

ELEN 4720: Machine Learning for Signals, Information and Data

Lecture 14

Prof. John Paisley

Department of Electrical Engineering

Columbia University

UNSUPERVISED LEARNING

SUPERVISED VS UNSUPERVISED LEARNING

Framework of supervised learning

Given: Pairs $(x_1, y_1), \dots, (x_n, y_n)$. Think of x as input and y as output.

Learn: A function $f(x)$ that accurately predicts $y_i \approx f(x_i)$ on this data.

Goal: Use the function $f(x)$ to predict new y_0 given x_0 .

Unsupervised learning

Given: A data set $x_1, \dots, x_n$, where $x_i \in \mathcal{X}$, e.g., $\mathcal{X} = \mathbb{R}^d$

Define: Some model of the data (probabilistic or non-probabilistic).

Goal: Learn structure within the data set *as defined by the model*.

- ▶ Supervised learning has a clear performance metric: accuracy
- ▶ Unsupervised learning is often (but not always) more subjective

SOME TYPES OF UNSUPERVISED LEARNING

Overview of second half of course

We will discuss a few types of unsupervised learning approaches in the second half of the course.

Clustering models: Learn a partition of data $x_1, \dots, x_n$ into groups.

- Image segmentation, data quantization, preprocessing for other models

Matrix factorization: Learn an underlying dot-product representation.

- User preference modeling, topic modeling

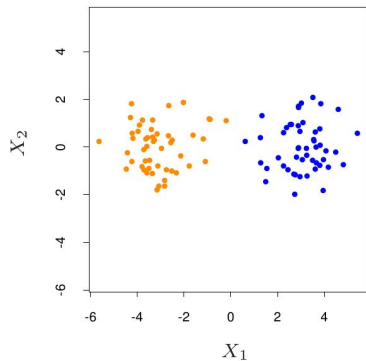
Sequential models: Learn a model based on sequential information.

- Learn how to rank objects, target tracking

CLUSTERING

Problem

- ▶ Given data $x_1, \dots, x_n$, partition it into groups called *clusters*.
- ▶ Find the clusters, given only the data.
- ▶ Observations in same group $\Rightarrow$ “similar,”
different groups $\Rightarrow$ “different.”



Cluster assignment representation

For K clusters, encode cluster assignments as an indicator $c \in \{1, \dots, K\}$,

$$c_i = k \quad \Longleftrightarrow \quad x_i \text{ is assigned to cluster } k$$

Clustering feels similar to classification in that we “label” an observation by its cluster assignment. The difference is that there is no ground truth.

THE K-MEANS ALGORITHM

CLUSTERING AND K-MEANS

K-means is the simplest and most fundamental clustering algorithm.

Input: $x_1, \dots, x_n$, where $x \in \mathbb{R}^d$.

Output: Vector $\mathbf{c}$ of cluster assignments, and K mean vectors $\boldsymbol{\mu}$

- ▶ $\mathbf{c} = (c_1, \dots, c_n)$, $c_i \in \{1, \dots, K\}$
 - If $c_i = c_j = k$, then x_i and x_j are *clustered together* in cluster k .
- ▶ $\boldsymbol{\mu} = (\mu_1, \dots, \mu_K)$, $\mu_k \in \mathbb{R}^d$ (same space as x_i)
 - Each μ_k (called a *centroid*) defines a cluster.

As usual, we need to define an *objective function*. We pick one that:

1. Tells us what are good $\mathbf{c}$ and $\boldsymbol{\mu}$, and
2. That is easy to optimize.

K-MEANS OBJECTIVE FUNCTION

The K-means objective function can be written as

$$\boldsymbol{\mu}^*, \mathbf{c}^* = \arg \min_{\boldsymbol{\mu}, \mathbf{c}} \sum_{i=1}^n \sum_{k=1}^K \mathbb{1}\{c_i = k\} \|x_i - \mu_k\|^2$$

Some observations:

- ▶ K-means uses the squared Euclidean distance of x_i to the centroid μ_k .
- ▶ It only penalizes the distance of x_i to the centroid it's assigned to by c_i .

$$\mathcal{L} = \sum_{i=1}^n \sum_{k=1}^K \mathbb{1}\{c_i = k\} \|x_i - \mu_k\|^2 = \sum_{k=1}^K \sum_{i:c_i=k} \|x_i - \mu_k\|^2$$

- ▶ The objective function is “non-convex”
 - ▶ This means that we can't actually find the *optimal* $\boldsymbol{\mu}^*$ and $\mathbf{c}^*$.
 - ▶ We can only derive an *algorithm* for finding a *local optimum* (more later).

