



Unsupervised Learning with Scikit-Learn

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Konferencja Inżynierii Oprogramowania



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- Co-founder & Board Member at **Gradient**
- ML & DL Enthusiast
- Fan of **Computer Vision**
- **MedTagger's** Team Leader
- **Graphics Software Engineer** at Intel Technology Poland



Agenda

1. Introduction to Machine Learning
2. Clustering (~30 minutes)
3. Hierarchical Clustering (~30 minutes)
4. Anomaly Detection (~40 minutes)

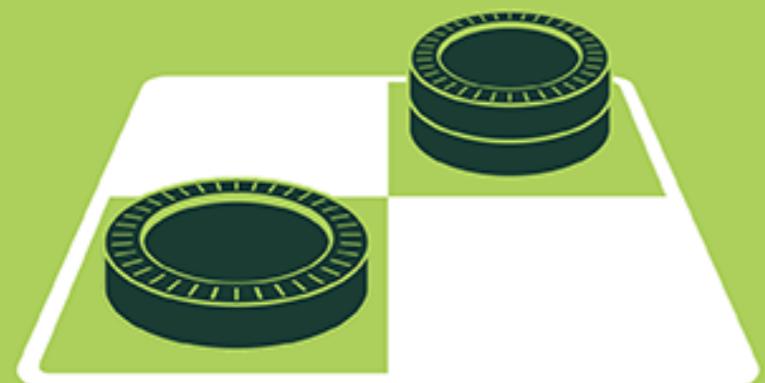
Ask Questions anytime! 😊

Introduction to Machine Learning

Before we will dive deep into Unsupervised Learning...

ARTIFICIAL INTELLIGENCE

Early artificial intelligence stirs excitement.



MACHINE LEARNING

Machine learning begins to flourish.



DEEP LEARNING

Deep learning breakthroughs drive AI boom.



