CS 480/680
Introduction to Machine Learning

Lecture 4
Non-Parametric Methods: KDE, k-NN, and k-Means

Kathryn Simone

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The algorithms we have encountered so far involved assuming a hypothesis class and parametrization

Perceptron: Separating Hyperplane

$$\mathcal{H}_+ = \{x : w^T x > -b\}$$
$$\mathcal{H}_- = \{x : w^T x < -b\}$$

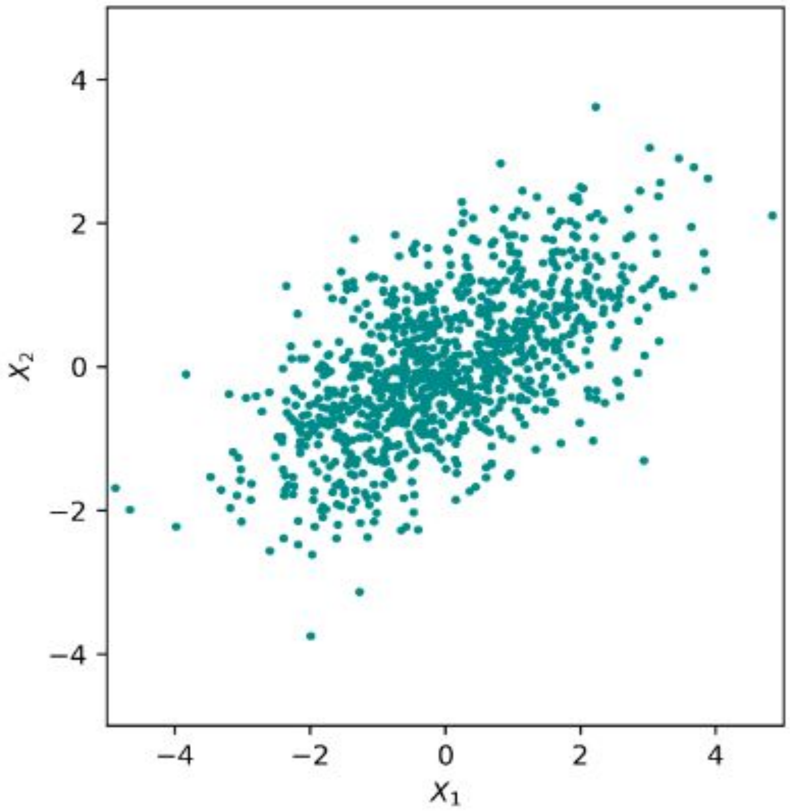
Linear Regression:

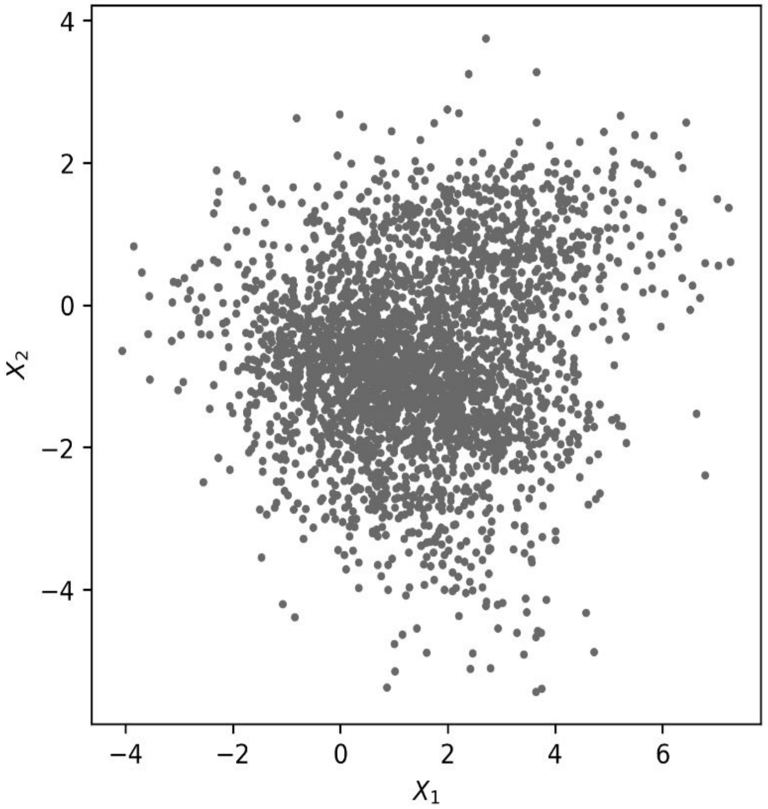
$$y(x) = w^T x + b$$

Gaussian distribution learning

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(x-\mu)^2}$$

Strong assumptions limit the class of functions you can approximate well





Learning a distribution without a hypothesis class
Kernel (Parzen) Density Estimation

Given a set of observations $\{x_1, x_2, \ldots x_n\}, x_i \in \mathbb{R}^d$, the Parzen estimate for the probability density at some arbitrary point x_o is calculated as

$$\hat{p}_X(x_o) = \frac{1}{n\lambda} \sum_{i=1}^{n} K_\lambda(x_0, x_i)$$

Where: $K_\lambda : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}_+$ is a non-negative kernel function, and λ is the length scale parameter. For KDE, we often desire K_λ to be symmetric and shift-invariant. That is:

$$K_\lambda(x_0, x_i) = K(x_0/\lambda - x_i\lambda)$$

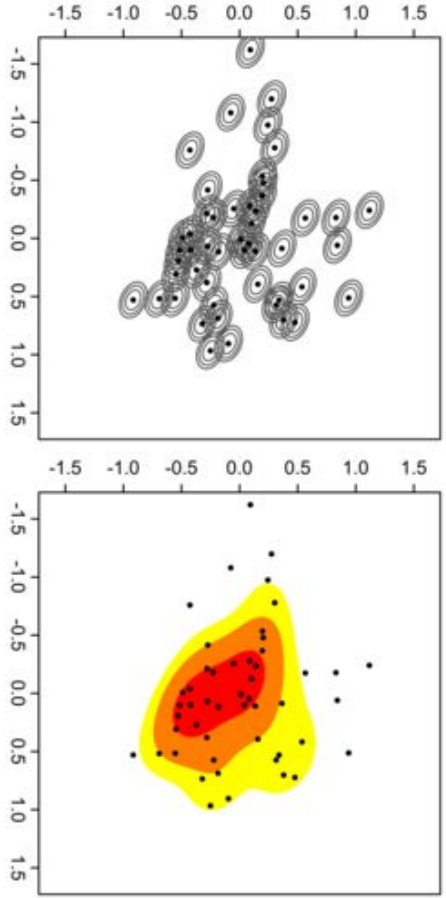
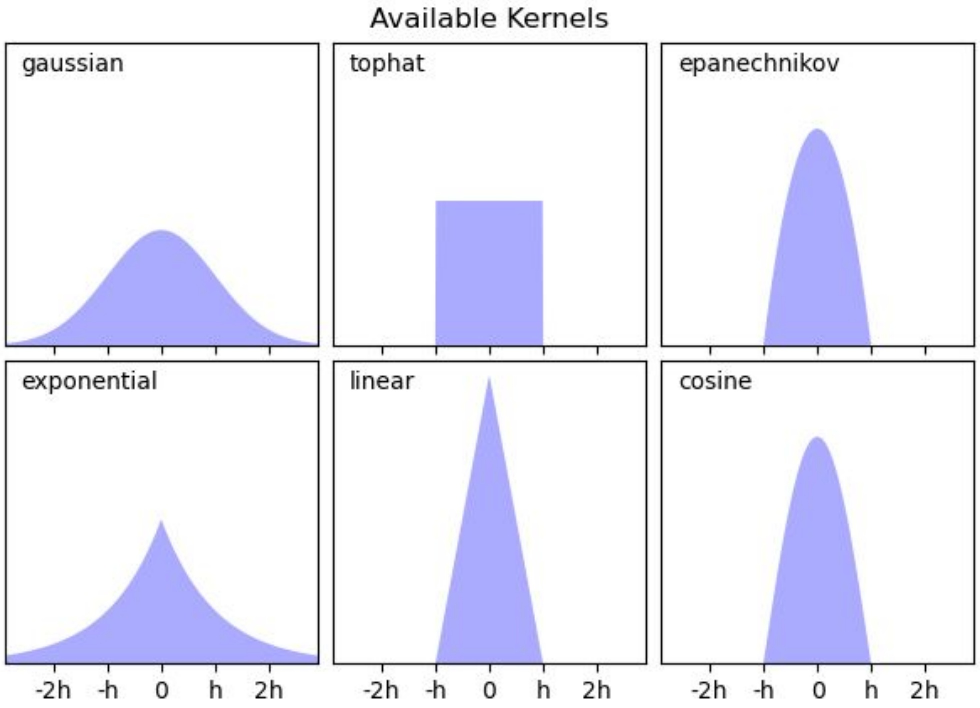


