CSC 480/580 Principles of Machine Learning

03 Geometry & Nearest Neighbors

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Outline

- Nearest neighbor methods for supervised learning

- Clustering and the k-means algorithm

Nearest neighbors for supervised learning

Motivation

Example Given student course survey data, predict whether Alice likes Algorithms course

Idea Find a student ``similar'' to Alice & has taken Algorithm course before, say Jeremy

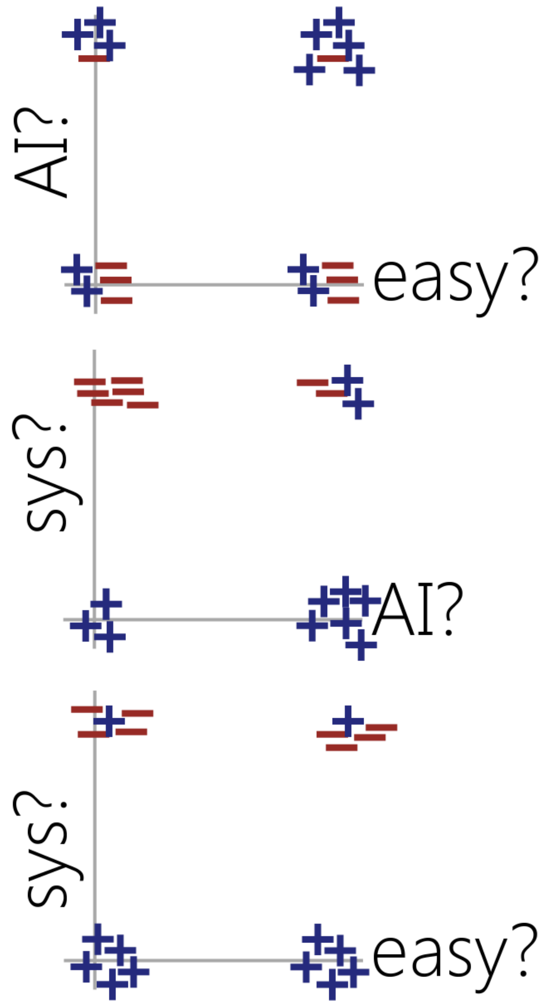
- If Jeremy likes Algorithms, then Alice is also likely to have the same preference.
- Or even better, find *several* similar students

- Prediction = mapping inputs to outputs
- Inputs = *features* that can be viewed as points in some space (possibly high-dimensional)
- "Similarity" = "distance" in feature space
- Suggests a **geometric** view of data

Example: Course Recommendation

Rating	Easy?	AI?	Sys?	Thy?	Morning?
+2	y	y	n	y	n
+2	y	y	n	y	n
+2	n	y	n	n	n
+2	n	n	n	y	n
+2	n	y	y	n	y
+1	y	y	n	n	n
+1	y	y	n	y	n
+1	n	y	n	y	n
0	n	n	n	n	y
0	y	n	n	y	y
0	n	y	n	y	n
0	y	y	y	y	y
-1	y	y	y	n	y
-1	n	n	y	y	n
-1	n	n	y	n	y
-1	y	n	y	n	y
-2	n	n	y	y	n
-2	n	y	y	n	y
-2	y	n	y	n	n
-2	y	n	y	n	y

Features



ML begins by mapping data to feature vectors

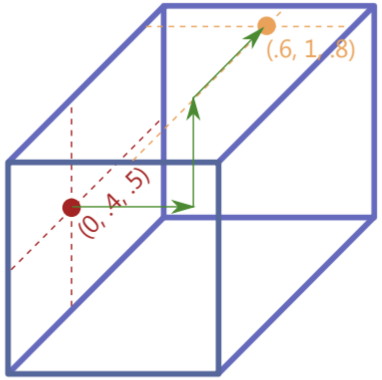
Represented as points in 5-dimensional space for this example

That's too many dimensions to plot…so we look at 2D projections…

Measuring nearest neighbors

- Oftentimes convenient to work with feature $x \in \mathrm{R}^d$
- Distances in R^d:

notation $x(f)$: $x = (x(1), \dots, x(d))$

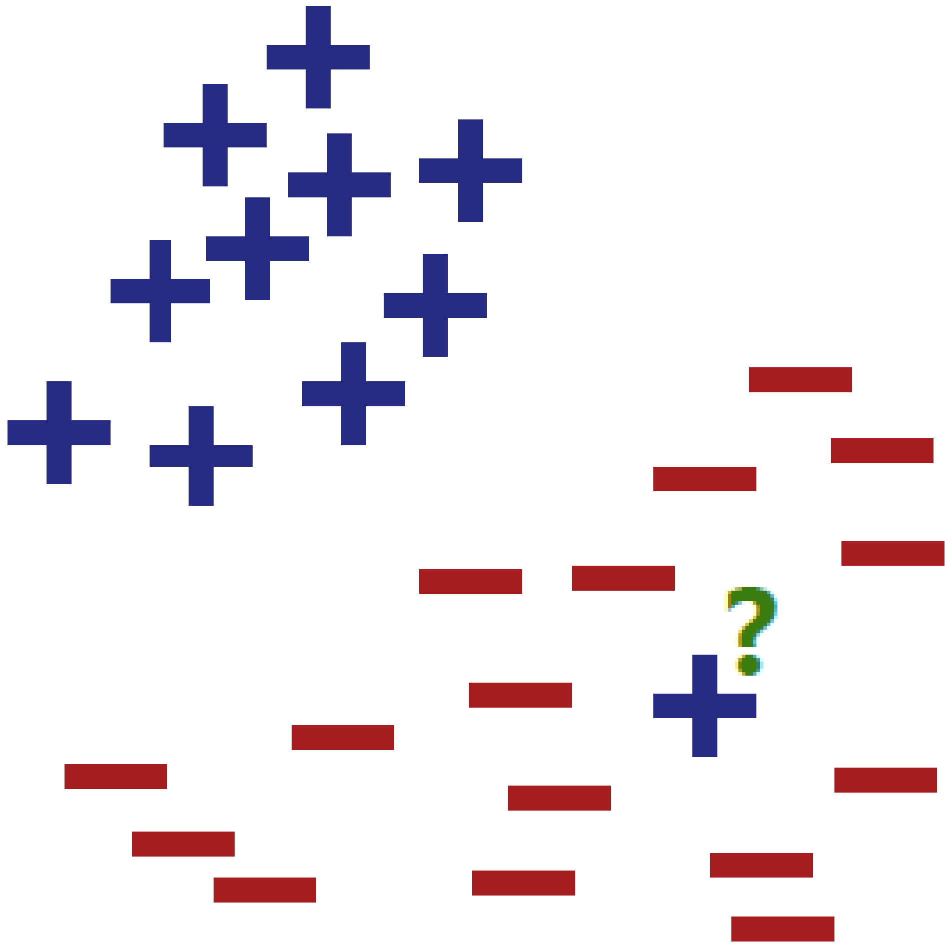


  - (popular) Euclidean distance $d_2(x, x') = \sqrt{\sum_{f=1}^{d} \left(x(f) - x'(f)\right)^2}$
  - Manhattan distance $d_1(x, x') = \sum_{f=1}^{d} |x(f) - x'(f)|$

  - If we shift a feature, would the distance change?
  - What about scaling a feature?

- How to extract features as **<u>real values</u>**?
  - Boolean features: {Y, N} -> {0,1}
  - Categorical features: {Red, Blue, Green, Black}
    - Convert to {1, 2, 3, 4}?
    - Better one-hot encoding: (1,0,0,0), .., (0,0,0,1) (IsRed?/isGreen?/isBlue?/IsBlack?)

Nearest Neighbor Classification



Query point ? Will be classified as +
but should be -

Problem: predicting using 1 nearest neighbor's label can be sensitive to noisy data

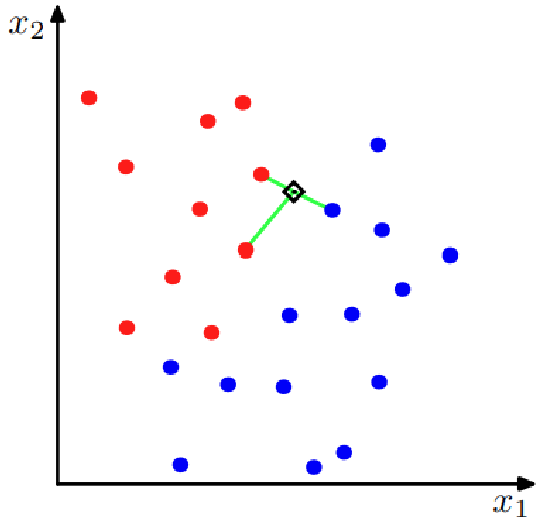
How to mitigate this?