OPTIMIZING THE K-MEANS OBJECTIVE

Gradient-based optimization

We can't optimize the K-means objective function exactly by taking derivatives and setting to zero, so we use an iterative algorithm.

However, the algorithm we will use is different from gradient methods:

$$w \leftarrow w - \eta \nabla_w \mathcal{L} \quad (\text{gradient descent})$$

Recall: With gradient descent, when we update a parameter “ w ” we move in the direction that decreases the objective function, but

- ▶ It will almost certainly not move to the *best* value for that parameter.
- ▶ It may not even move to a better value if the step size η is too big.
- ▶ We also need the parameter w to be continuous-valued.

K-MEANS AND COORDINATE DESCENT

Coordinate descent

We will discuss a new and widely used optimization procedure in the context of K -means clustering. We want to minimize the objective function

$$\mathcal{L} = \sum_{i=1}^n \sum_{k=1}^K \mathbb{1}\{c_i = k\} \|x_i - \mu_k\|^2.$$

We split the variables into two unknown sets μ and c . We can't find their best values *at the same time* to minimize $\mathcal{L}$. However, we will see that

- ▶ Fixing μ we can find the best c exactly.
- ▶ Fixing c we can find the best μ exactly.

This optimization approach is called *coordinate descent*: Hold one set of parameters fixed, and optimize the other set. Then switch which set is fixed.

COORDINATE DESCENT

Coordinate descent (in the context of K-means)

Input: $x_1, \dots, x_n$ where $x_i \in \mathbb{R}^d$. Randomly initialize $\mu = (\mu_1, \dots, \mu_K)$.

► Iterate back-and-forth between the following two steps:

1. Given μ , find the best value $c_i \in \{1, \dots, K\}$ for $i = 1, \dots, n$.
 2. Given c , find the best vector $\mu_k \in \mathbb{R}^d$ for $k = 1, \dots, K$.
-

There's a circular way of thinking about why we need to iterate:

1. Given a particular μ , we may be able to find *the best* c , but once we *change* c we can probably find a better μ .
2. Then find *the best* μ for the new-and-improved c found in #1, but now that we've changed μ , there is probably a better c .

We have to iterate because the values of μ and c *depend on each other*.
This happens very frequently in unsupervised models.

K-MEANS ALGORITHM: UPDATING $\mathbf{c}$

Assignment step

Given $\boldsymbol{\mu} = (\mu_1, \dots, \mu_K)$, update $\mathbf{c} = (c_1, \dots, c_n)$. By rewriting $\mathcal{L}$, we notice the independence of each c_i given $\boldsymbol{\mu}$,

$$\mathcal{L} = \underbrace{\left(\sum_{k=1}^K \mathbb{1}\{c_1 = k\} \|x_1 - \mu_k\|^2 \right)}_{\text{distance of } x_1 \text{ to its assigned centroid}} + \dots + \underbrace{\left(\sum_{k=1}^K \mathbb{1}\{c_n = k\} \|x_n - \mu_k\|^2 \right)}_{\text{distance of } x_n \text{ to its assigned centroid}}.$$

We can minimize $\mathcal{L}$ with respect to each c_i by minimizing each term above separately. The solution is to assign x_i to the closest centroid

$$c_i = \arg \min_k \|x_i - \mu_k\|^2.$$

Because there are only K options for each c_i , there are no derivatives. Simply calculate all the possible values for c_i and pick the best (smallest) one.