1950's

1960's

1970's

1980's

1990's

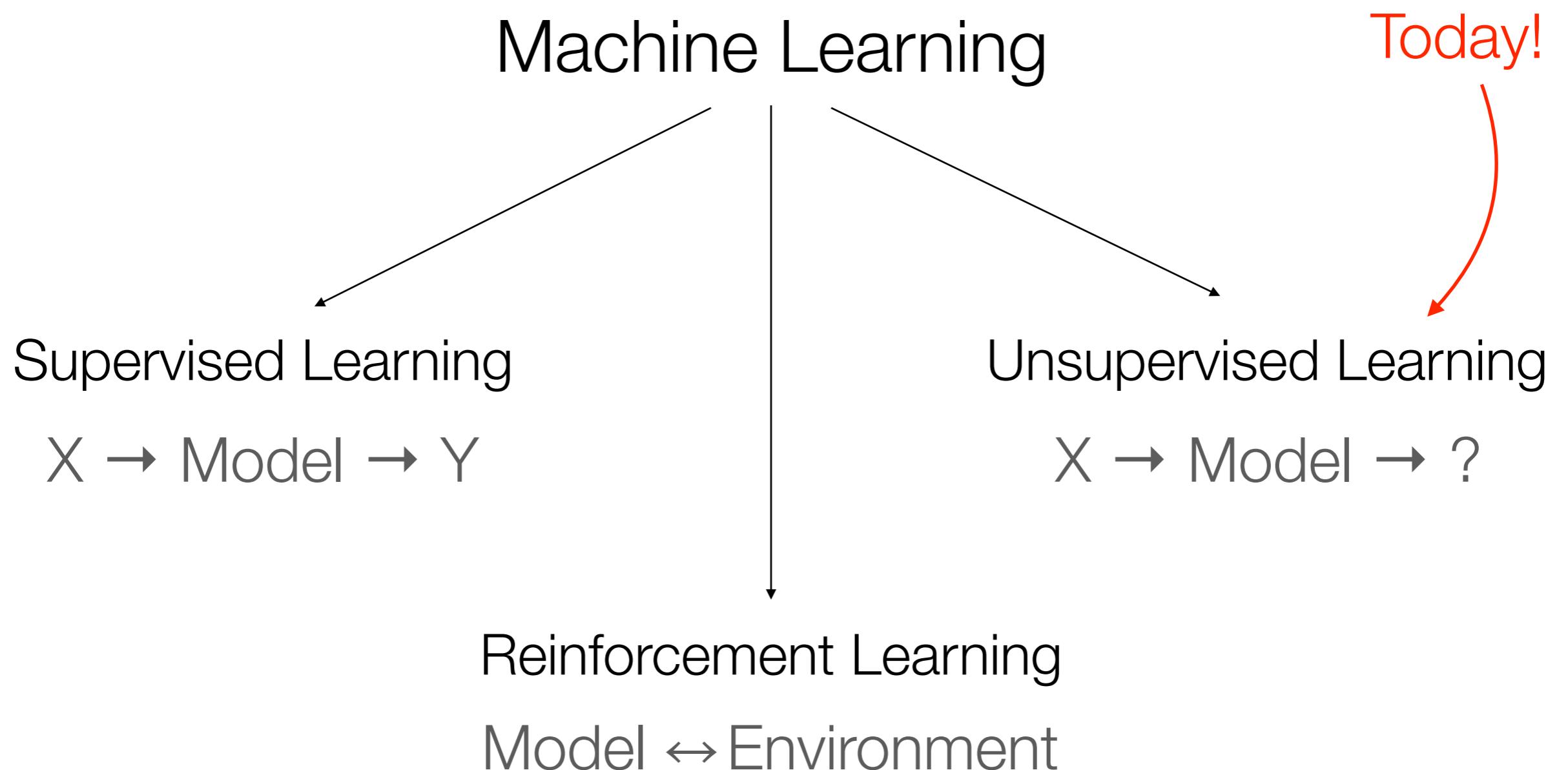
2000's

2010's

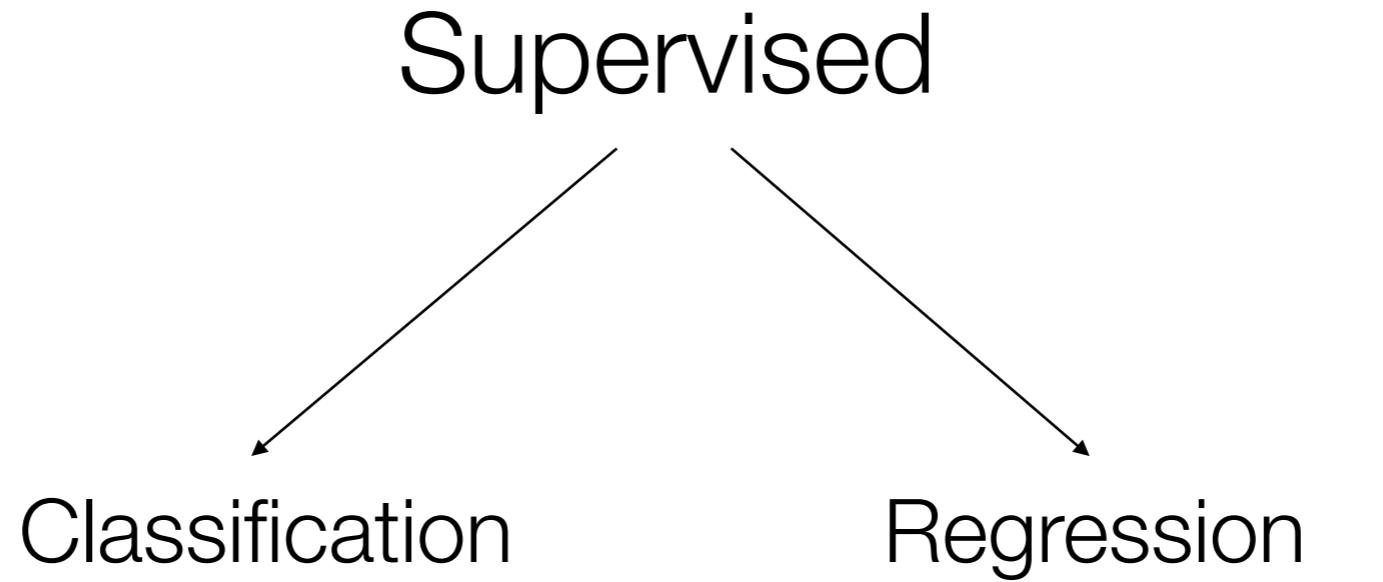
Since an early flush of optimism in the 1950s, smaller subsets of artificial intelligence – first machine learning, then deep learning, a subset of machine learning – have created ever larger disruptions.