Figure: Wikipedia
Elements of Statistical Learning, Section 6.6

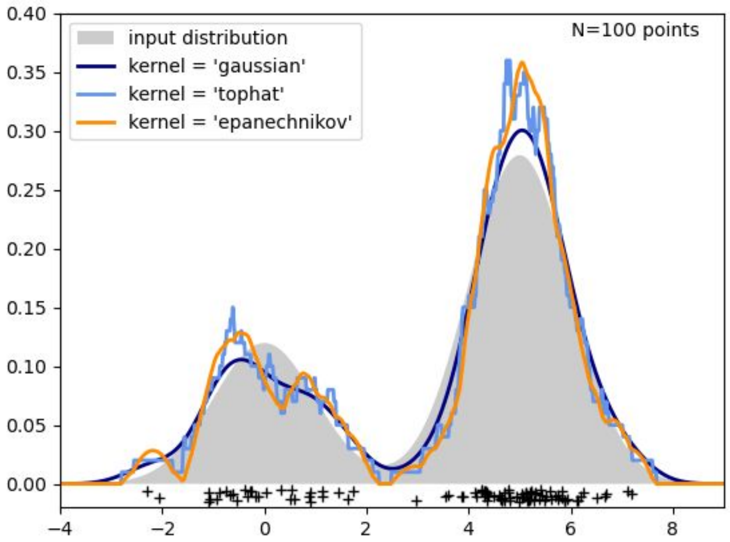
Many admissible kernels for density estimation



Source: Sci-Kit Learn

Using KDE to approximate the reference in KL divergence

$$D_{\mathrm{KL}}(P \,||\, Q) = \int_{-\infty}^{\infty} p(x) \log \frac{p(x)}{q(x)} dx \text{ (Continuous Random Variable)}$$



Source: Sci-Kit Learn

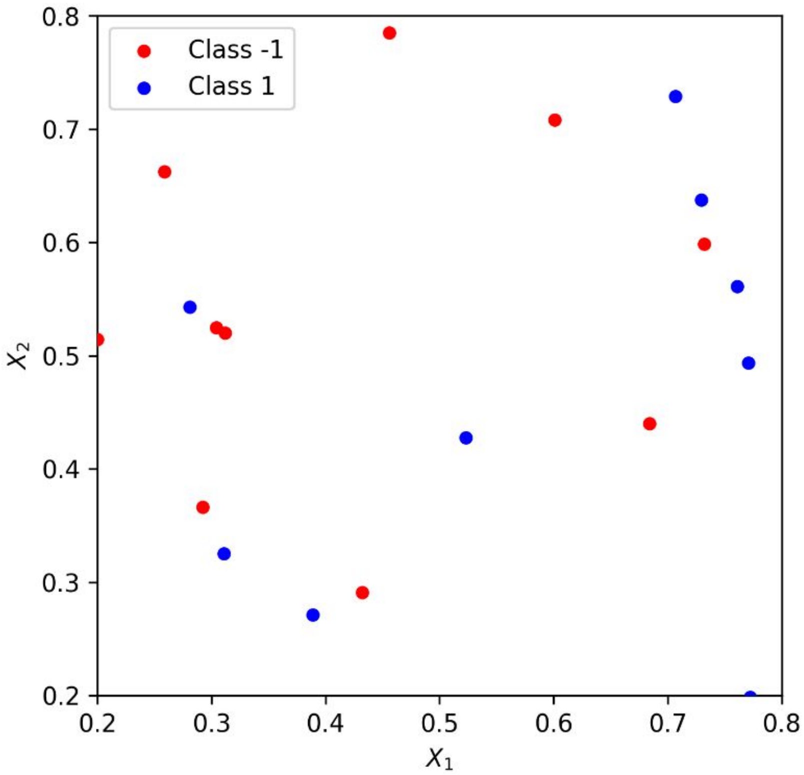
Today we'll look at examples of non-parametric algorithms

I. Classification (k-Nearest Neighbors)
II. Clustering (k-Means)

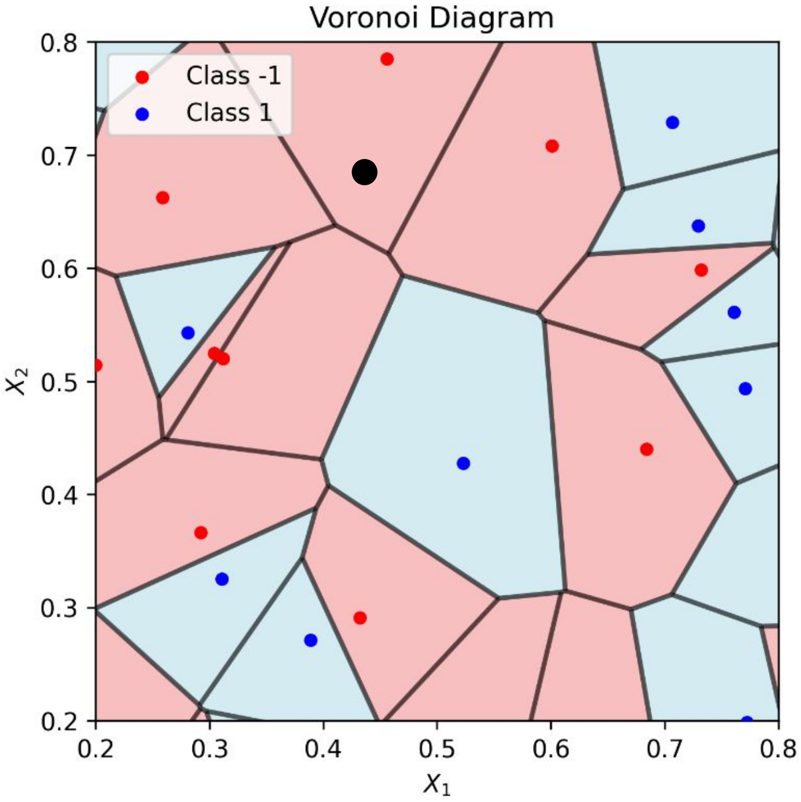
Non-Parametric Supervised Learning

K-Nearest Neighbors (k-NN)