k-nearest neighbors (k-NN): main concept

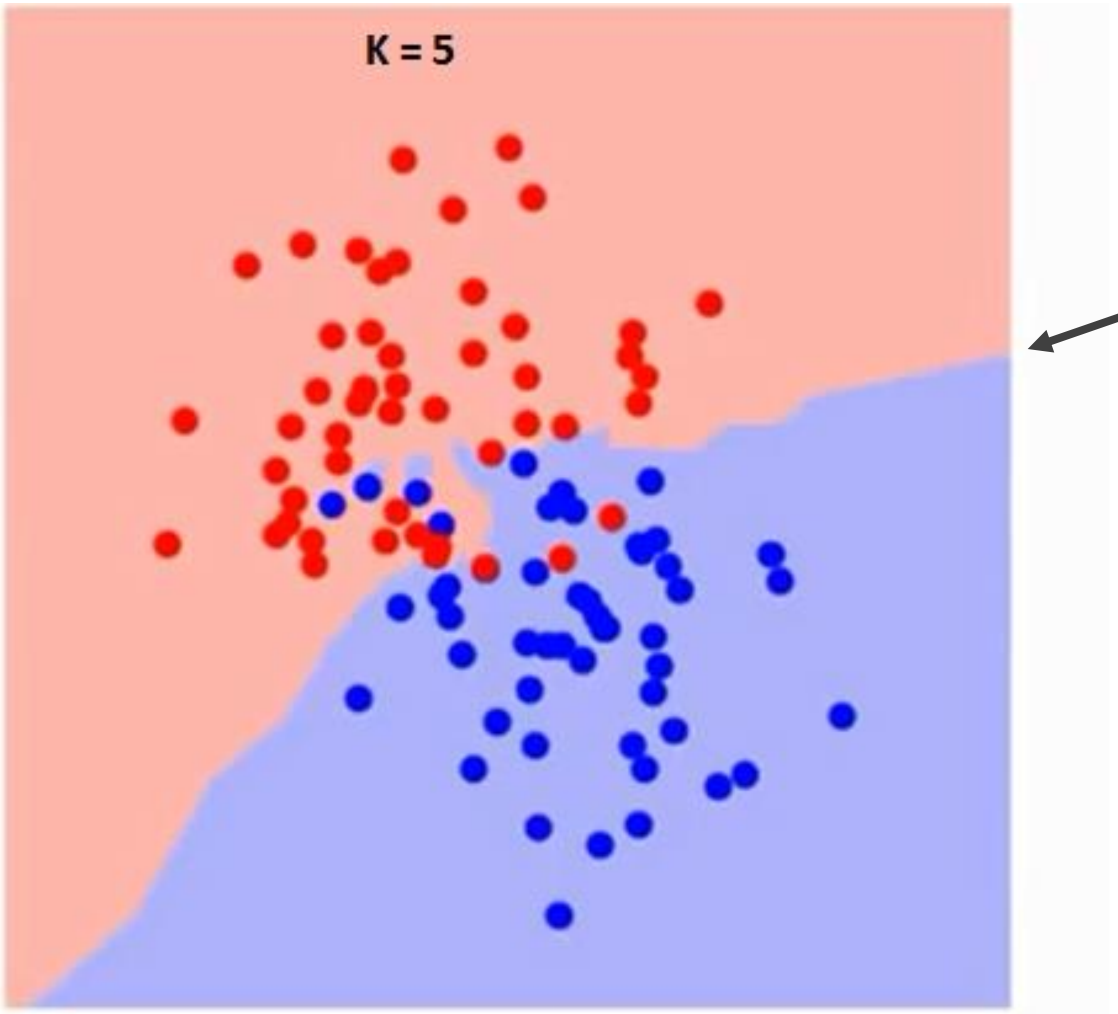
- Training set: $S = \{ (x_1, y_1), \ldots , (x_m, y_m)\}$

- **<u>Inductive bias</u>**: given test example x, its label should resemble the labels of **nearby points**

- Function
  - input: x
  - find the k nearest points to x from S; call their indices $N(x)$
  - output:
    - (classification) the majority vote of $\{y_i : i \in N(x)\}$
    - (regression) the average of $\{y_i : i \in N(x)\}$



k-NN classification example



decision boundary

k-NN classification: pseudocode

- Training is trivial: store the training set
- Test:

Algorithm 3 KNN-PREDICT($\mathbf{D}$, K, $\hat{x}$)

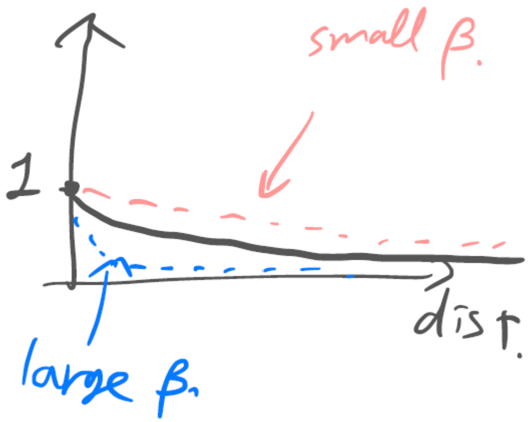
list	$S \leftarrow [\,]$	
	for $n = 1$ **to** N **do**	
append to list	$\quad S \leftarrow S \oplus \langle \mathrm{d}(x_n, \hat{x}), n \rangle$	// store distance to training example n
	end for	
sort in first coordinate (distance)	$S \leftarrow \textsc{sort}(S)$	// put lowest-distance objects first
	$\hat{y} \leftarrow 0$	
	for $k = 1$ **to** K **do**	
	$\quad \langle dist, n \rangle \leftarrow S_k$	// n this is the kth closest data point
	$\quad \hat{y} \leftarrow \hat{y} + y_n$	// vote according to the label for the nth training point
	end for	
Majority vote of $\{y_i : i \in N(x)\}$	**return** $\textsc{sign}(\hat{y})$	// return $+1$ if $\hat{y} > 0$ and -1 if $\hat{y} < 0$

- Time complexity (assuming distance calculation takes $O(d)$ time)
  - $O(m\,d + m\log m + k) = O\big(m(d + \log m)\big)$
- Faster nearest neighbor search: k-d trees, locality sensitive hashing

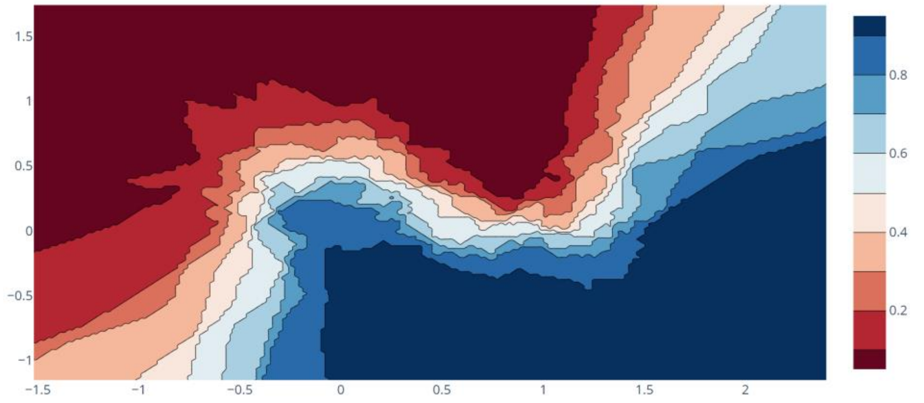
Variations

- Classification
  - Recall the majority vote rule: $\hat{y} = \underset{y \in \{1,\ldots,C\}}{\operatorname{argmax}} \sum_{i \in N(x)} 1\{y_i = y\}$
  - Soft weighting nearest neighbors: $\hat{y} = \underset{y \in \{1,\ldots,C\}}{\operatorname{argmax}} \sum_{i=1}^{m} w_i \, 1\{y_i = y\}$,

    where $w_i \propto \exp(-\beta \, d(x, x_i))$, or $\propto \frac{1}{1+d(x,x_i)^\beta}$



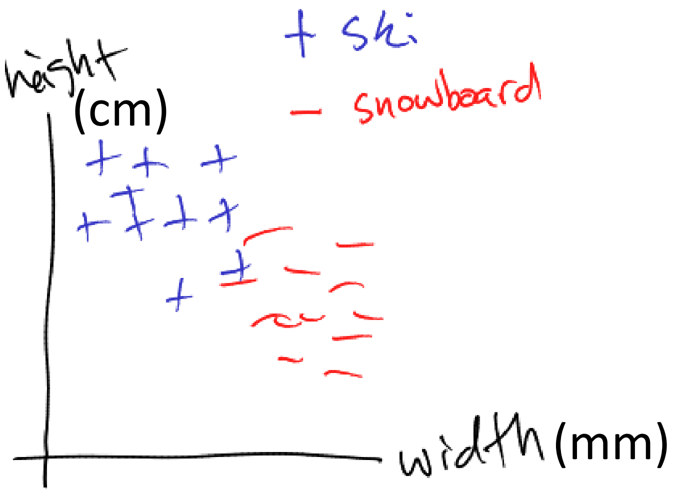
- Class probability estimates
  - $\hat{P}(Y = y \mid x) = \frac{1}{k} \sum_{i \in N(x)} 1\{y_i = y\}$
  - Useful for “classification with rejection” / label uncertainty quantification

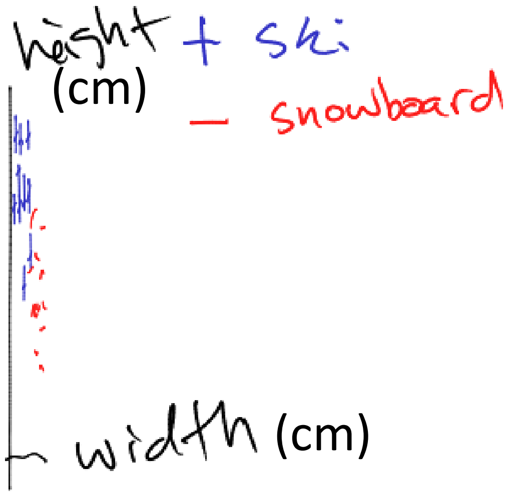


Feature issue 1: scaling

- Features having different scales can be problematic.