K-MEANS ALGORITHM: UPDATING μ

Update step

Given $\mathbf{c} = (c_1, \dots, c_n)$, update $\mu = (\mu_1, \dots, \mu_K)$. For a given $\mathbf{c}$, we can break $\mathcal{L}$ into K clusters defined by $\mathbf{c}$ so that each μ_i is independent.

$$\mathcal{L} = \underbrace{\left(\sum_{i=1}^N \mathbb{1}\{c_i = 1\} \|x_i - \mu_1\|^2 \right)}_{\text{sum squared distance of data in cluster \#1}} + \dots + \underbrace{\left(\sum_{i=1}^N \mathbb{1}\{c_i = K\} \|x_i - \mu_K\|^2 \right)}_{\text{sum squared distance of data in cluster \#K}} .$$

For each k , we then optimize. Let $n_k = \sum_{i=1}^n \mathbb{1}\{c_i = k\}$. Then

$$\mu_k = \arg \min_{\mu} \sum_{i=1}^n \mathbb{1}\{c_i = k\} \|x_i - \mu\|^2 \quad \longrightarrow \quad \mu_k = \frac{1}{n_k} \sum_{i=1}^n x_i \mathbb{1}\{c_i = k\} .$$

That is, μ_k is the *mean* of the data assigned to cluster k .

K-MEANS CLUSTERING ALGORITHM

Algorithm: K-means clustering

Given: $x_1, \dots, x_n$ where each $x \in \mathbb{R}^d$

Goal: Minimize $\mathcal{L} = \sum_{i=1}^n \sum_{k=1}^K \mathbb{1}\{c_i = k\} \|x_i - \mu_k\|^2$.

- ▶ Randomly initialize $\boldsymbol{\mu} = (\mu_1, \dots, \mu_K)$.
- ▶ Iterate until $\boldsymbol{c}$ and $\boldsymbol{\mu}$ stop changing

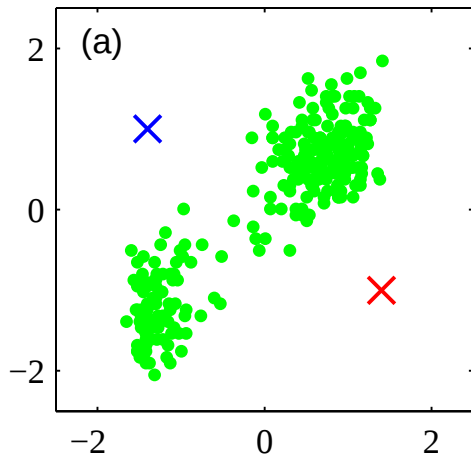
1. Update each c_i :

$$c_i = \arg \min_k \|x_i - \mu_k\|^2$$

2. Update each μ_k : Set

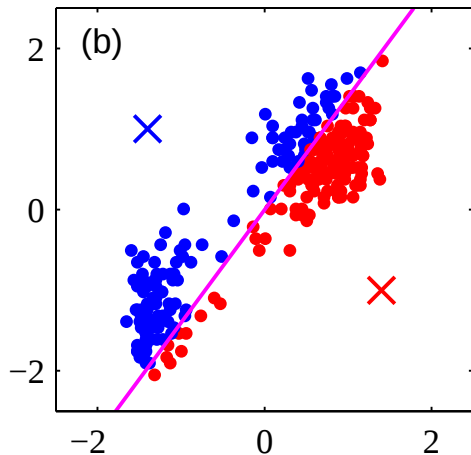
$$n_k = \sum_{i=1}^n \mathbb{1}\{c_i = k\} \quad \text{and} \quad \mu_k = \frac{1}{n_k} \sum_{i=1}^n x_i \mathbb{1}\{c_i = k\}$$