Classification with non-linearly separable data



Approach: assume that points that are near to one another are likely to have the same label



k-Nearest Neighbors (k-NN) Classification

Algorithm 1 k Nearest Neighbors (binary classification)

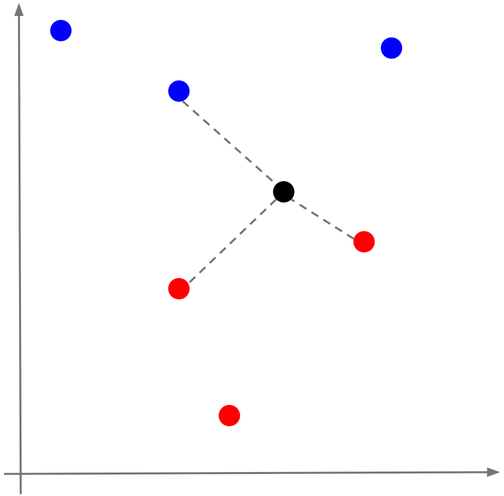
Input:

Dataset $\{(x_1, y_1), \ldots, (x_n, y_n)\}$, $x_i \in \mathbb{R}^d$, $y_i \in \{\pm 1\}$
Number of neighbors k
New instance $x \in \mathbb{R}^d$
for $i = \{1, 2, \ldots n\}$ **do**
    $d_i = \text{dist}(x, x_i)$
end for
Find smallest k indices of d
return Majority vote of $\{y_i, \ldots y_k\}$

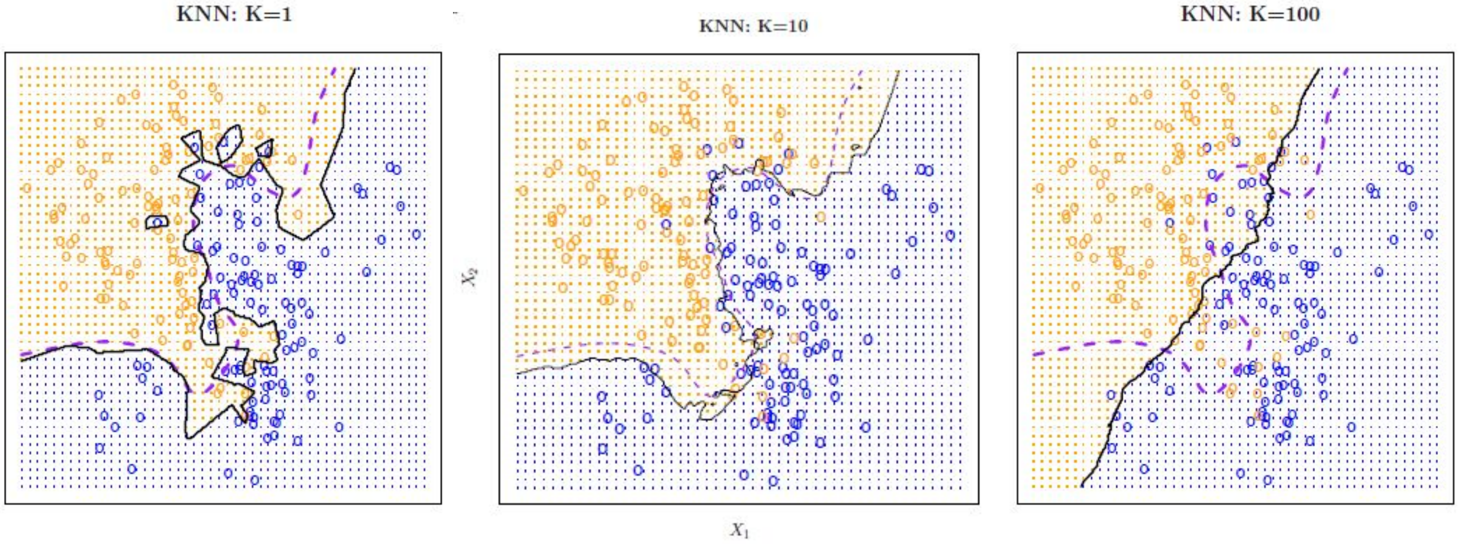
KNN requires a distance function
$d : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$

- Euclidean: $d(x, x') = \sqrt{\sum_{m=1}^{d} (x_m - x'_m)^2}$
- Manhattan: $d(x, x') = \sum_{m=1}^{d} \|x_m - x'_m\|_1$

$k = 3$



The bias-variance tradeoff and the role of hyperparameter *k*



Variable:
Predictions depend strongly on training dataset

Biased:
systematic error due to simplified model

Introduction to Statistical Learning, Section 2.2

Computational complexity of KNN

	Time	Space
Train	0	O(nd)
Test	Computing distances: O(nd) Fast sorting: O(n log k) O(nd+ nlogk) ≈ O(nd) for small k	O(nd)

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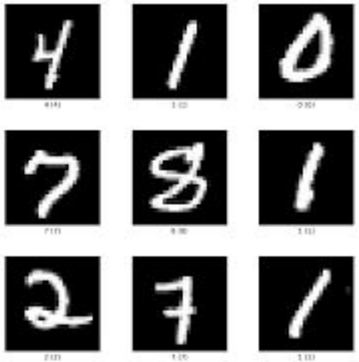
KNN on handwritten digit recognition (MNIST)

CLASSIFIER	PREPROCESSING	TEST ERROR RATE (%)
Linear Classifiers		
linear classifier (1-layer NN)	none	12.0
linear classifier (1-layer NN)	deskewing	8.4
pairwise linear classifier	deskewing	7.6
K-Nearest Neighbors		
K-nearest-neighbors, Euclidean (L2)	none	5.0
K-nearest-neighbors, Euclidean (L2)	none	3.09
K-nearest-neighbors, L3	none	2.83
K-nearest-neighbors, Euclidean (L2)	deskewing	2.4
Convolutional nets		
Convolutional net LeNet-1	subsampling to 16x16 pixels	1.7
Convolutional net LeNet-4	none	1.1
Convolutional net LeNet-4 with K-NN instead of last layer	none	1.1
Convolutional net LeNet-4 with local learning instead of last layer	none	1.1
Convolutional net LeNet-5, [no distortions]	none	0.95
Convolutional net LeNet-5, [huge distortions]	none	0.85
Convolutional net LeNet-5, [distortions]	none	0.8
Convolutional net Boosted LeNet-4, [distortions]	none	0.7
Trainable feature extractor + SVMs [no distortions]	none	0.83
Trainable feature extractor + SVMs [elastic distortions]	none	0.56



https://yann.lecun.com/exdb/mnist/

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An upper bound on KNN error rate (Cover and Hart, 1967)

The Bayes optimal classifier outputs the most likely class under a known distribution P:

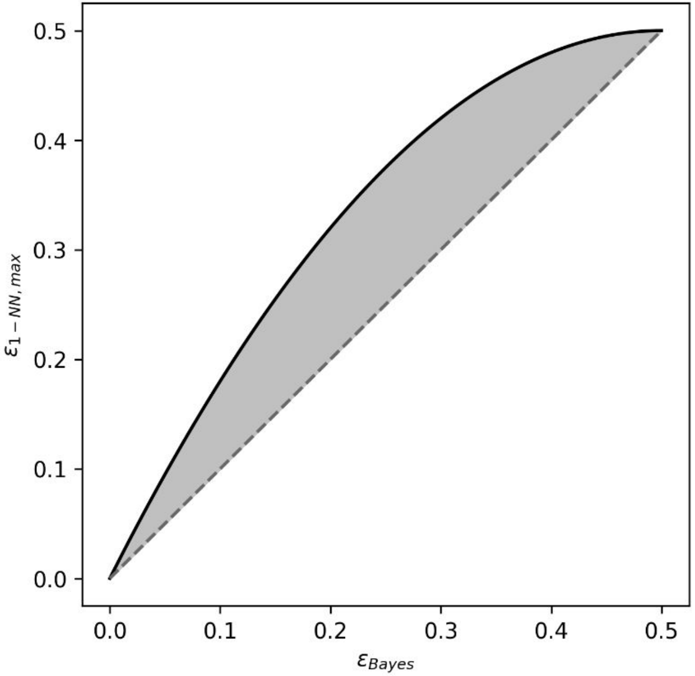
$$\hat{y}(x) = \text{argmax}_c \Pr[y = c|x, P]$$

- Given a point x, look at the distribution of labels given that feature vector
- Pick whichever label is most likely to be generated
- Error rate ϵ : $E[1 - \max_c Pr[y = c|x, P]]$

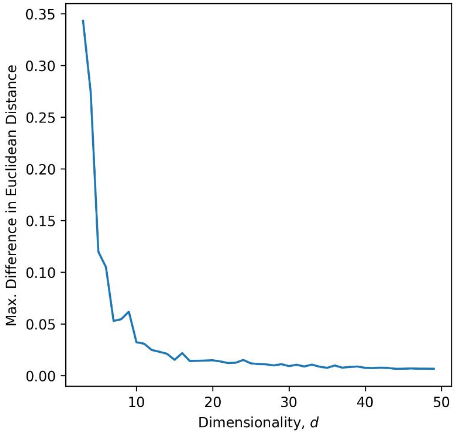
Suppose $KNN(x)$ is a Nearest Neighbor binary classifier with k=1, then its error rate ϵ_h

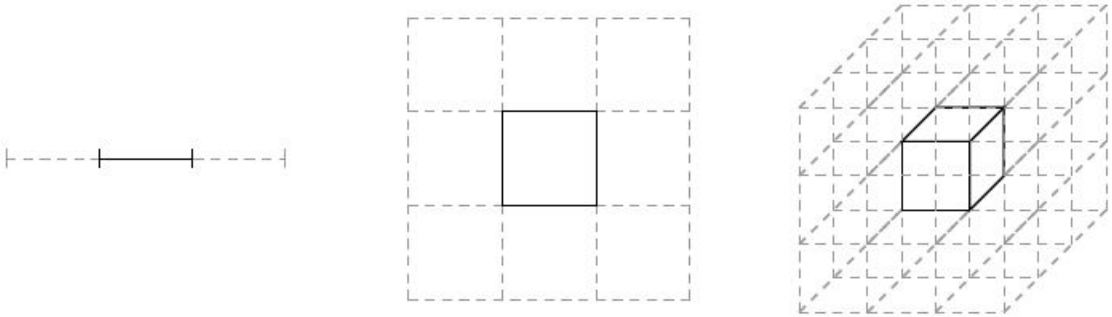
$$\lim_{n\to\infty} \epsilon_{KNN} < 2\epsilon_{Bayes}(1 - \epsilon_{Bayes})$$

Where ϵ_{Bayes} is the error rate of the Bayes optimal classifier, and n is the number of samples.



Caveat of the Cover-Hart Theorem
The “curse of dimensionality” (Bellman, 1961)





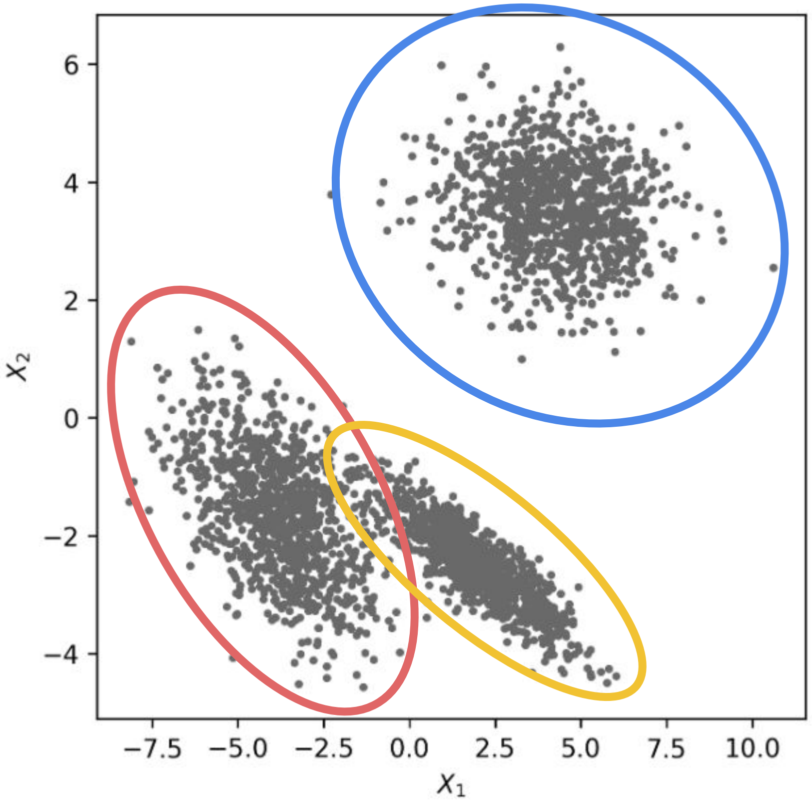
The number of samples needed to train the KNN classifier to reach the lower bound on the error rate grows exponentially with the number of features.

Right: Michael Betancourt, 2018
Discussion: Elements of Statistical Learning, Section 2.5,
Proof: Understanding Machine Learning, Section 19.2.2