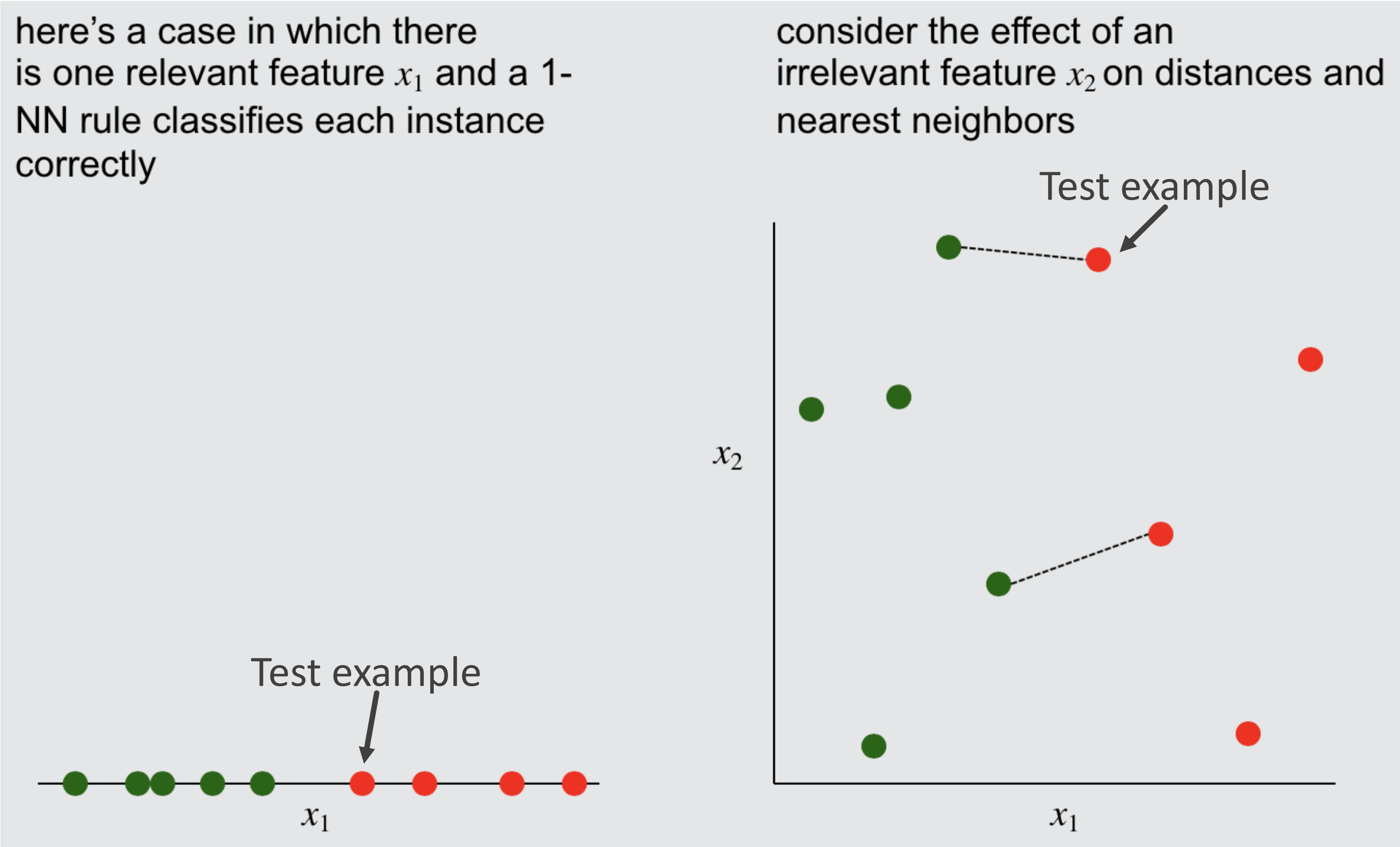
- Ex: ski vs. snowboard classification





- One solution: feature standardization (later in the course)

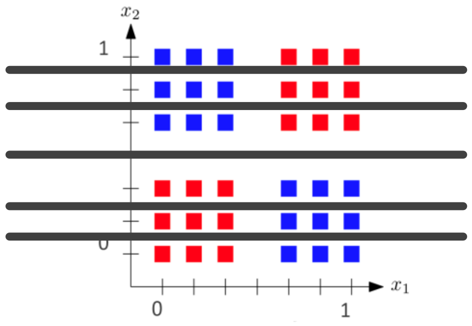
Feature issue 2: irrelevant features



- Recall: how did we deal with irrelevant features in training decision trees?
- Solution: feature selection (later in the course)

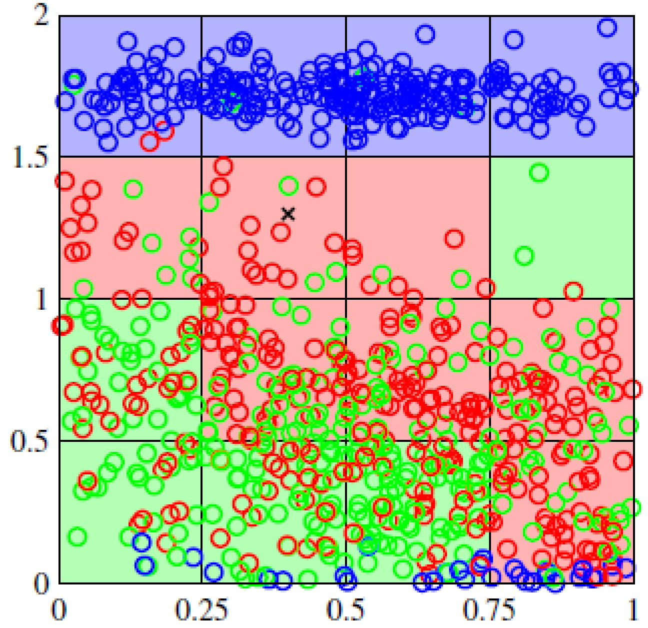
Comparison (feature $x \in \mathrm{R}^d$)

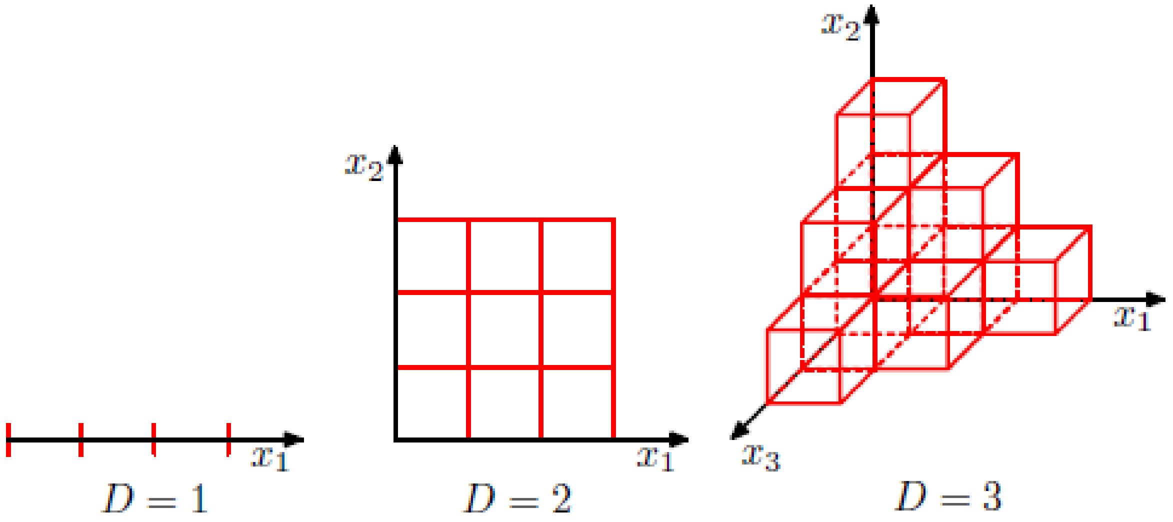
	Decision Tree	k-NN
• Interpretability	High	Medium (example-based)
• Sensitivity to irrelevant features	Low	High
• training time	$O(\#\text{nodes} \cdot d \cdot \ (m + m \log m)\ )$ $\leq \tilde{O}(d\, m^2)$ (when no two points have the same feature)	0
• test time per example	$O(\text{depth})$	$O\big(m(d \ + \log m)\big)$



Curse of Dimensionality

Divide space into regular intervals





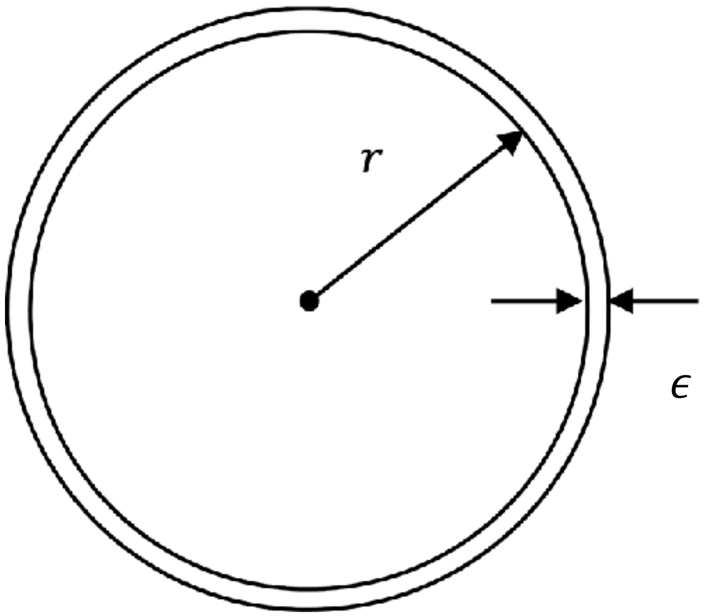
Number of required cells grows exponentially in dimension!

