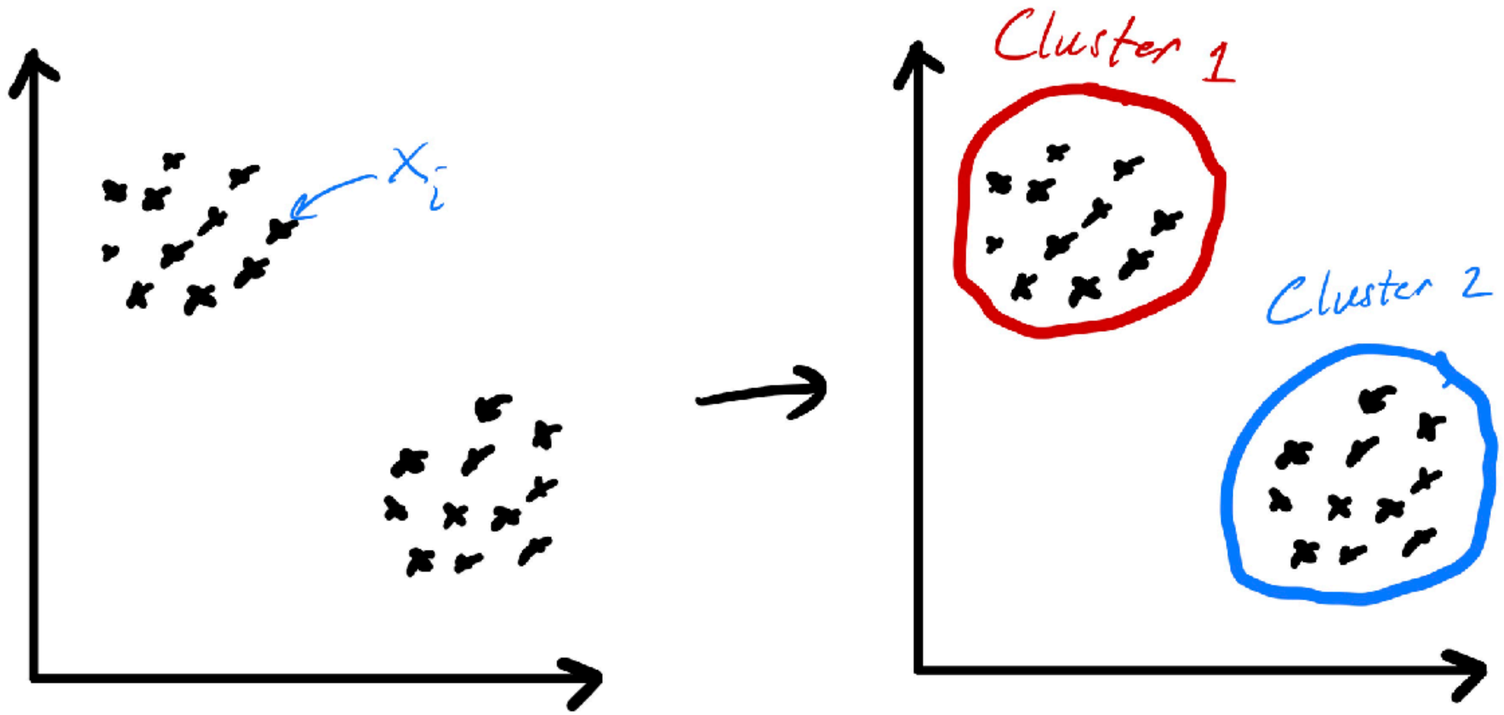
2. Unsupervised Learning: Clustering and the K-means algorithm

3. Convergence of K-means

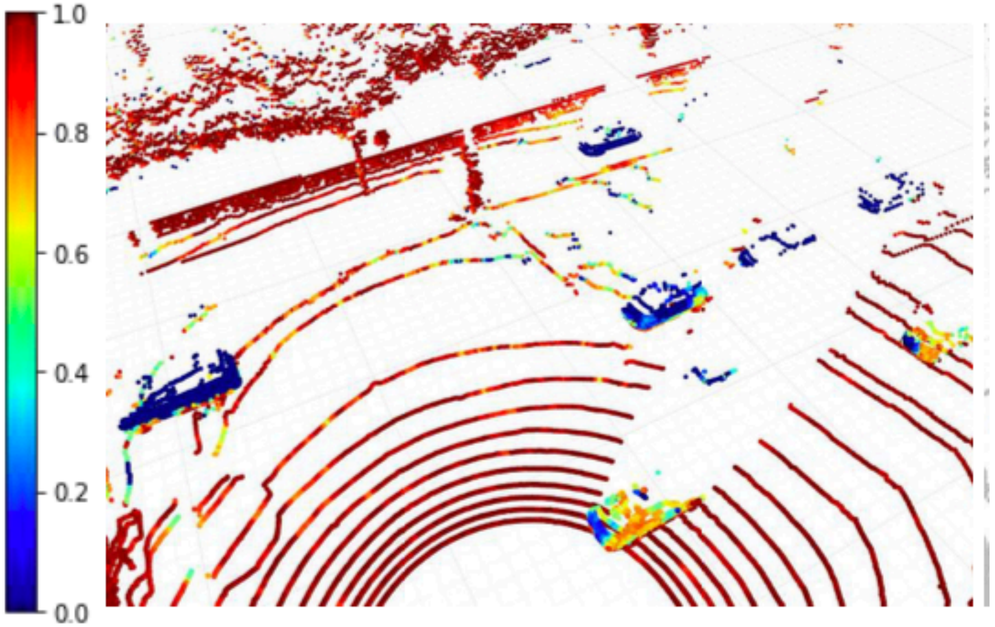
What is clustering?