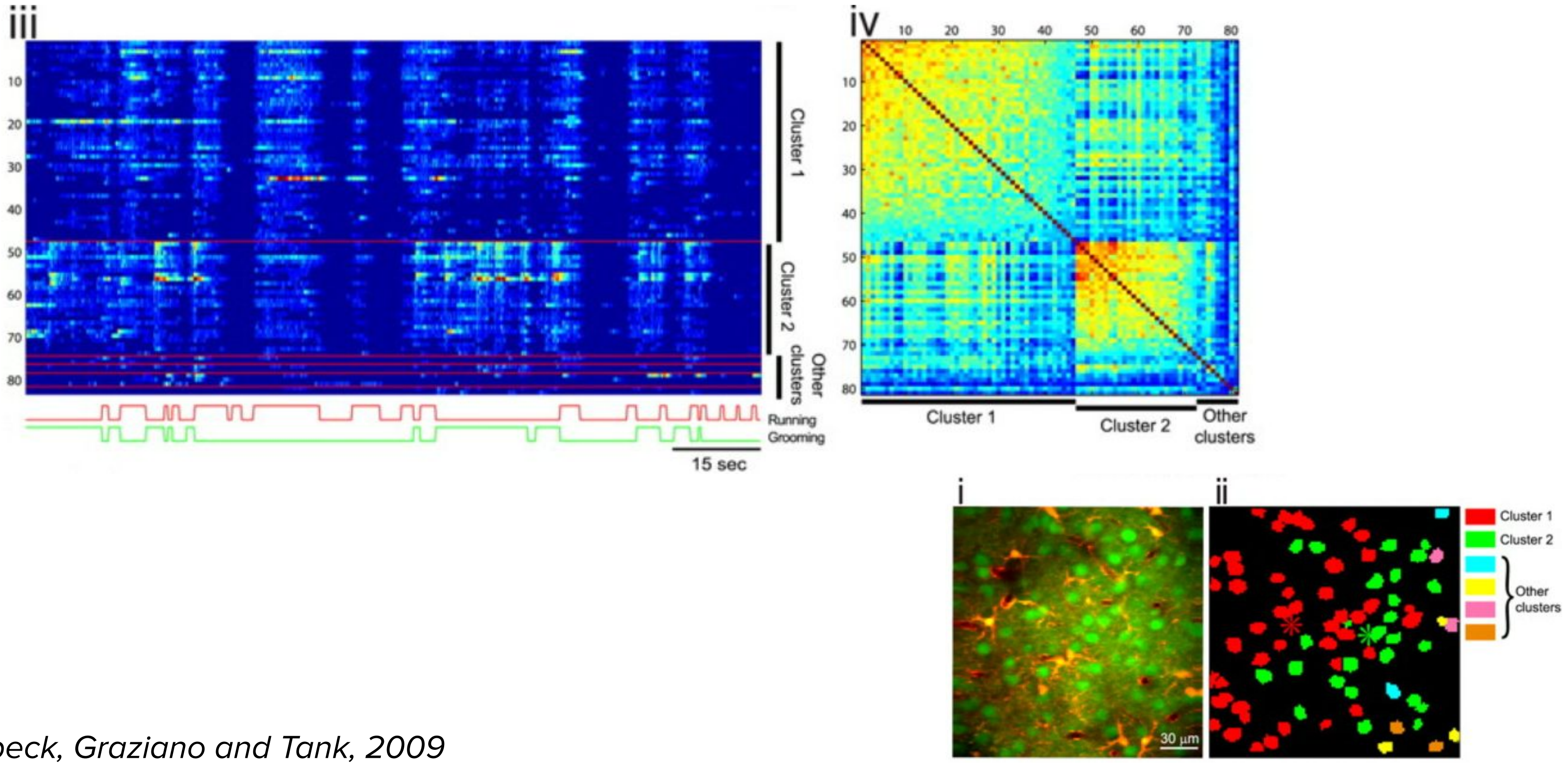
K-Means Clustering

Non-Parametric Clustering

The clustering task concerns grouping unlabelled data



Example: Clustering applied to neural data in motor cortex



Dombeck, Graziano and Tank, 2009

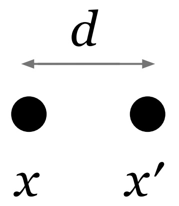
A common clustering problem

Given: A dataset of n observations, $D = \{x_1, x_2, \ldots, x_n\}$, $x_i \in \mathbb{R}^d$, and function $f : \mathbb{R}^d \rightarrow \mathbb{R}_+$

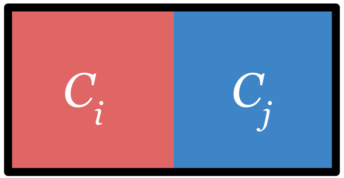
- f is symmetric: $f(x, x') = f(x', x) \;\; \forall x, x'$
- If f is a distance function, $f(x, x) = 0 \;\; \forall x$, and $f(x, z) \leq f(x, y) + f(y, z)$
- If f is a similarity measure, $f : \mathbb{R}^d \rightarrow [0, 1]$, $f(x, x) = 1 \;\; \forall x$

Goal: A partition of the set into a set of subsets $C = \{C_1, C_2, \ldots C_k\}$.

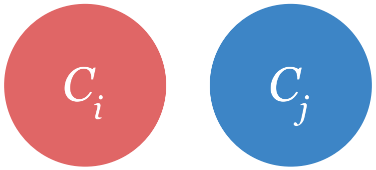
- Each observation belongs to a subset: $\cup_{i=1}^{k} C_i = D$
- Each observation belongs to only one subset: $C_i \cap C_j = 0, \forall \;\; i \neq j$