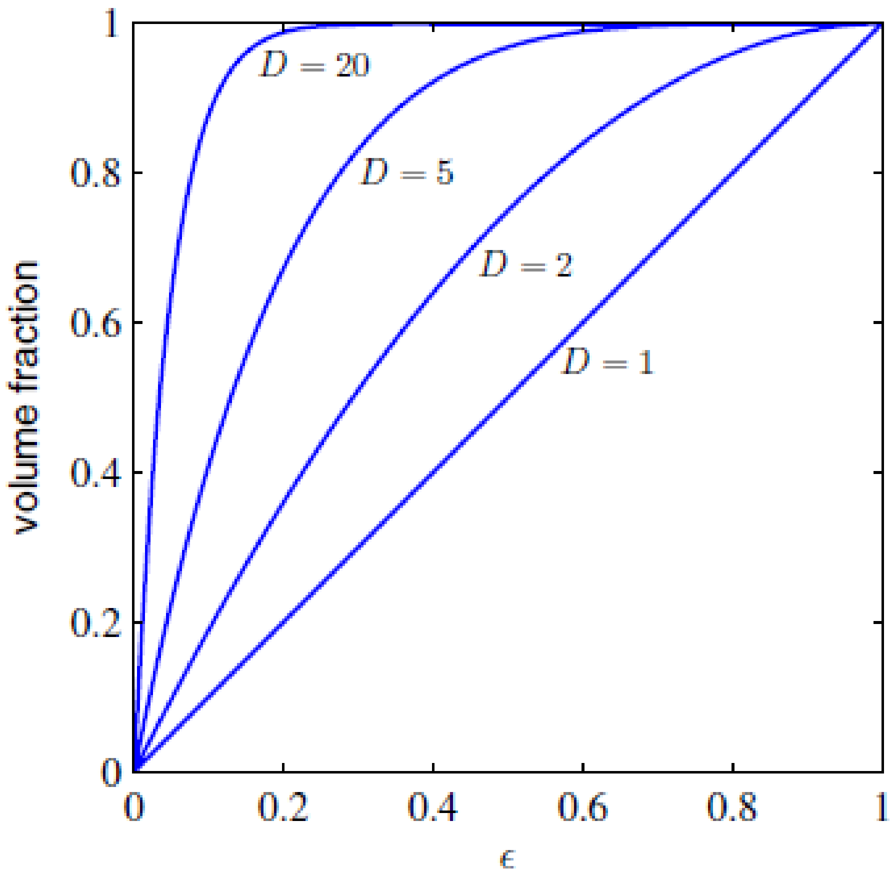
Implications for high-dimensional data:

- Nearest neighbors may actually be far away
- k-NN classifier may not perform very well

Curse of Dimensionality – Distance Weirdness

- Consider *D*-dimensional hypersphere of radius *r=1*
- What is the fraction of volume within shell of width ϵ?



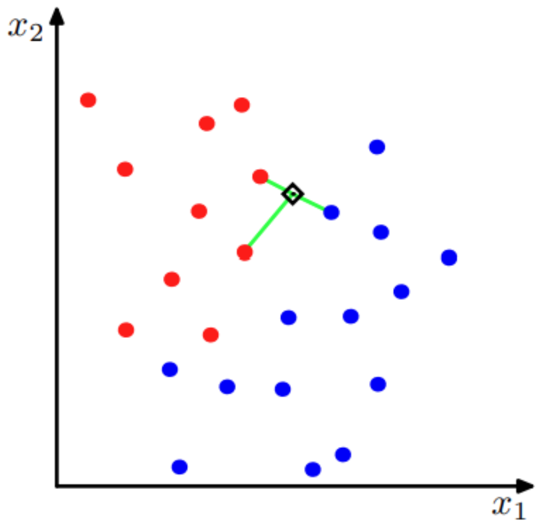


- Total volume of hypersphere concentrates onto shell at the surface!

Intuition about lower dimensions doesn't extend to high dimensions

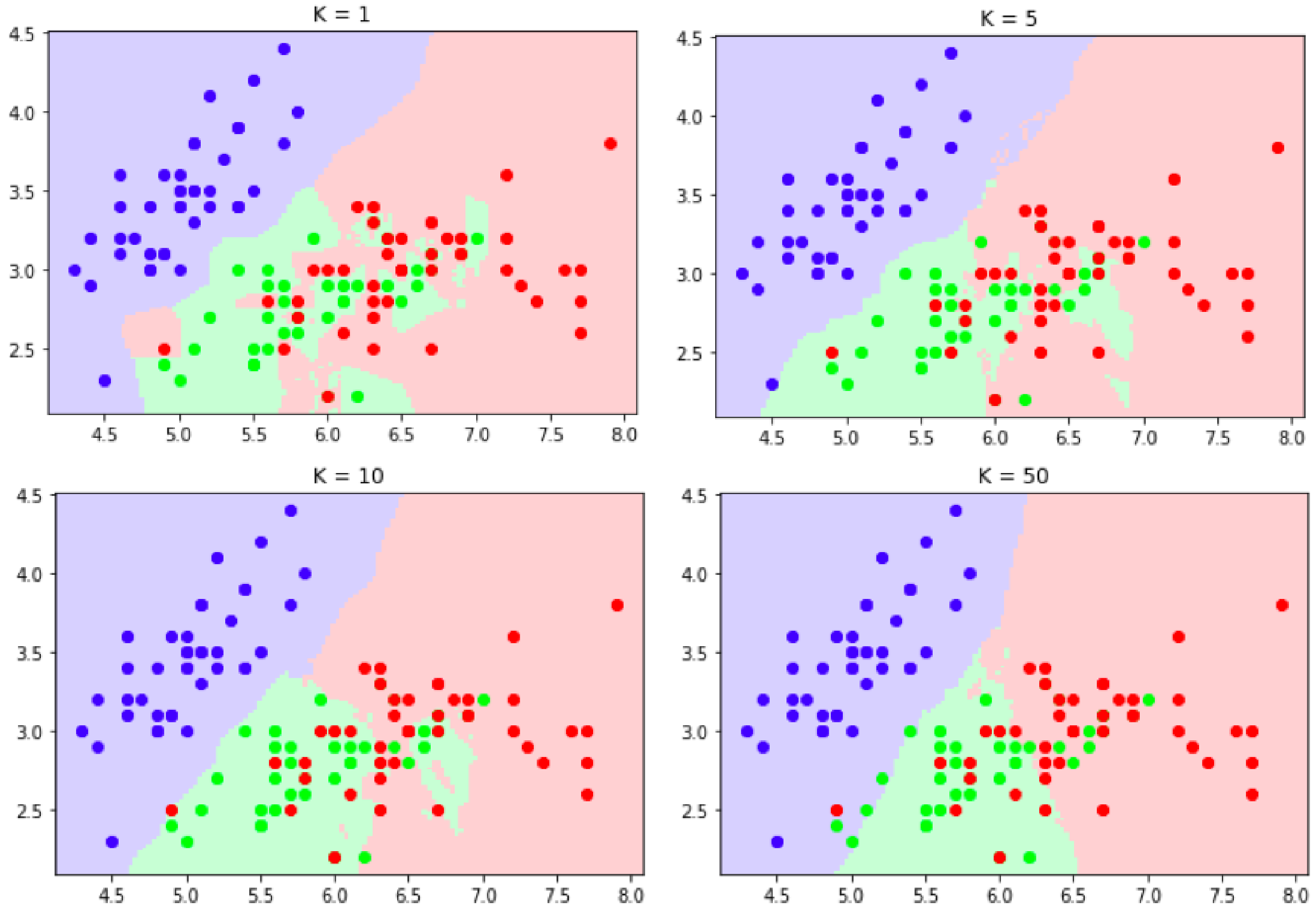
Hyperparameter tuning in k-NN

- Q: What are the hyperparameters for k-NN?
  - k, # of neighbors used for prediction