It is an unsupervised learning procedure (i.e., applies to data without ground truth labels)



Usage of clustering algorithms in real world

Example: Learning to detect cars without ground truth label



A point cloud from a Lidar sweep (4-d data)

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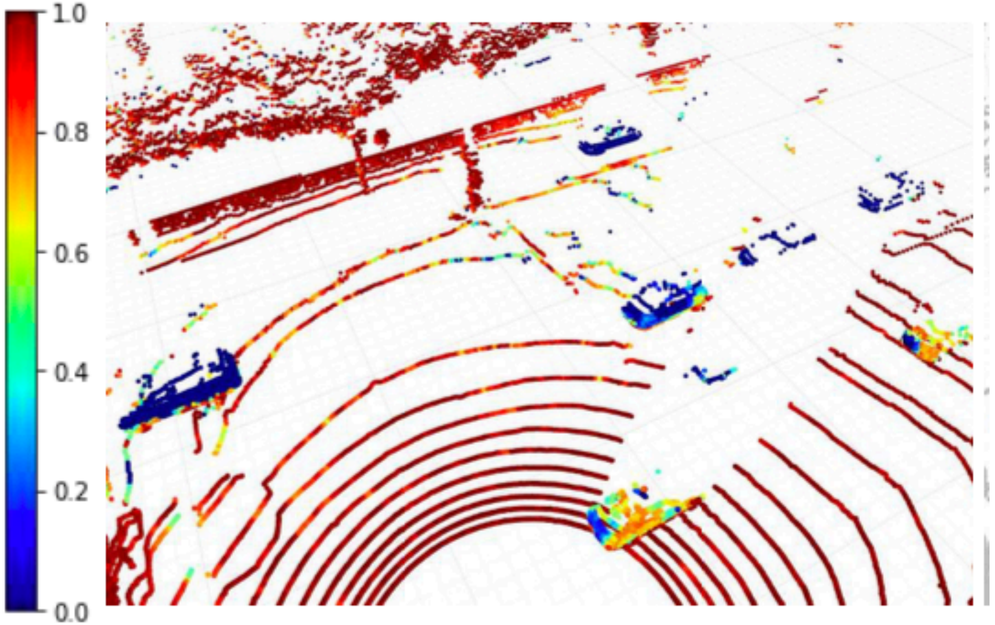
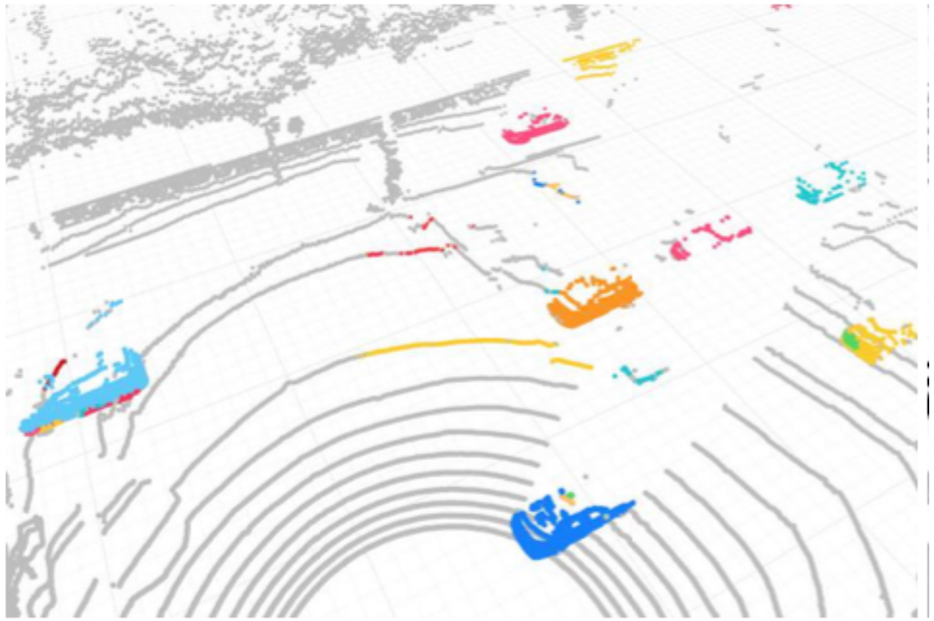