K-MEANS ALGORITHM: EXAMPLE RUN



A random initialization

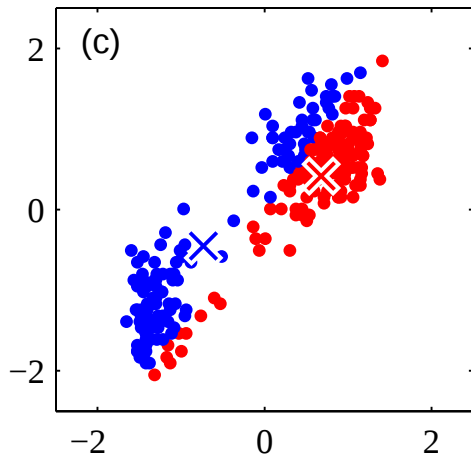
K-MEANS ALGORITHM: EXAMPLE RUN



Iteration 1

Assign data to clusters

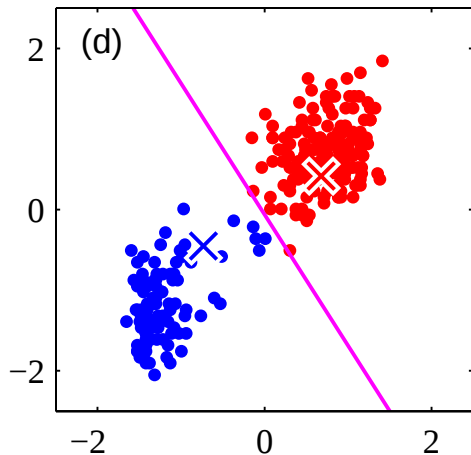
K-MEANS ALGORITHM: EXAMPLE RUN



Iteration 1

Update the centroids

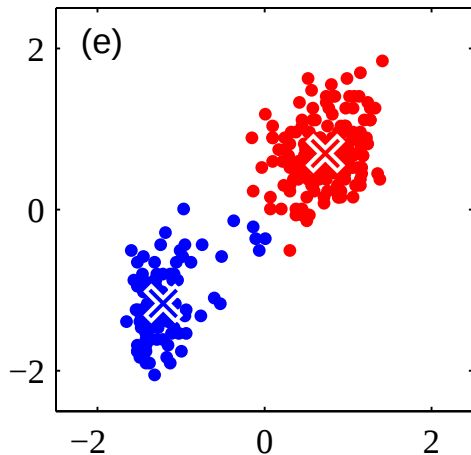
K-MEANS ALGORITHM: EXAMPLE RUN



Iteration 2

Assign data to clusters

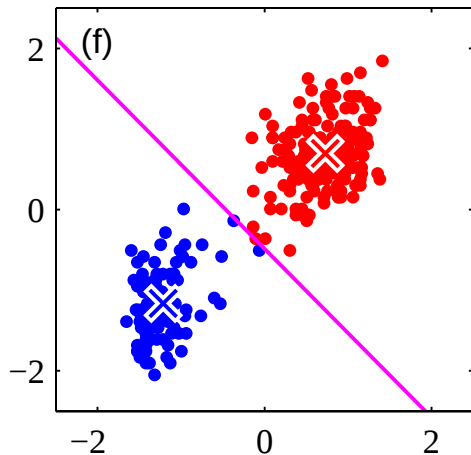
K-MEANS ALGORITHM: EXAMPLE RUN



Iteration 2

Update the centroids

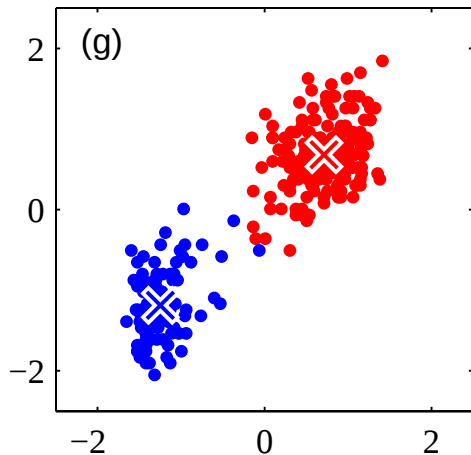
K-MEANS ALGORITHM: EXAMPLE RUN



Iteration 3

Assign data to clusters

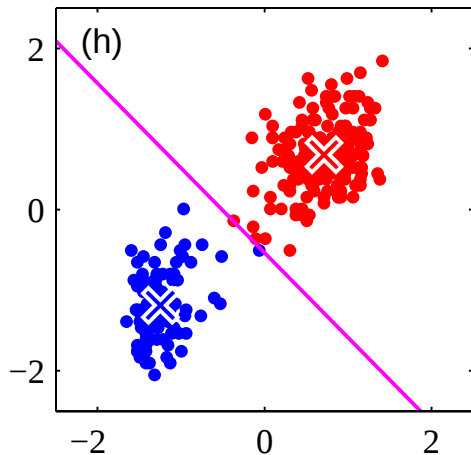
K-MEANS ALGORITHM: EXAMPLE RUN



Iteration 3

Update the centroids

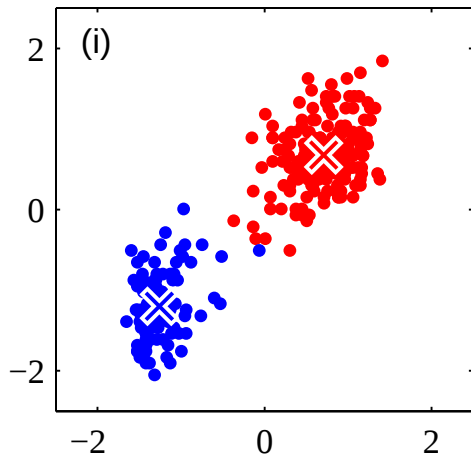
K-MEANS ALGORITHM: EXAMPLE RUN



Iteration 4

Assign data to clusters

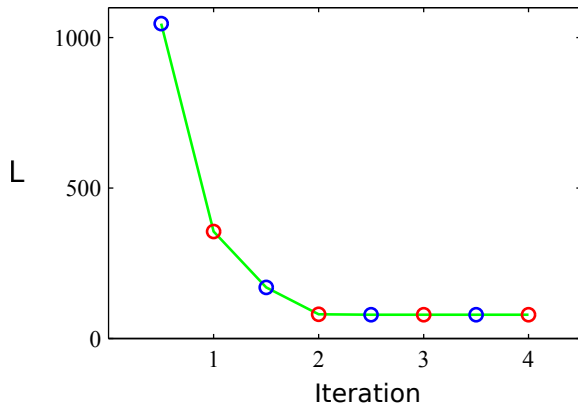
K-MEANS ALGORITHM: EXAMPLE RUN



Iteration 4

Update the centroids

CONVERGENCE OF K-MEANS



Objective function after

- ▶ the “assignment” step (blue: corresponding to c), and
- ▶ the “update” step (red: corresponding to μ).

CONVERGENCE OF K-MEANS

The outline of why this converges is straightforward:

1. Every update to c_i or μ_k decreases $\mathcal{L}$ compared to the previous value.
2. Therefore, $\mathcal{L}$ is *monotonically decreasing*.
3. $\mathcal{L} \geq 0$, so Step 1 converges to some point (but probably not to 0).

When $\mathbf{c}$ stops changing, the algorithm has converged to a *local* optimal solution. This is a result of $\mathcal{L}$ not being convex.

Non-convexity means that different initializations will give different results:

- ▶ Often the results will be similar in quality, but no guarantees.
- ▶ In practice, the algorithm can be run multiple times with different initializations. Then use the result with the lowest $\mathcal{L}$.

SELECTING K

We don't know how many clusters there are, but selecting K is tricky.
The K-means objective function decreases as K increases,

$$\mathcal{L} = \sum_{i=1}^n \sum_{k=1}^K \mathbb{1}\{c_i = k\} \|x_i - \mu_k\|^2.$$

For example, if $K = n$ then let $\mu_k = x_k$ and as a result $\mathcal{L} = 0$.

Methods for choosing K include:

- ▶ Using additional knowledge. e.g., if you want to split a set of tasks among K people, then you already know K .
- ▶ Looking at the *relative* decrease in $\mathcal{L}$. If K^* is best, then increasing K when $K \leq K^*$ should decrease $\mathcal{L}$ much more than when $K > K^*$.
- ▶ Often the K-means result is part of a larger application. The main application may start to perform worse even though $\mathcal{L}$ is decreasing.

EXTENSIONS: K-MEDOIDS

Algorithm: K-medoids clustering

Input: Data $x_1, \dots, x_n$ and distance measure $D(x, \mu)$. Randomly initialize μ .

► Iterate until c is no longer changing

1. For each c_i : Set

$$c_i = \arg \min_k D(x_i, \mu_k)$$

2. For each μ_k : Set

$$\mu_k = \arg \min_{\mu} \sum_{i:c_i=k} D(x_i, \mu)$$

Comment: Step #2 may require an algorithm.

K-medoids is a straightforward extension of K-means where the distance measure isn't the squared error. That is,

- K-means uses $D(x, \mu) = \|x - \mu\|^2$.
- Could set $D(x, \mu) = \|x - \mu\|_1$, which would be more robust to outliers.
- If $x \notin \mathbb{R}^d$, we could define $D(x, \mu)$ to be more complex.