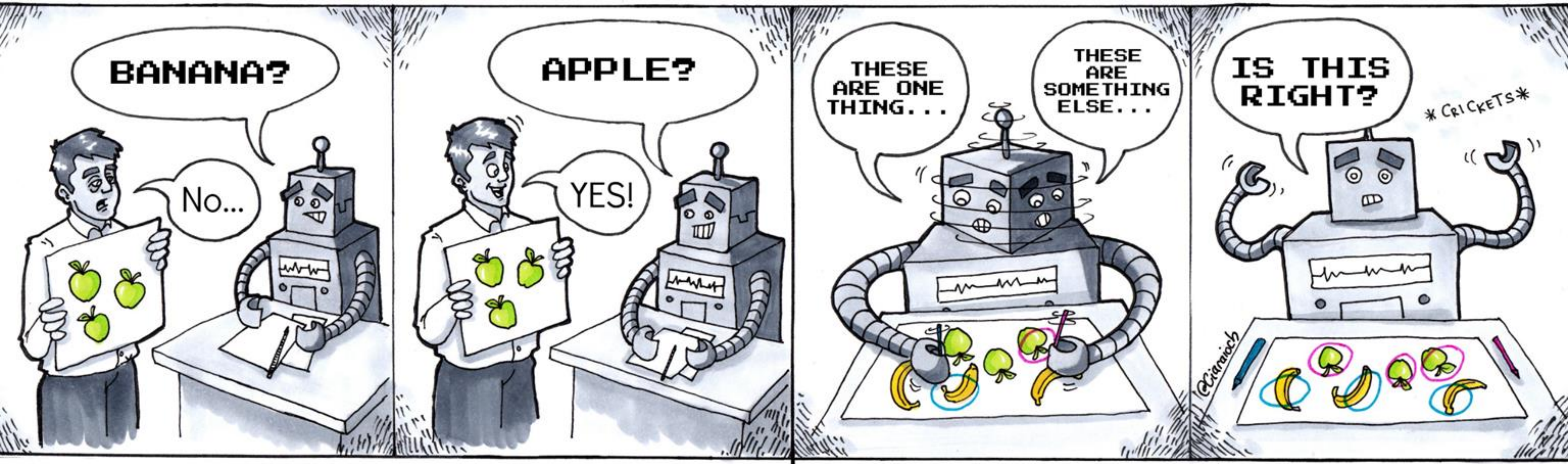


- $k = 1$:
  - Training error = 0, overfitting
- $k = m$:
  - Output a constant (majority class) prediction, underfitting
- From last lecture: can use hold-out validation set to perform hyperparameter tuning, i.e., choose k

Hyperparameter tuning in k-NN



Clustering; k-means algorithm



Supervised Learning

Unsupervised Learning

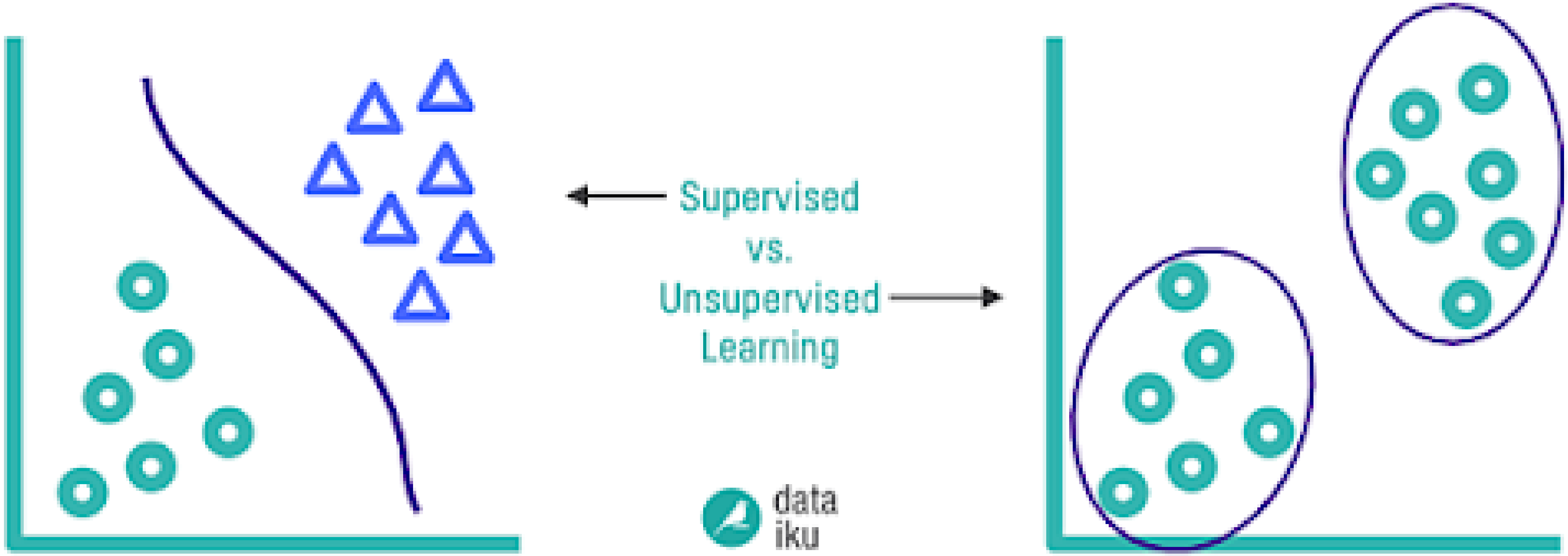
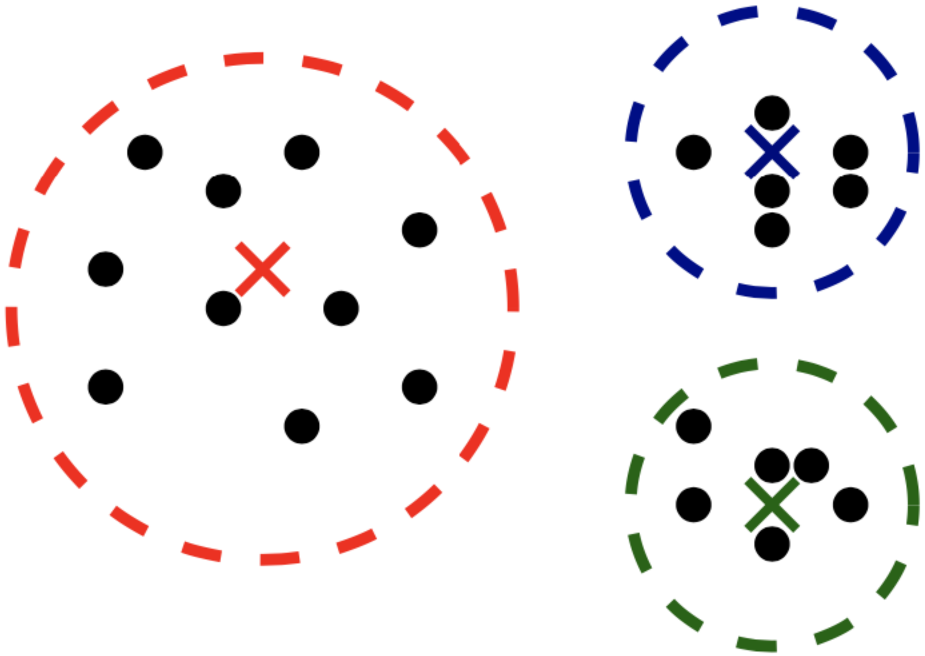


Image from [Dataiku]

Clustering

- Input: k: the number of clusters (hyperparameter)

  dataset: $S = \{x_1, \ldots, x_n\}$
- Output:
  - partition $\{G_i\}_{i=1}^k$ s.t. $S = \cup_i G_i$ (disjoint union).
  - often, we also obtain 'centroids'



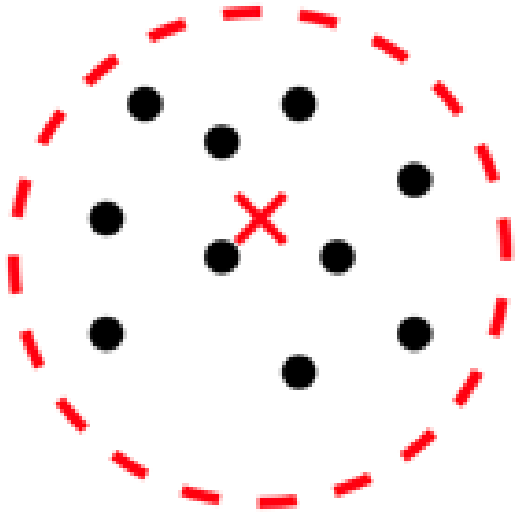
- Q: what would be a reasonable definition of centroids?