Apply clustering
on this dataset
(point cloud)



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Different color represents different clusters

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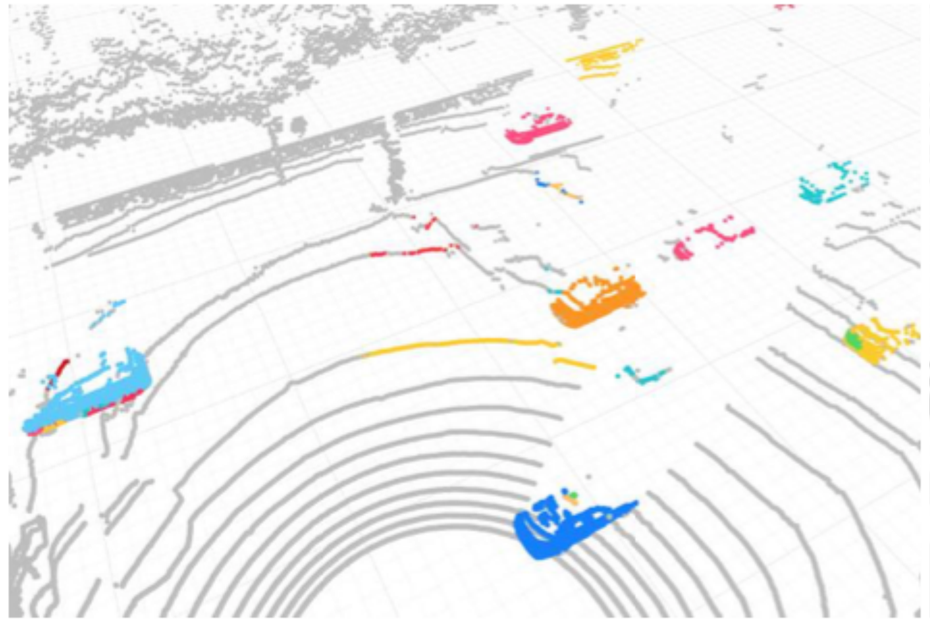
3. Fit Bounding Boxes

These boxes are the pseudo-labels we use to train detector

Fitting bounding box around clusters



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The K-means algorithm

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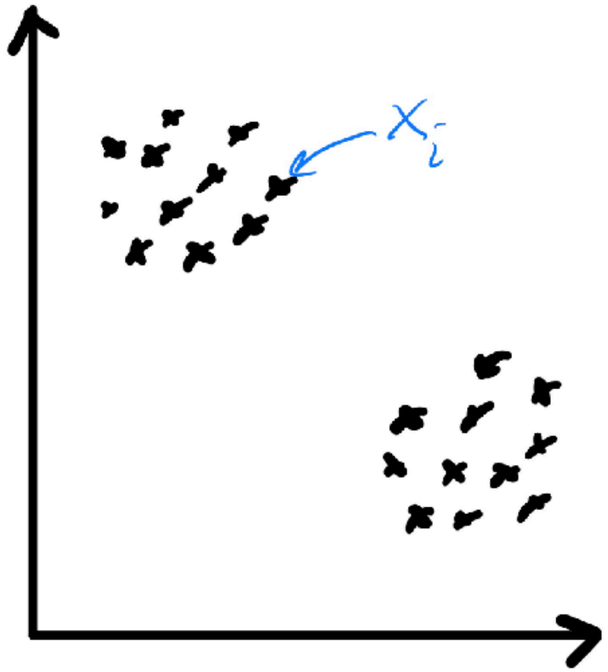

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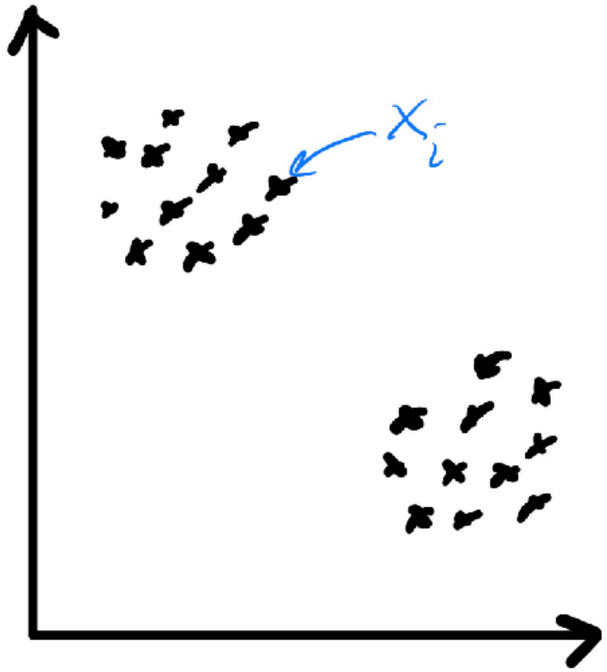