Collectively Exhaustive

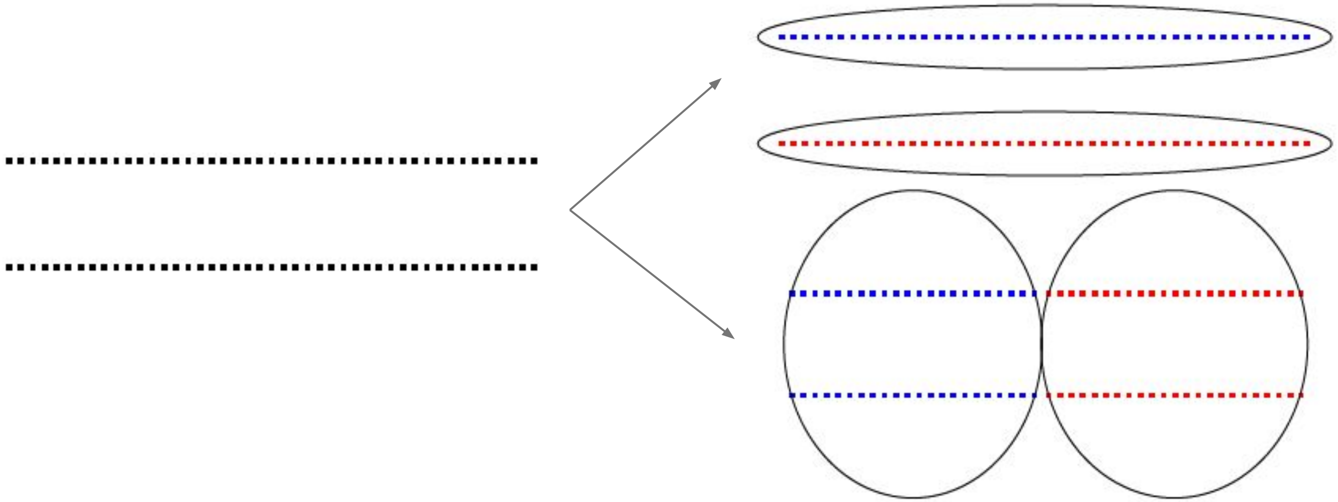


Disjoint or mutually exclusive



Understanding Machine Learning, Chapter 22

Clustering output depends on what we mean by similarity



Understanding Machine Learning, Chapter 22, pg. 308

The k-Means clustering objective

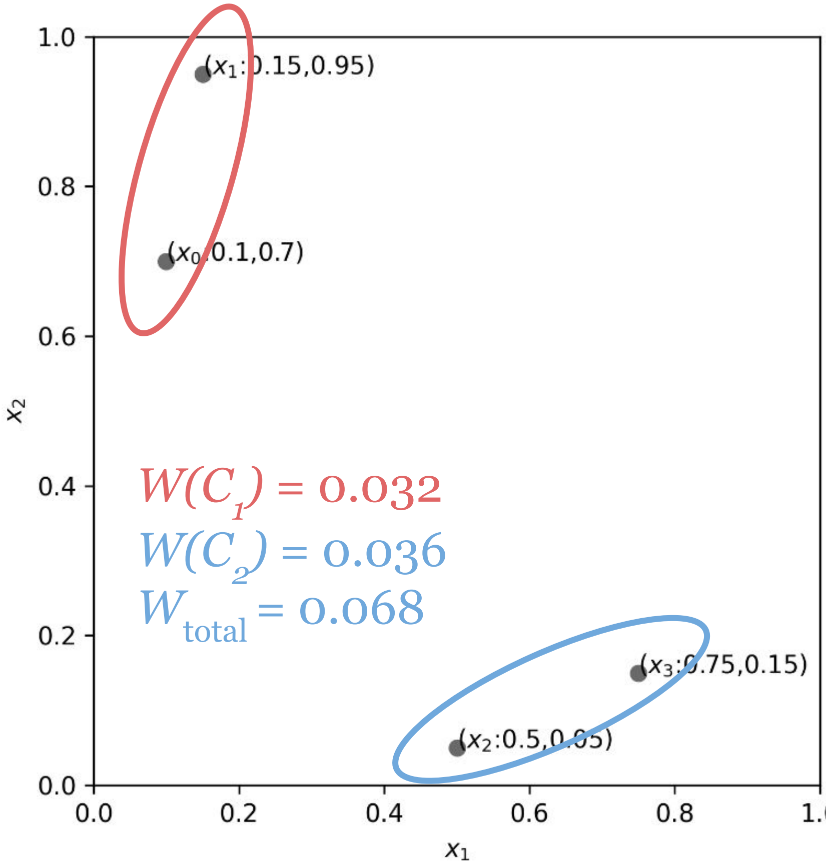
Objective:

Cost of C_j, $W(C_j)$

$$\min_{C_1,\ldots C_k} \sum_{j=1}^{k} \frac{1}{|C_j|} \sum_{x_i, x_i' \in C_j} \|x_i - x_i'\|_2^2,$$

Where:

$|C_j|$ is the number of points in cluster j



Understanding Machine Learning, Chapter 22

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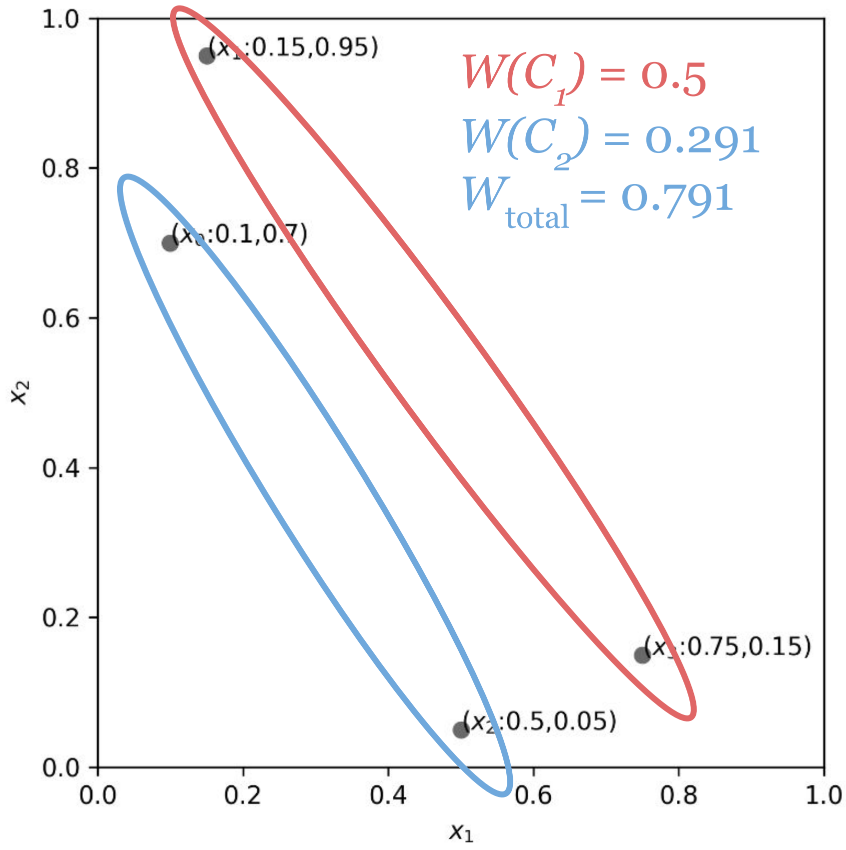


Understanding Machine Learning, Chapter 22

Reformulating the *k*-Means objective

The j^{th} cluster has a centroid $\mu_j \in \mathbb{R}^d$:

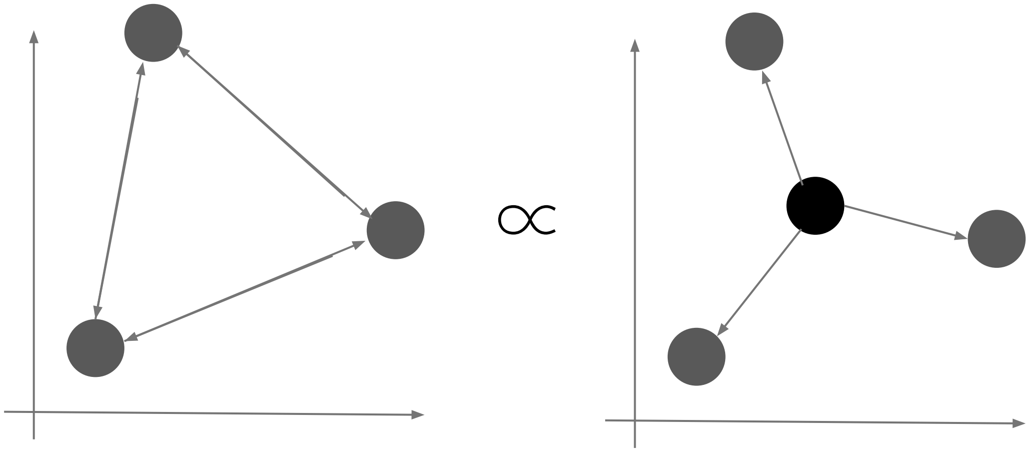
$$\mu_j = \frac{1}{|C_j|} \sum_{x_i \in C_j} x_i$$

It can be shown that

$$\sum_{x_i, x_i' \in C_j} \|x_i - x_i'\|_2^2 \propto \sum_{x_i \in C_j} \|x_i - \mu_j\|_2^2,$$

therefore, the objective can be rewritten as:

$$\min_{C_1,\dots C_k} \sum_{j=1}^{k} \frac{1}{|C_j|} \sum_{x_i \in C_j} \|x_i - \mu_j\|_2^2.$$



$\propto$

How to minimize the objective function?