Centroid of a point set

- Intuition: a centroid c of point set $S = \{z_1, \dots, z_n\}$ should be close to all points in that set

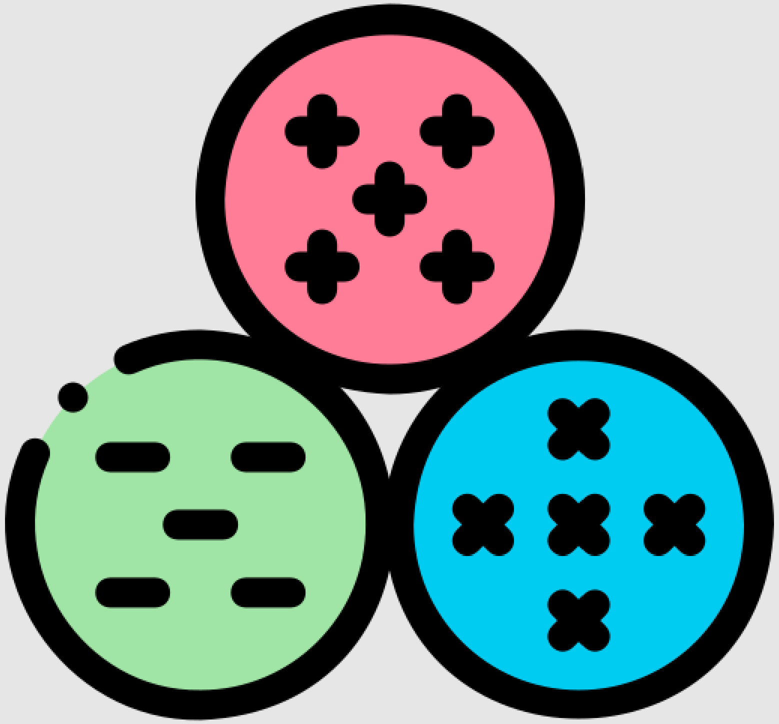
- A reasonable definition: c minimizes the sum of squared distances to points in S:

$$c = \underset{w \in \mathbb{R}^d}{\operatorname{argmin}} \|z_1 - w\|^2 + \cdots + \|z_n - w\|^2$$

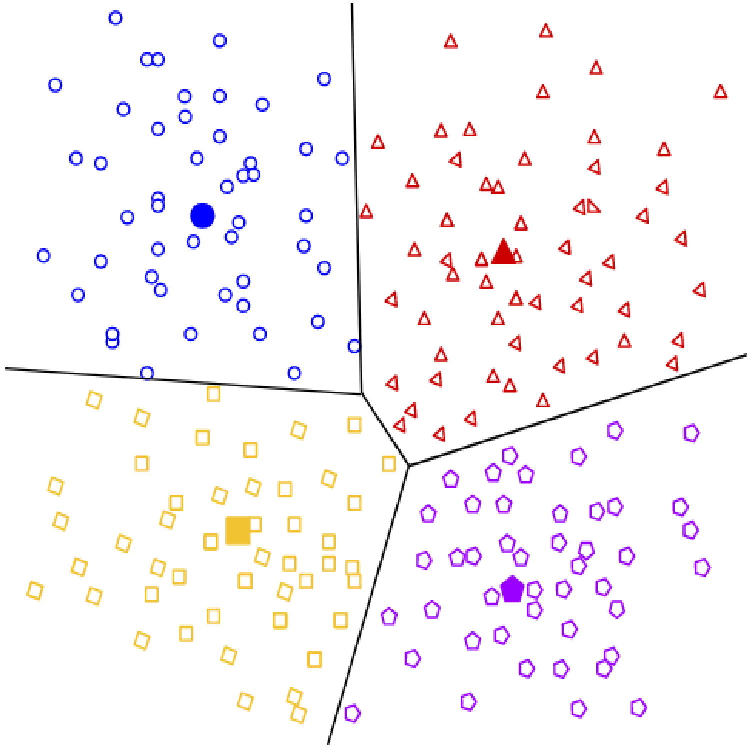


- When $d = 1$: $c = \bar{z} = \frac{1}{\mathrm{n}} \sum_{i=1}^{n} z_i$ (*)
- Fact: (*) is still true for general d

K-means algorithm [Lloyd'82]: Intuition



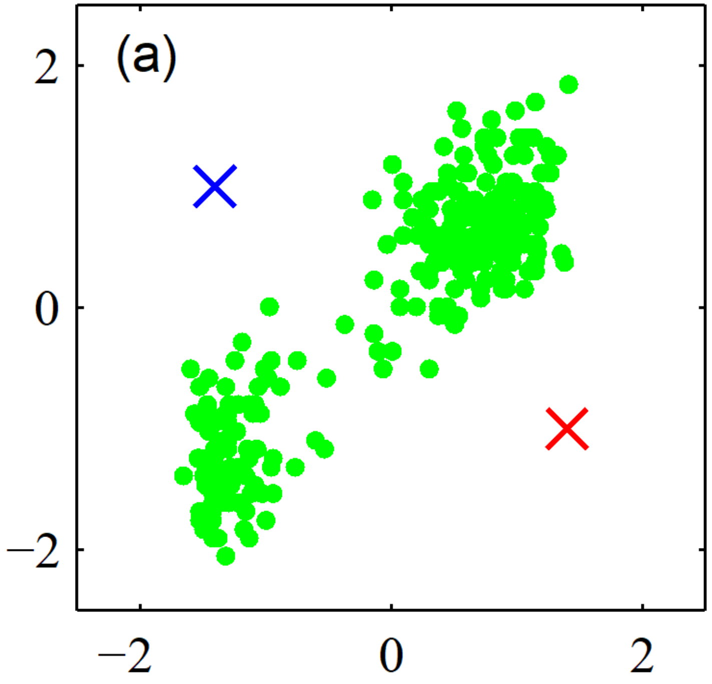
K-means algorithm



- Initialize Cluster Centroids

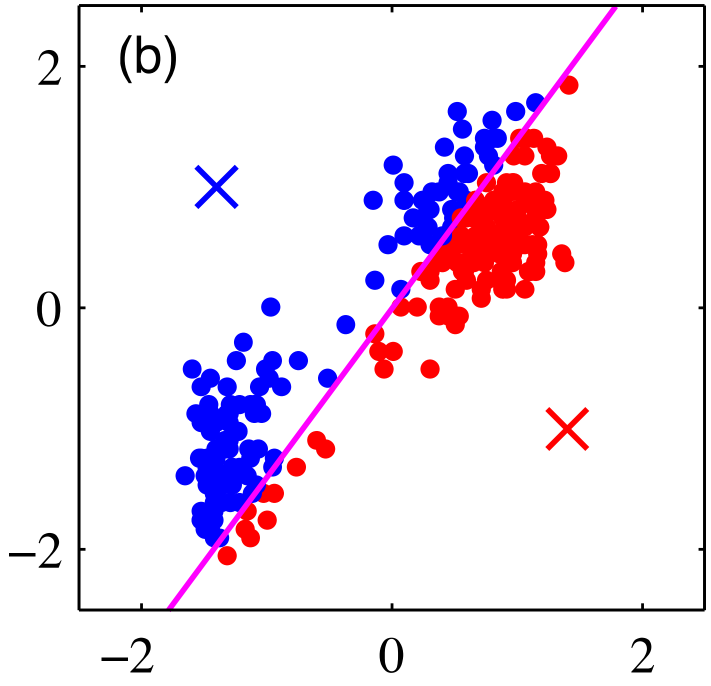
- Until Convergence:
    - **Cluster Assignment:** for each point, assign it to the cluster with the nearest centroid
    - **Recompute Centroid:** for each cluster, recompute its centroid to be the cluster mean

Initialization

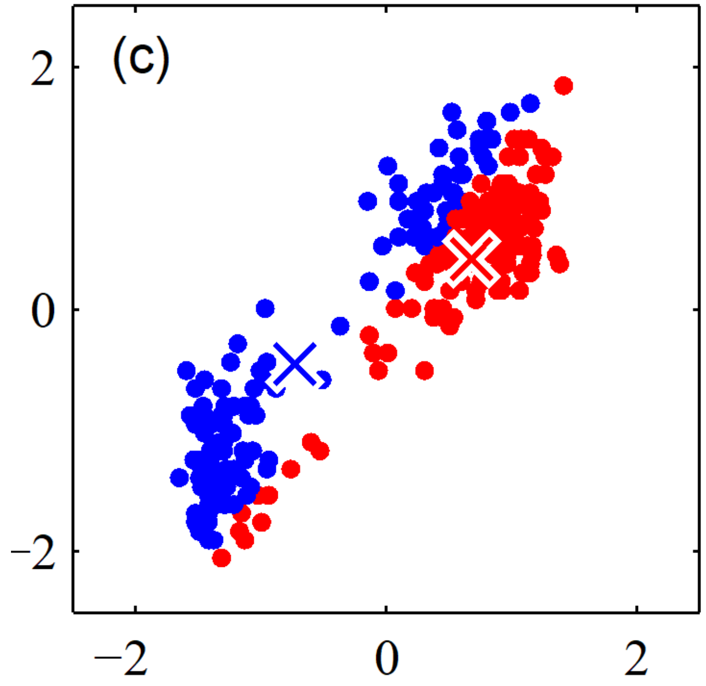


Arbitrary/random initialization of c_1 and c_2

Iteration 1

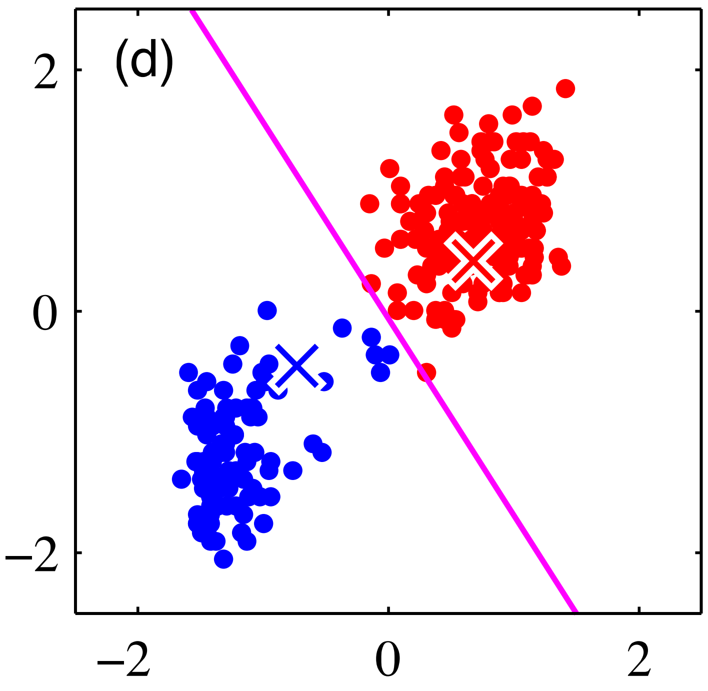


(A) update the cluster assignments.