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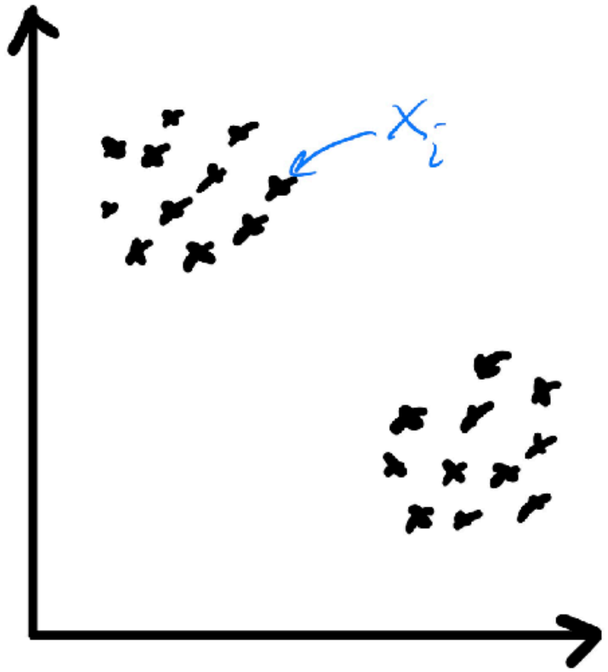

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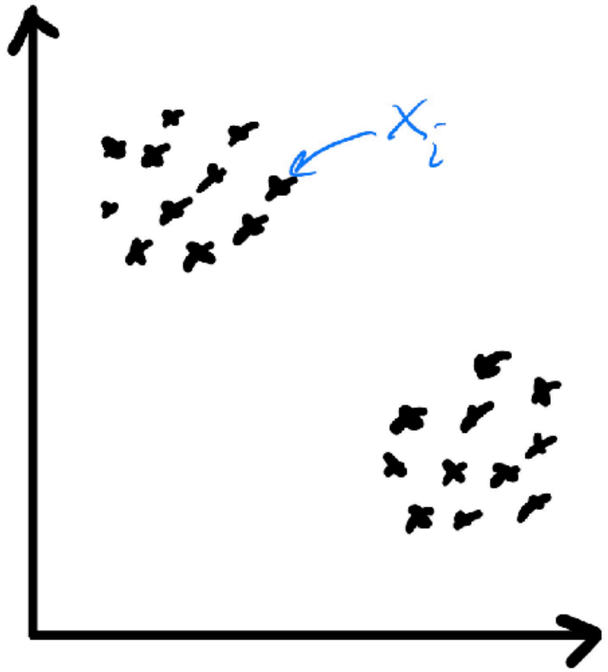

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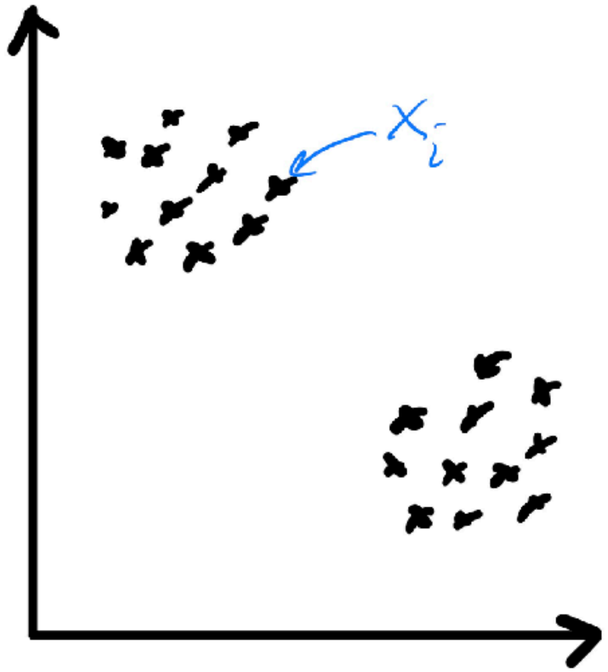