Source: Nvidia's blog

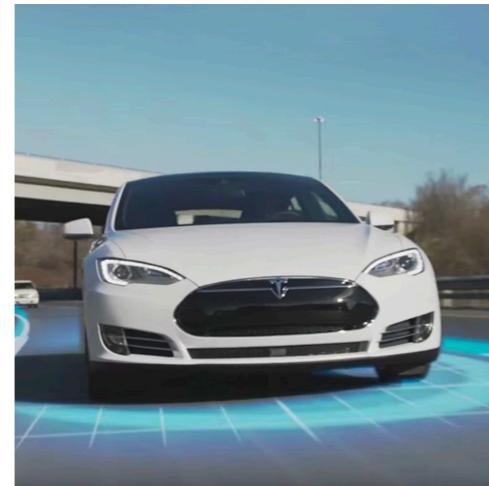
Machine Learning Tasks



Machine Learning Problems



“This is a cat!”

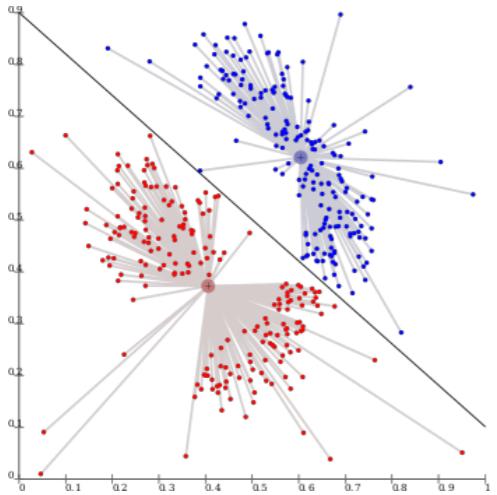


“5 degrees to the left”

Machine Learning Problems

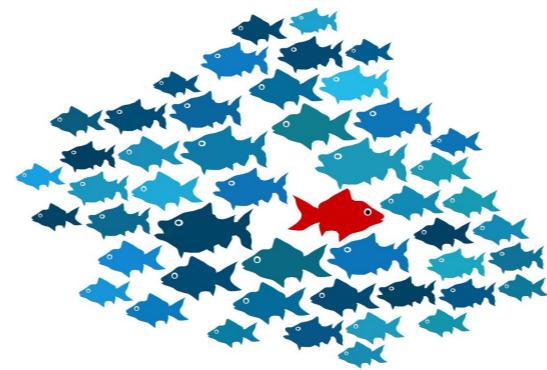
Unsupervised

Clustering



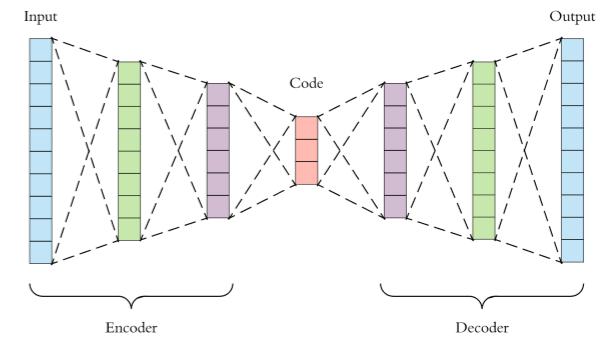
“Looks very similar
to others”

Anomaly detection



“Looks abnormal...”

Autoencoders



“Here is the encoding
for this example!”