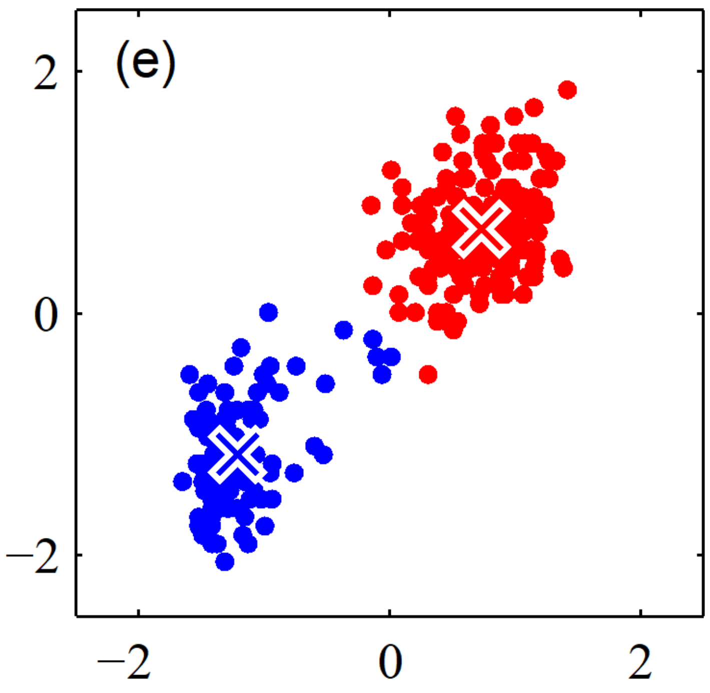


(B) Update the centroids $\{c_j\}$

Iteration 2

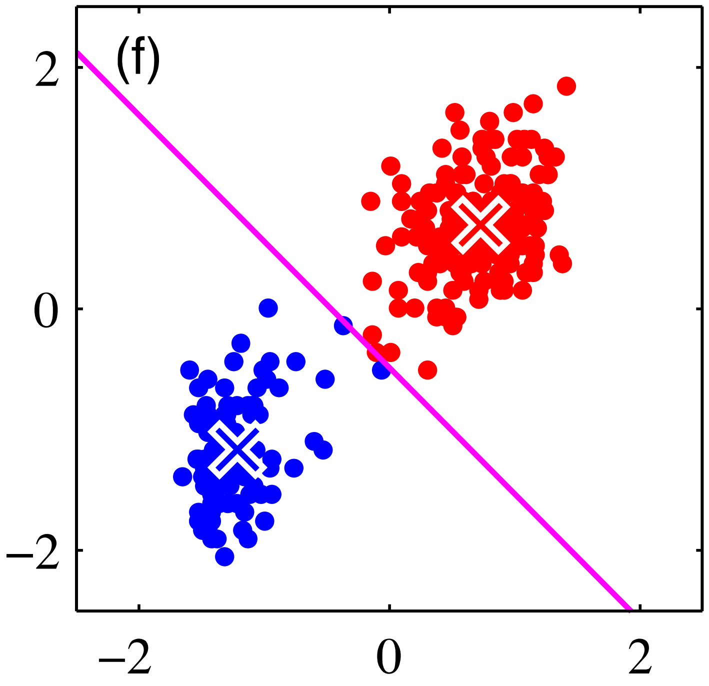


(A) update the cluster assignments.

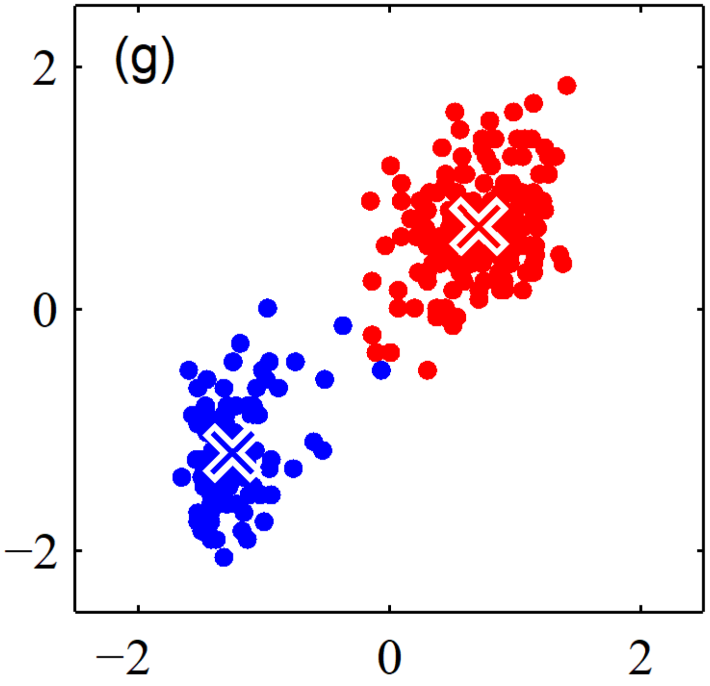


(B) Update the centroids $\{c_j\}$

Iteration 3

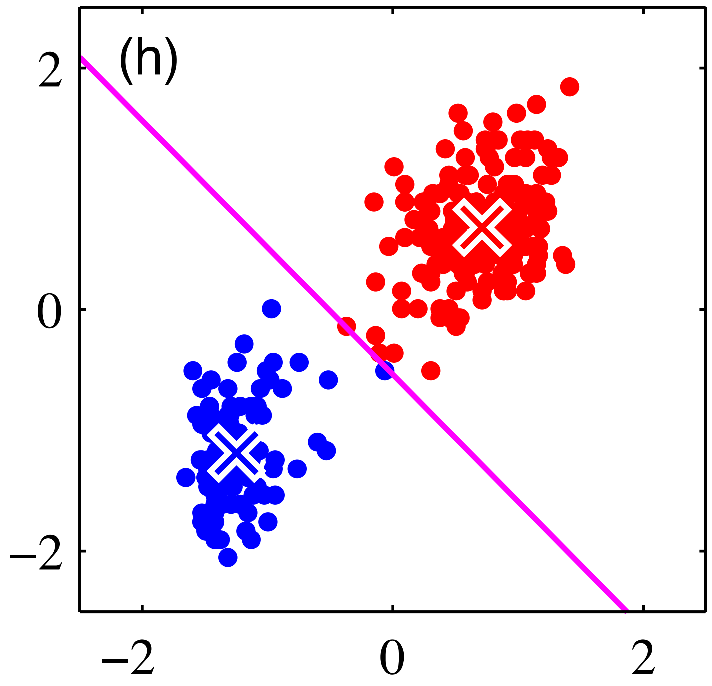


(A) update the cluster assignments.