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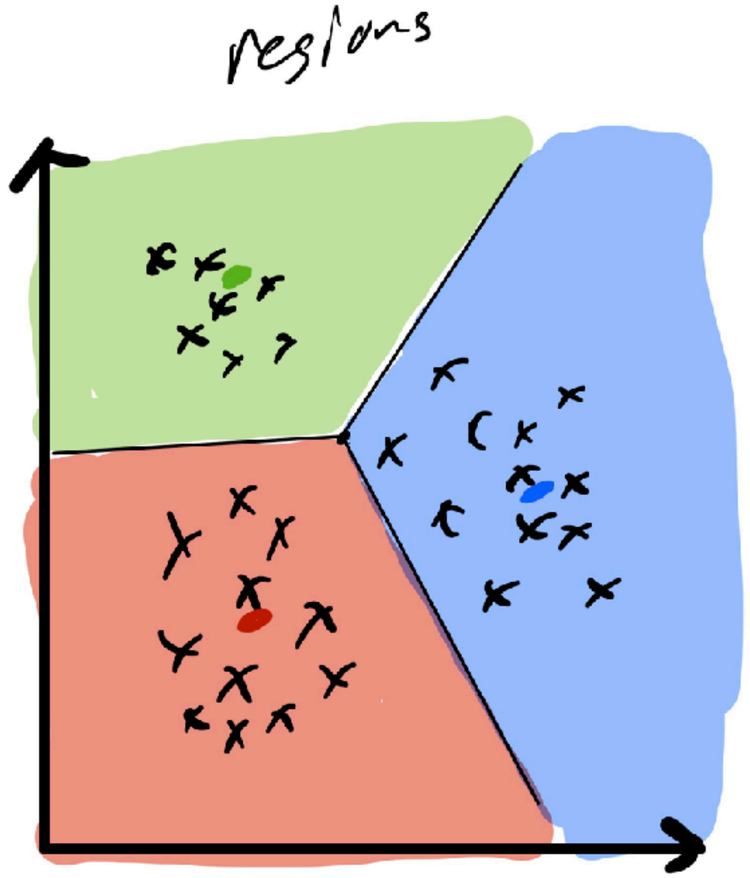
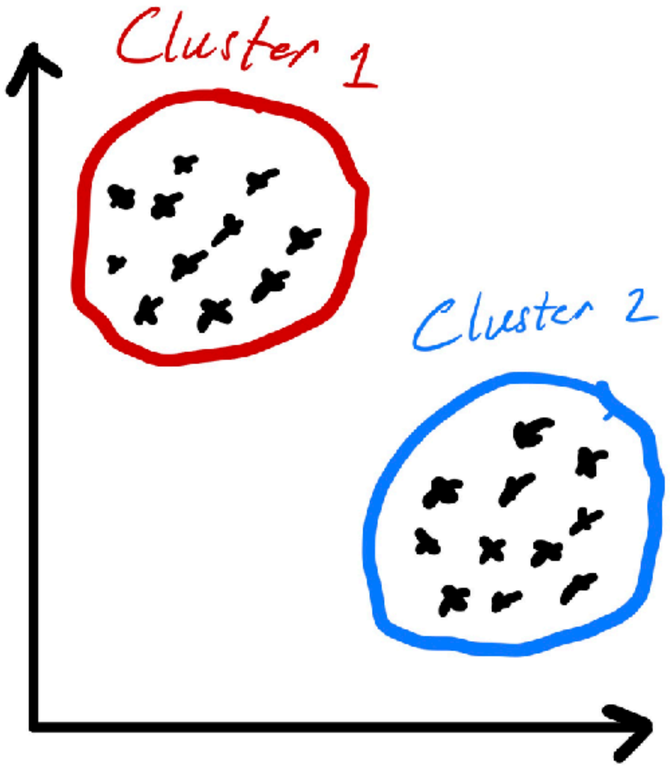
$$C_i = \{x \in \mathcal{D} \text{ s.t., } \mu_i \text{ is the closest centroid to } x\}$$

The data assignment procedure

K centroids $\mu_1, \ldots, \mu_k$ splits the space into a voronoi diagram



The centroid computation procedure



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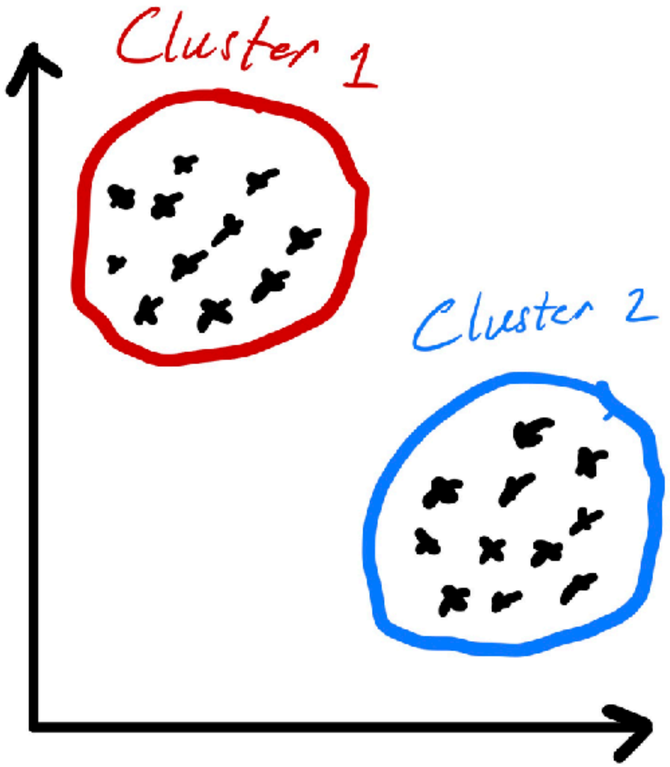

If we magically had the clusters $C_1, \ldots, C_K$, we could compute centroids as follows:

μ_i : the mean of the data in C_i

The K-means algorithm

Iterate between Centroid computation and Data Assignment!