- If you do brute-force search, you'll have a bad time
  - There are K^{n} possible clusters (an NP-hard problem)
  - Would only work for small k and n
- Partial derivative won't be as helpful here
  - Hard-membership means the gradient is non-smooth
  - Multiple local minima

Lloyd’s algorithm for K-Means clustering

Algorithm 1 Lloyd’s k-Clustering method

Input:

Dataset $D = \{x_1, x_2 \dots, x_n\}$ $x_i \in \mathbb{R}^d$

Number of clusters k

Output: Partition $C = \{C_1, C_2, \dots C_k\}$

Randomly initialize partition $C^0 = \{C_1, C_2, \dots C_k\}$

while $\exists i C_i^{(t)} \neq C_i^{(t-1)}$ **do**

  for $C^t = \{C_1^t, C_2^t, \dots C_k^t\}$ **do**

   $\mu_j = \frac{1}{|C_j^t|} \sum_{x_i \in C_j^t} x_i$

   ▷ Compute centroid of cluster j

  end for

  for $\{x_1, x_2 \dots, x_n\}$ **do**

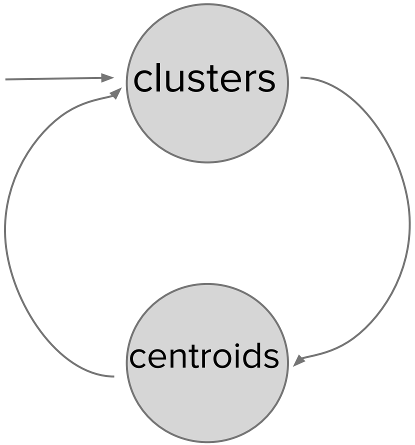
   $j = \text{argmin}_j \|x_i - \mu_j\|_2^2$

   $C_j^{t+1} \cup \{x_i\}$ ▷ Reassign sample i to cluster j

  end for

end while

return Partition $C^{(t)} = \{C_1, C_2, \dots C_k\}$



Lloyd's algorithm in action

Algorithm 1 Lloyd's k-Clustering method

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  end for

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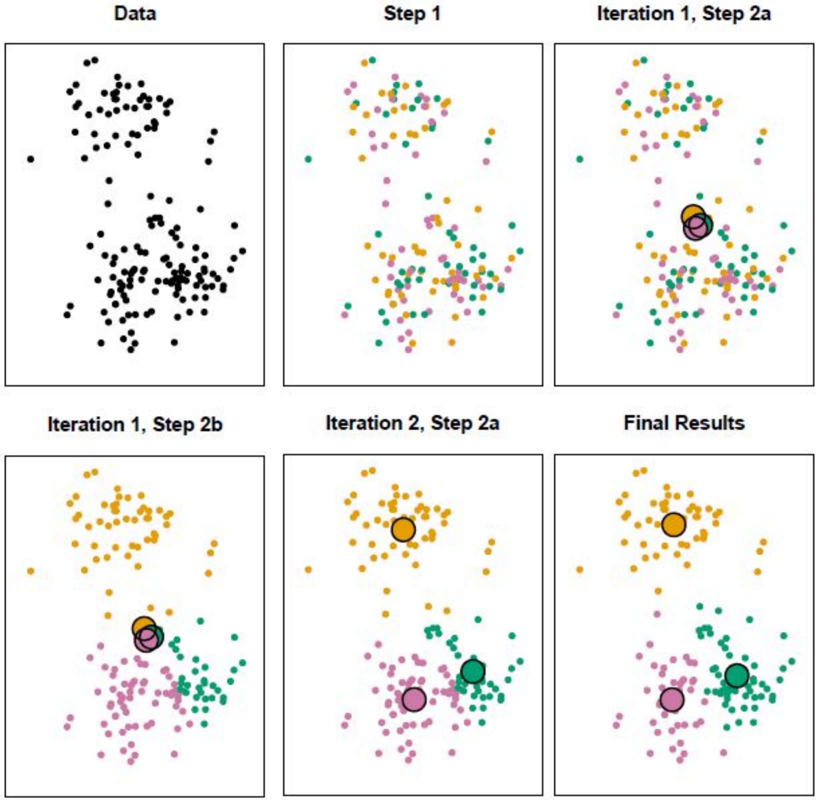
  end for