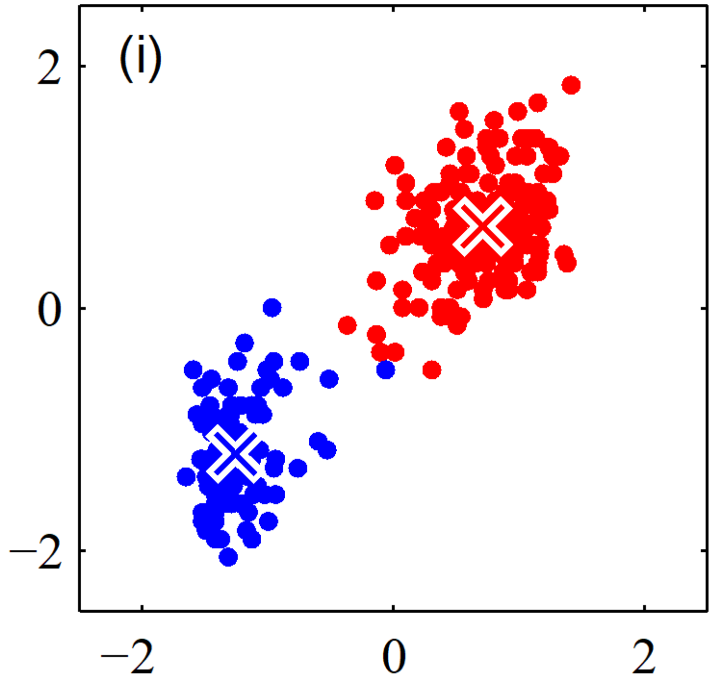


(B) Update the centroids $\{c_j\}$

Iteration 4

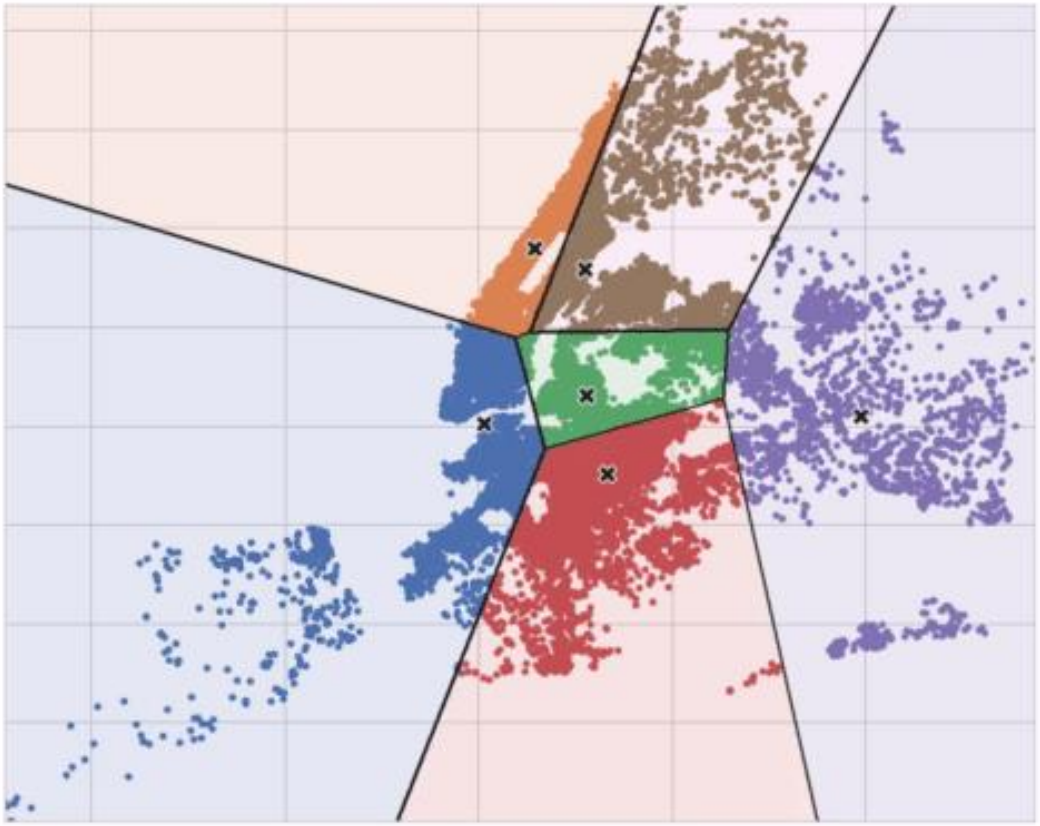


(A) update the cluster assignments.



(B) Update the centroids $\{c_j\}$

Iterating until Convergence



Animation from [Kaggle]

Promise of Convergence

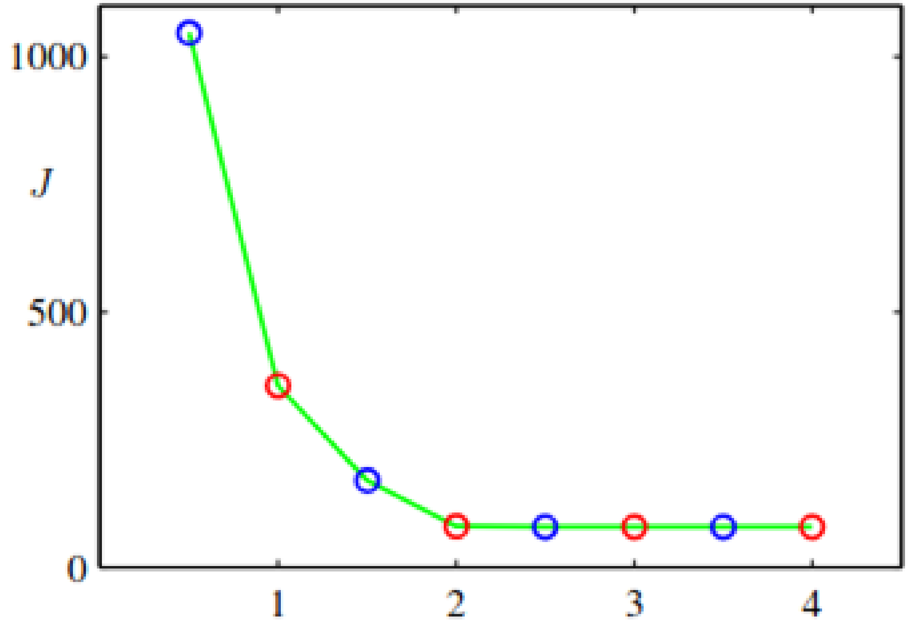
$$J = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \|\mathbf{x}_n - \boldsymbol{\mu}_k\|^2$$

=1 if x_n is assigned to cluster k
=0 otherwise

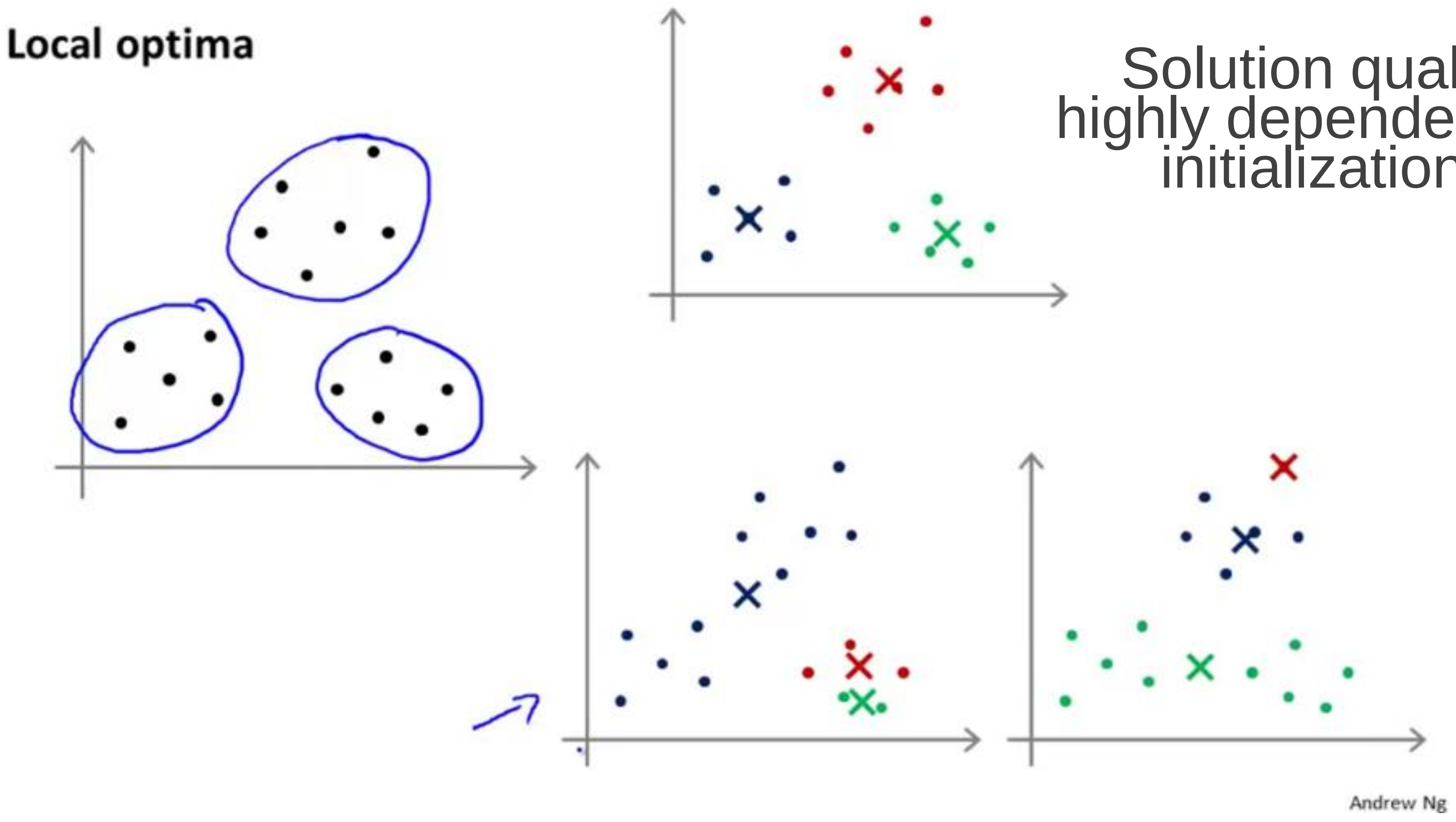
Location of centroid k

But, may converge to a local rather than global minimum of J.

Solution quality highly dependent on initialization!



Plot of the cost function J after each cluster assignment step (blue points) and recompute centroid step (red points)



Solution quality highly dependent on initialization!

Image from Andrew NG Coursera Machine Learning Course

Next lecture (1/30)

- Linear classification; the Perceptron algorithm

- Assigned reading: CIML Chap. 4