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Initialize K clusters $C_1, C_2, \ldots, C_K$, where $\cup_{i=1}^{K} C_i = \mathscr{D}$, and $C_i \cap C_j = \emptyset$, for $i \neq j$

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1. centroids computation using $C_1, \ldots, C_K$, i.e.,for all i,
   $\mu_i = \sum_{x \in C_i} x / |C_i|$ (i.e., the mean of the data in C_i)

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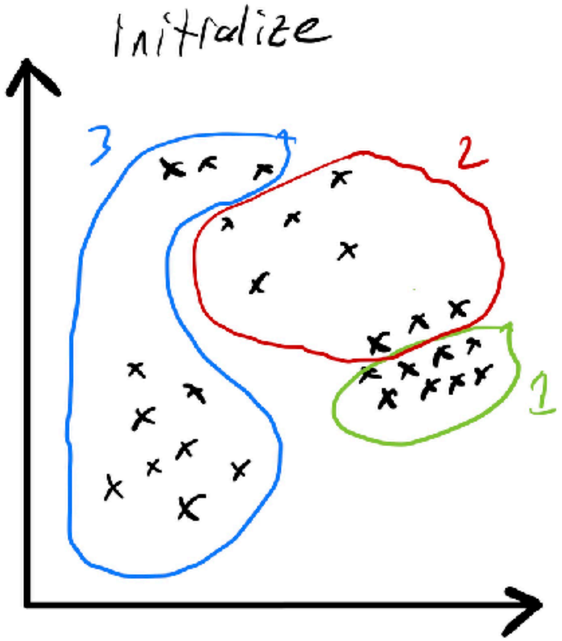
2. the data assignment procedure, i.e., re-split data into $C_1, \ldots, C_K$, using $\mu_1, \ldots, \mu_k$

The K-means algorithm



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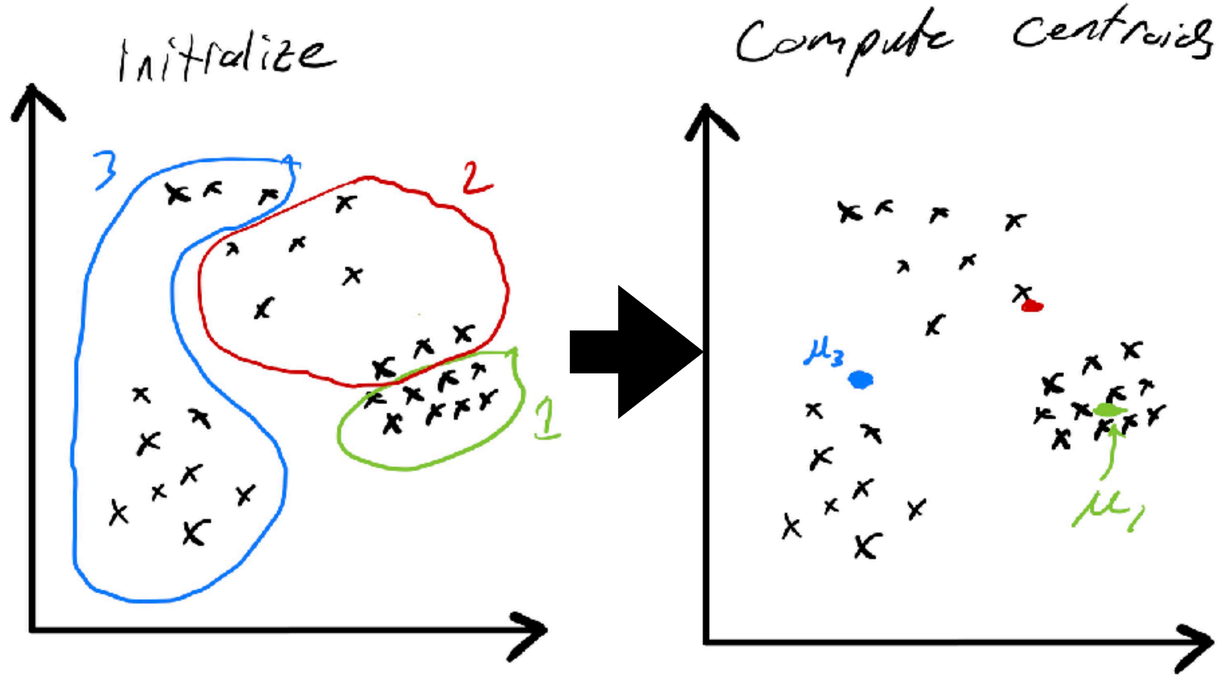