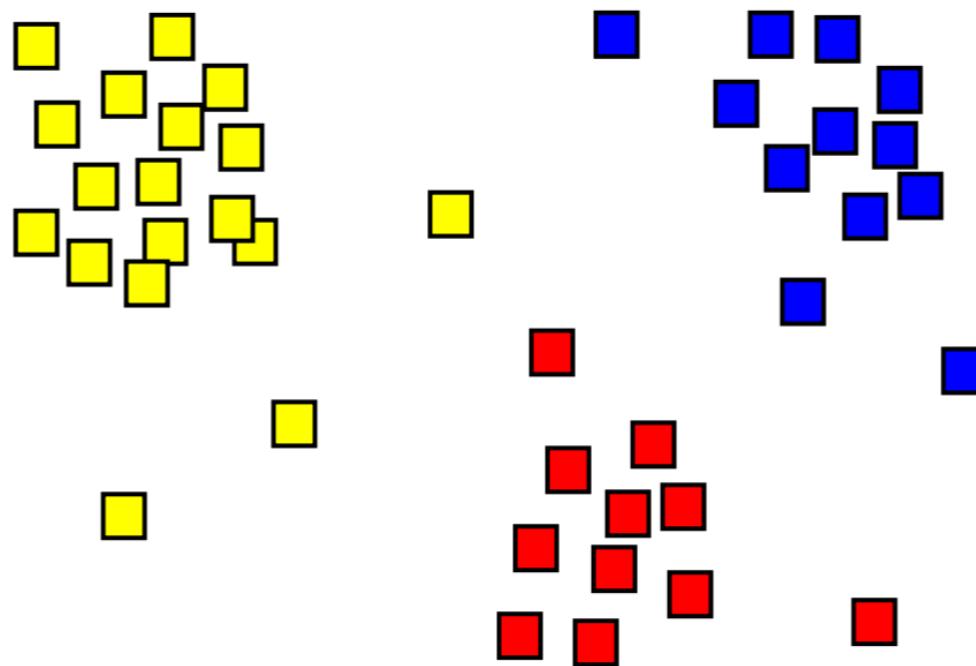
Questions? 😊

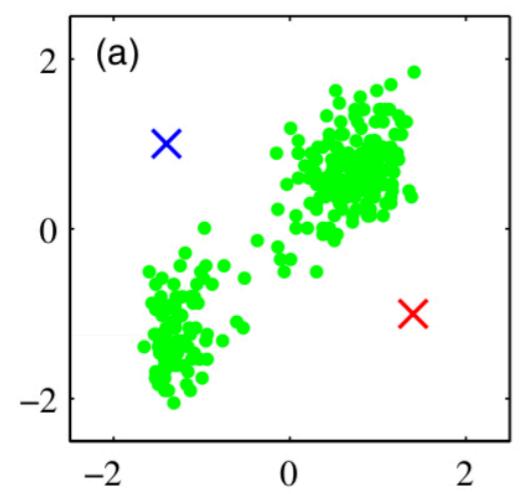
Clustering

A few words about K-Means algorithm

What is clustering?

A clustering algorithm will help you **group the data** into distinct groups, guaranteeing that data points in each group are **similar to each other**.

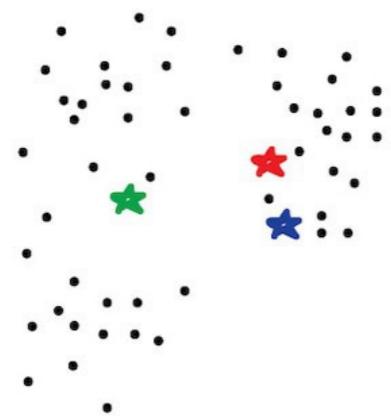




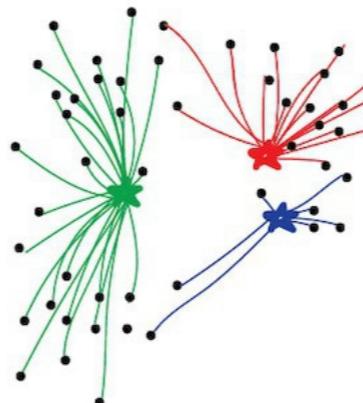
Source: *Pattern Recognition and Machine Learning*

PUT KEBAB KIOSKS IN THE OPTIMAL WAY

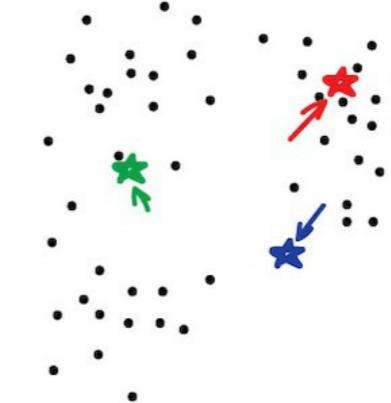
(also illustrating the K-means method)