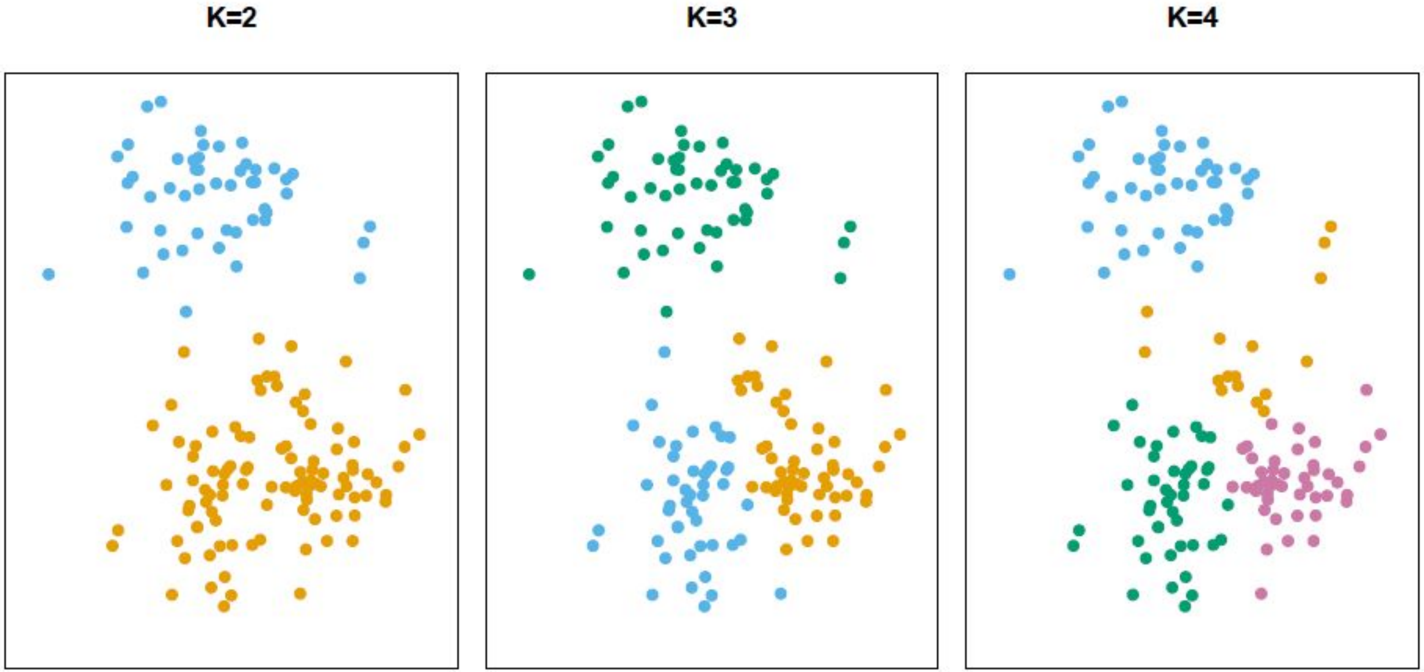
end while

return Partition $C^{(t)} = \{C_1, C_2, \ldots C_k\}$



Introduction to Statistical Learning, Section 12.4

Limitations of *k*-Means



Introduction to Statistical Learning, Section 12.4

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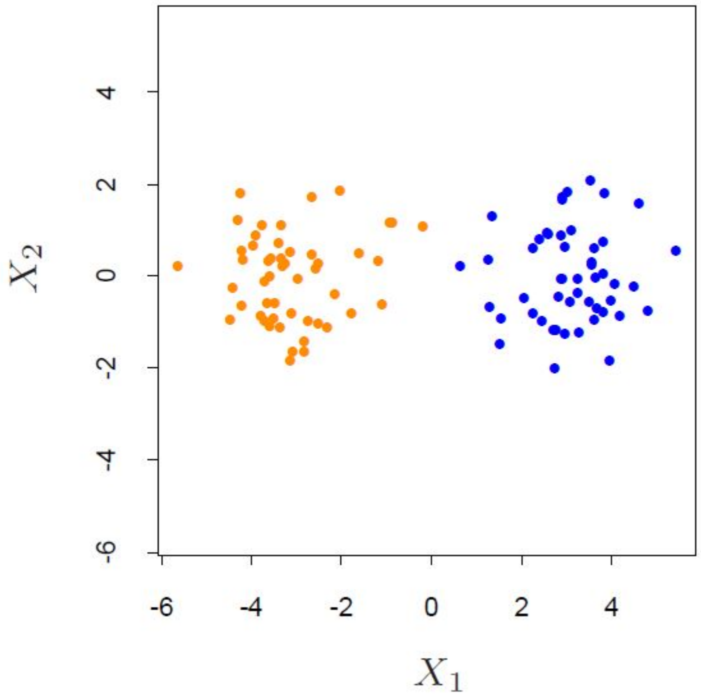
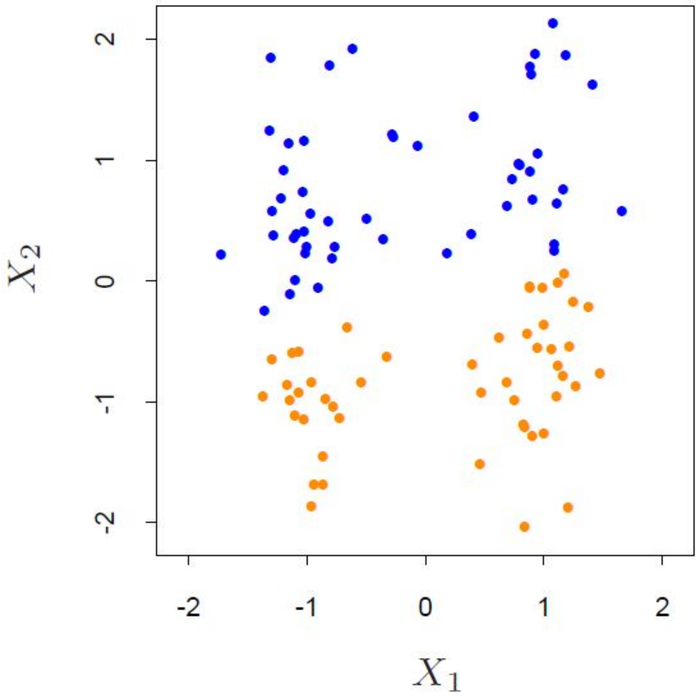
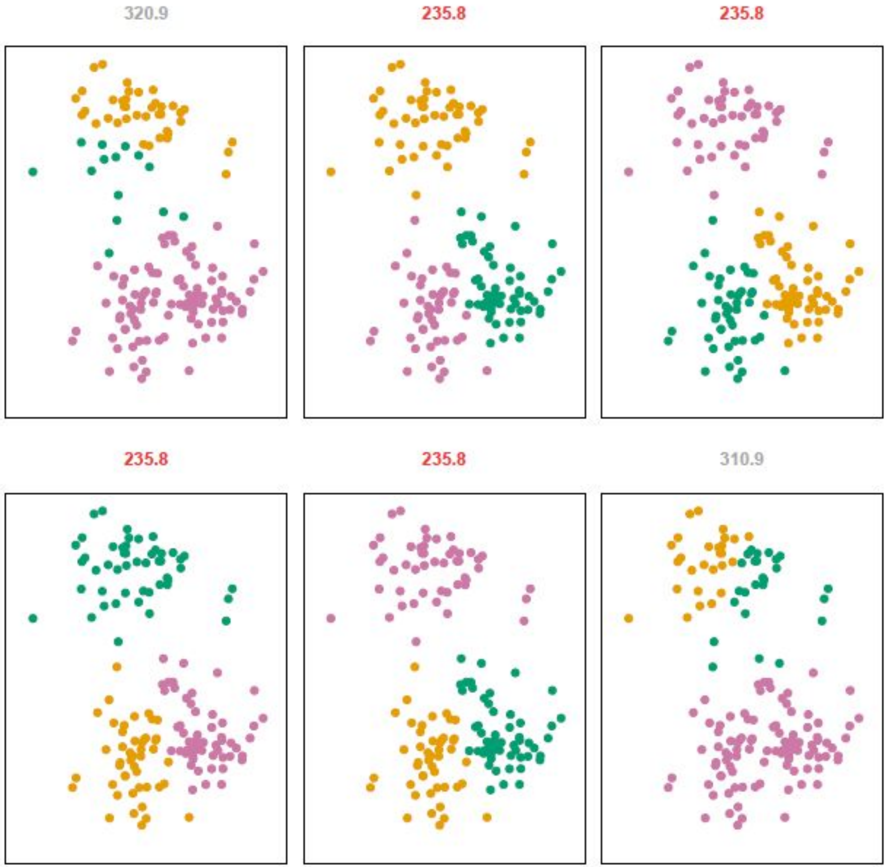




Elements of Statistical Learning, Section 14.3

Limitations of Lloyd’s Algorithm



Introduction to Statistical Learning, Section 12.4

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Summary

Now that we're at the end of the lecture, you should be able to…

- ★ Differentiate **parametric and non-parametric algorithms**, and give examples of algorithms in unsupervised and supervised settings.
- ★ Defend *k*-NN on both empirical and theoretical grounds, with reference to the **Bayes optimal classifier**.
- ★ State the Cover-Hart theorem and anticipate its implications on real datasets, with reference to the **curse of dimensionality**.
- ★ Characterize ML algorithms by their compromise of the **bias-variance** tradeoff.
- ★ Use kernel density estimation (KDE) to fit an empirical distribution.
- ★ Apply KDE to assess a learned parametric model with KL divergence.
- ★ State the clustering problem and differentiate it from classification.
- ★ Implement Lloyd's algorithm for K-Means clustering.
- ★ Implement *k*-NN classification with O(ndk) at test.
- ★ Design *k*-NN algorithms and justify choices against alternatives.
- ★ Recommend k-NN in appropriate supervised learning settings.

Errata

- On the slide titled "Reformulating the k-Means objective", there appeared a reference to u_j'. This has been corrected to μ_j, denoting the centroid of cluster j.
- On the slides titled "LLoyd's algorithm for K-Means clustering" and "Lloyd's algorithm in action", the algorithm should have returned the partition at iteration t, which is now captured on line 11 of the algorithm pseudocode.

Added Context

- On the slide titled "An upper bound on KNN error rate (Cover and Hart, 1967) there was a figure depicting how the KNN error rate is bounded by twice the error of the Bayes optimal classifier. The plot explored the case where the Bayes optimal classifier has an error rate greater than 50%, but this is non-sensical. The figure now restricts the exploration to the case where the Bayes rate is at most 50%, and also emphasizes that the actual KNN error rate can be anywhere from the Bayes error rate up to twie the Bayes error rate adjusted by a factor involving that rate.
- On the slide titled "Learning a distribution without a hypothesis class", details covered during the recitation about the mapping of the kernel function and the effect of lambda have now been spelled out in the text of the slide.
- On the slide titled "Computational complexity of KNN" nuance has been added to the complexity of the algorithm at test time.