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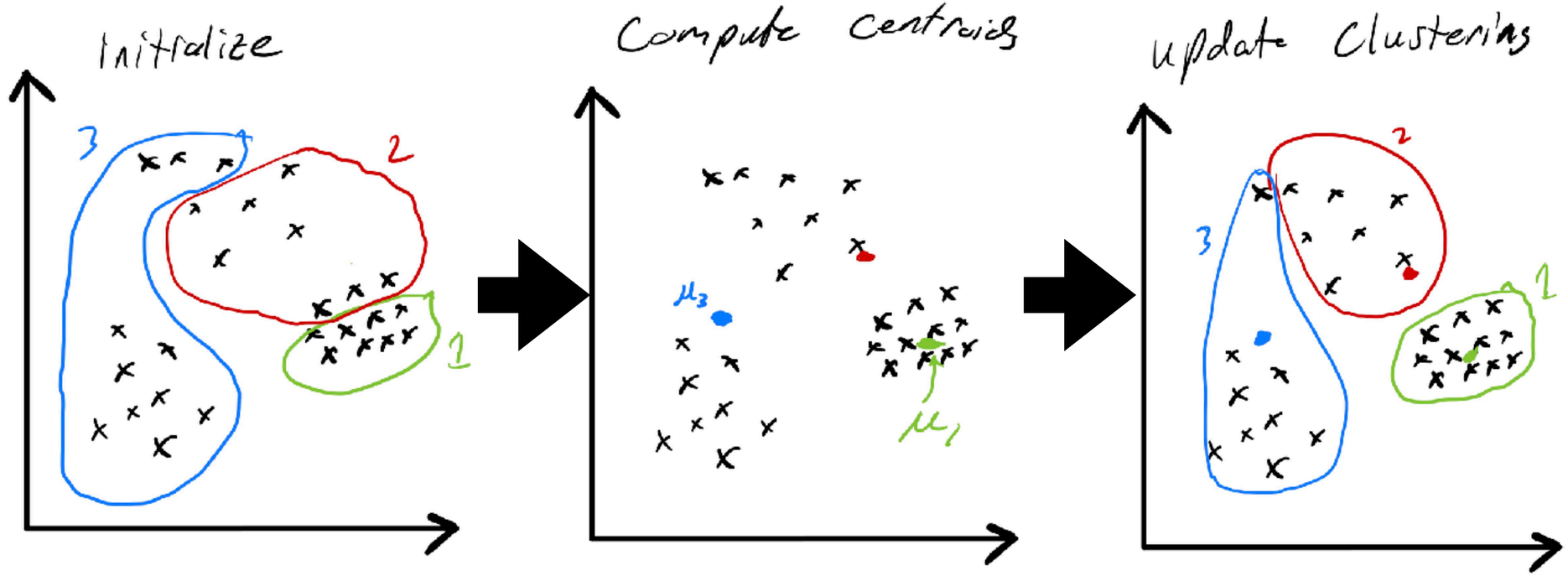

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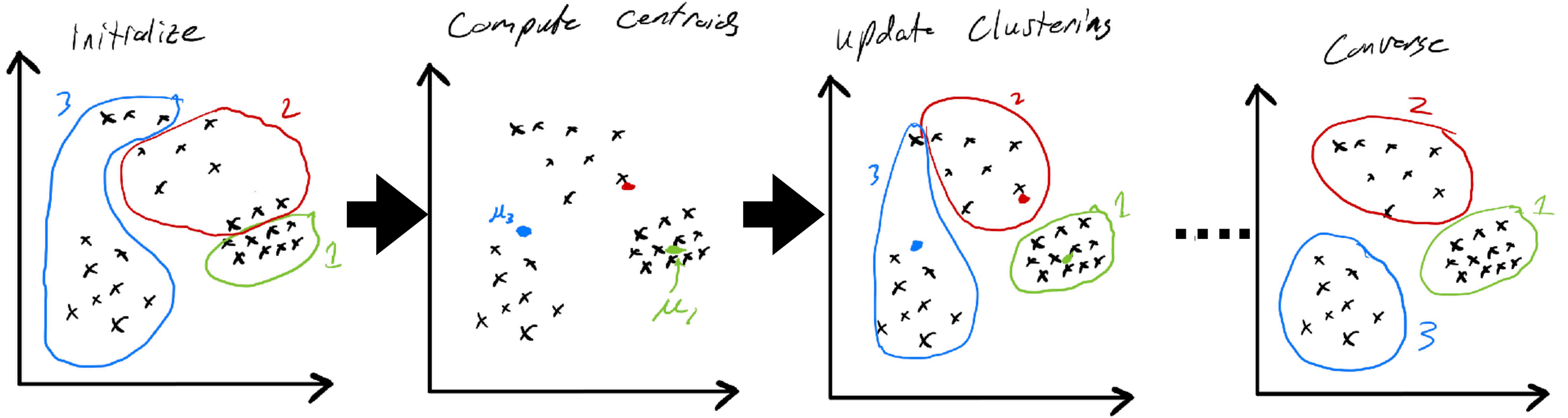

Outline for Today

1. Curse of dimensionality ✓

2. Unsupervised Learning: Clustering and the K-means algorithm ✓

3. Convergence of K-means

Does K-means algorithm converge?

Yes, though it does not guarantee to return the globally optimal solution

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Given any K disjoint groups $C_1, C_2, \ldots, C_K$, and any K centroids, define a loss function:

$$\ell(\{C_i\}, \{\mu_i\}) = \sum_{i=1}^{K} \left[\sum_{x \in C_i} \|x - \mu_i\|_2^2 \right]$$

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Total distance of points in C_i to μ_i

K-means as a Coordinate Descent Algorithm

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K means is doing Coordinate Descent here

$$\ell(\{C_i\}, \{\mu_i\}) = \sum_{i=1}^{K} \left[\sum_{x \in C_i} \|x - \mu_i\|_2^2 \right]$$

K-means Algorithm: (re-stated from a different perspective)

Initialize $\mu_1, \ldots, \mu_K$

Repeat until convergence:

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Given K, we can look at the minimum loss

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No! When $K = n$, loss is zero (every data point is a cluster!)

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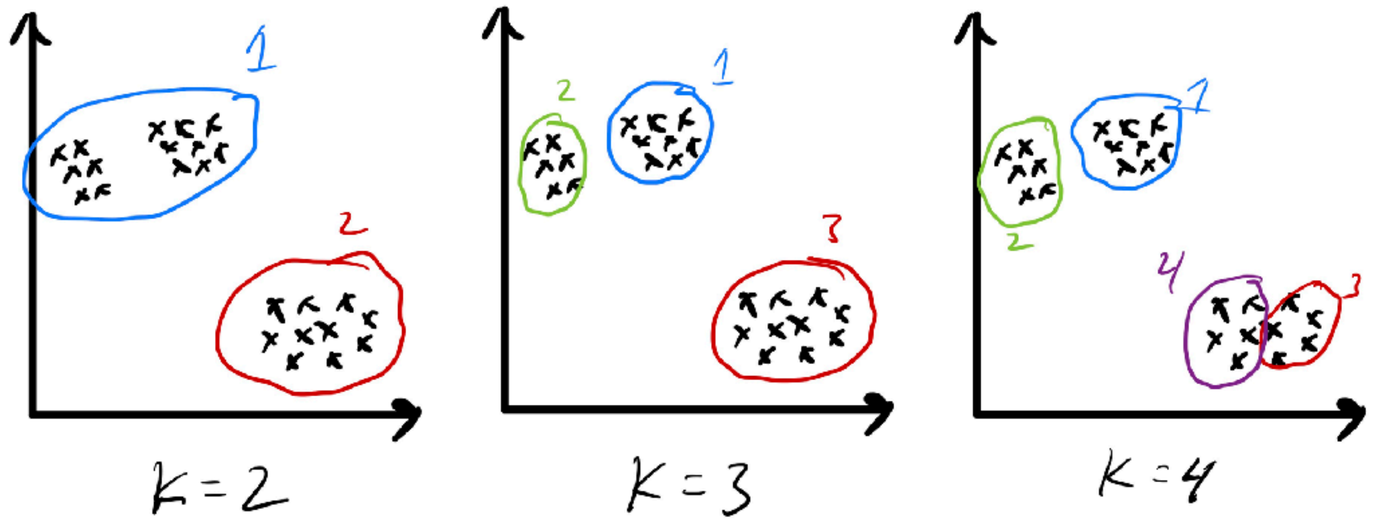

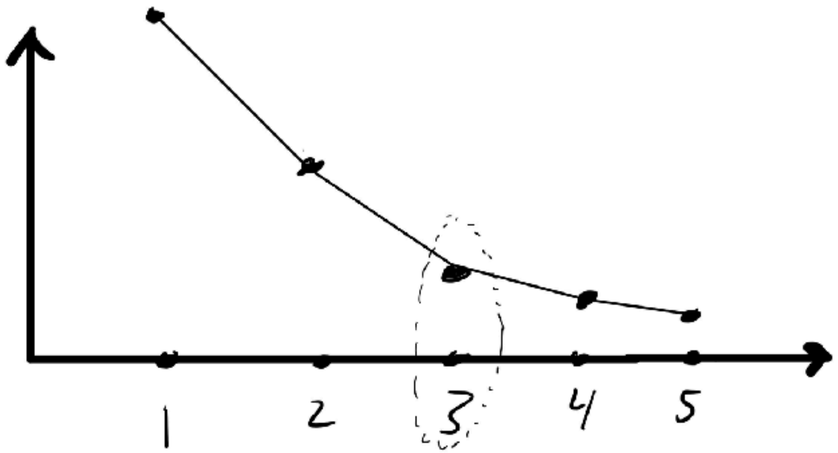

Summary

1. Curse of Dimensionality:

Data points in high-dim space tends to spread far from each other

2. The first Unsupervised Learning Algorithm — K means

Coordinate Descent on the loss $\ell(\{C_i\}, \{\mu_i\})$