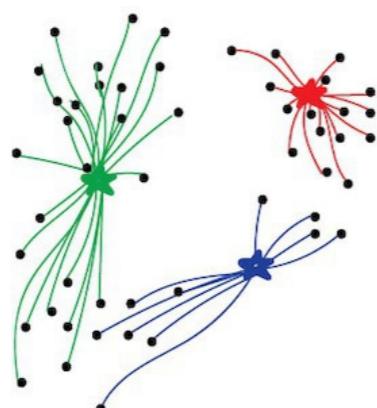
1. Put kebab kiosks in random places in city



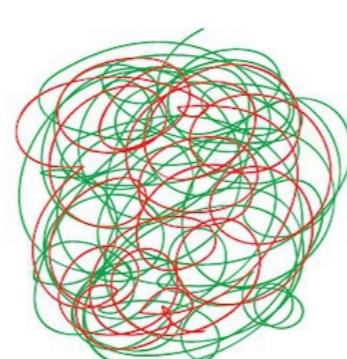
2. Watch how buyers choose the nearest one



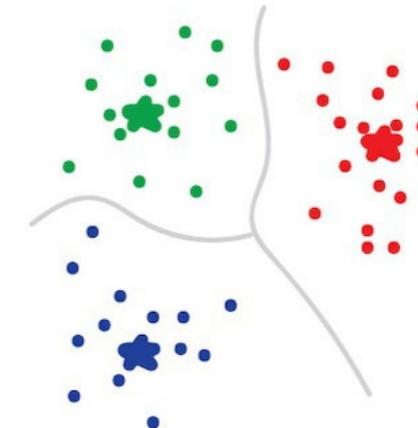
3. Move kiosks closer to the centers of their popularity



4. Watch and move again



5. Repeat a million times



6. Done!
You're god of kebabs!

Source: Vas3k's blog

K-Means Algorithm

1. Select K clusters randomly,
2. For each point select the closest cluster,
3. Update your clusters by taking mean value of all your data points,
4. Check for convergence and move to Step 2 if needed.

How to measure the distance?

Euclidean distance

$$\|a - b\|_2 = \sqrt{\sum_i (a_i - b_i)^2}$$

Squared Euclidean distance

$$\|a - b\|_2^2 = \sum_i (a_i - b_i)^2$$

Manhattan distance

$$\|a - b\|_1 = \sum_i |a_i - b_i|$$

Why/Why not to use K-Means Clustering?

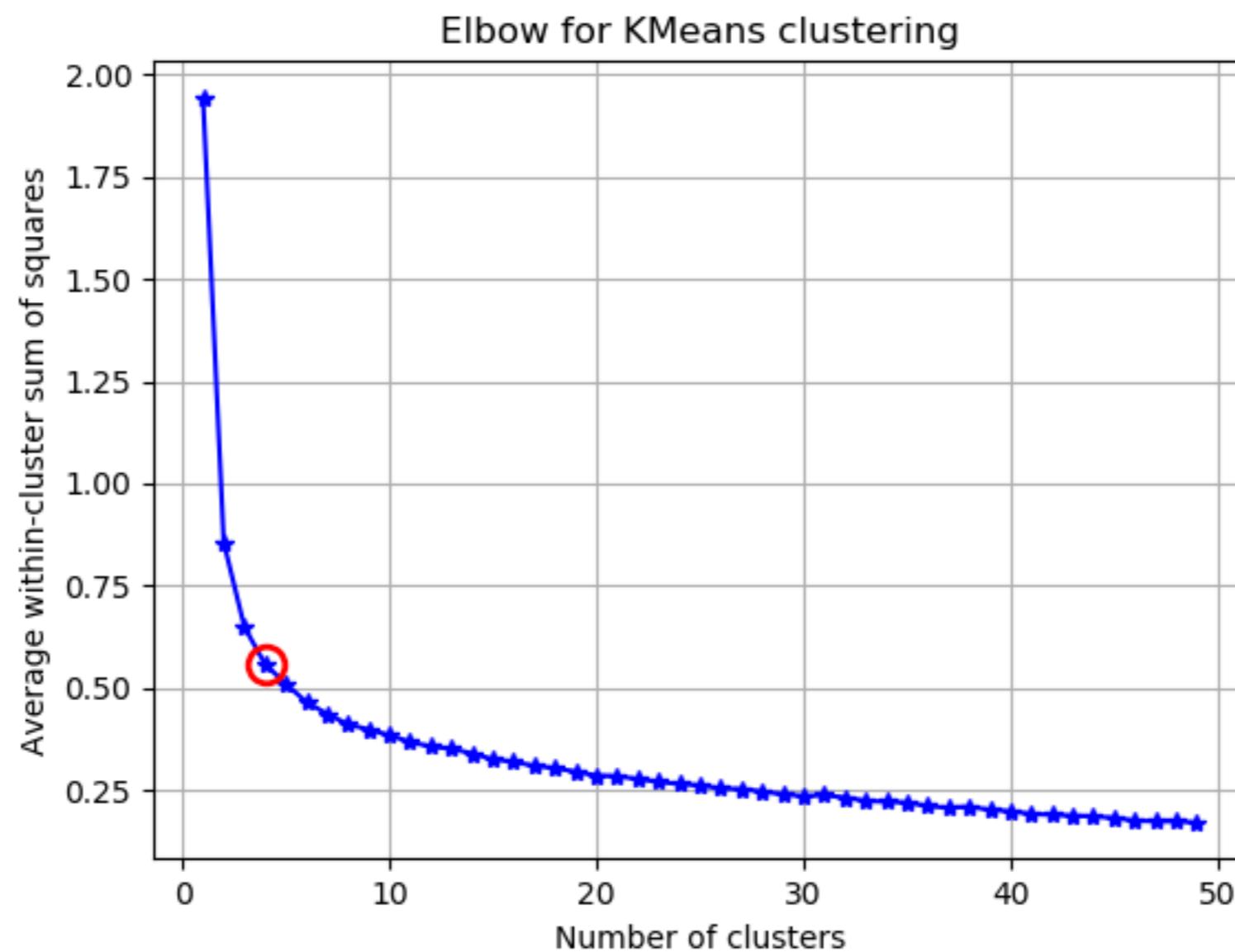
Advantages:

- Easy to implement,
- Relatively fast and efficient,
- Only one hyperparameter - K.

Disdvantages:

- Hyperparameter for number of clusters,
- Random points at the beginning.

How to choose the number of clusters?



<http://bit.ly/2OZetLC>

Let's use it in practice! 

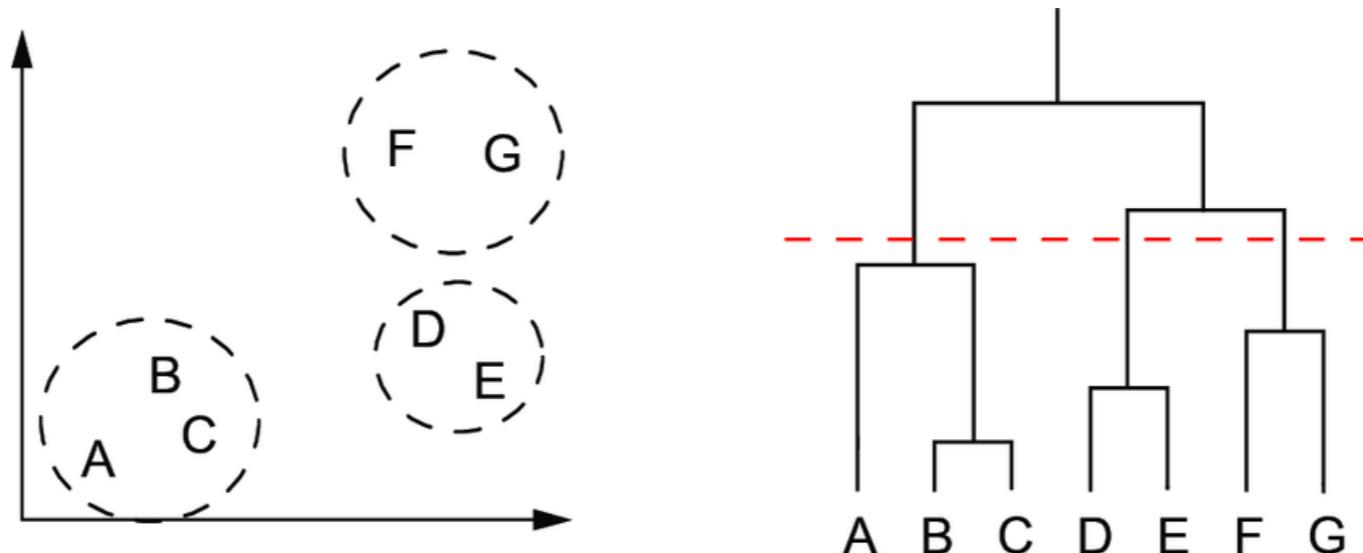
Questions? 😊

Hierarchical Clustering

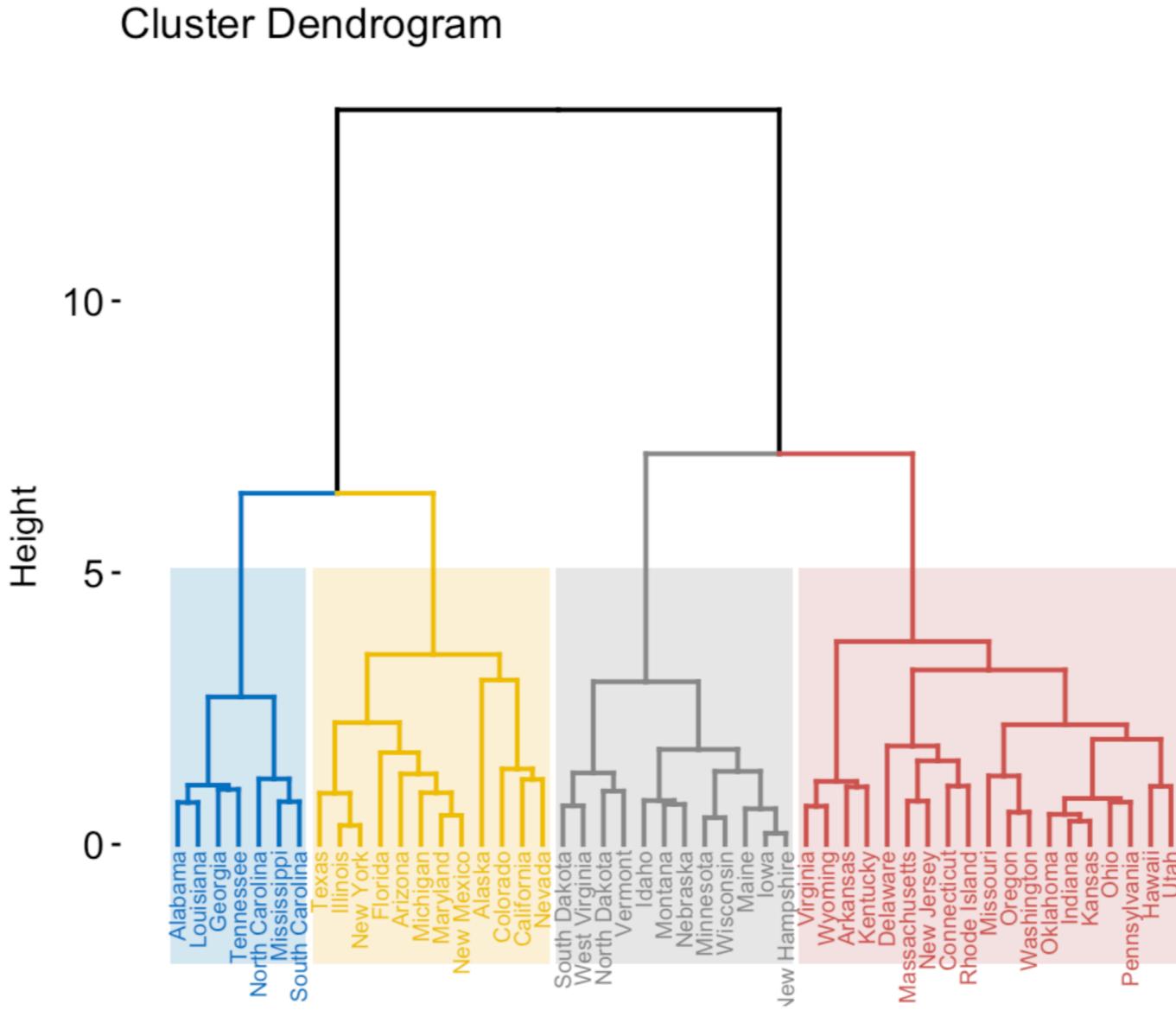
Is it really different than K-Means?

Hierarchical Clustering

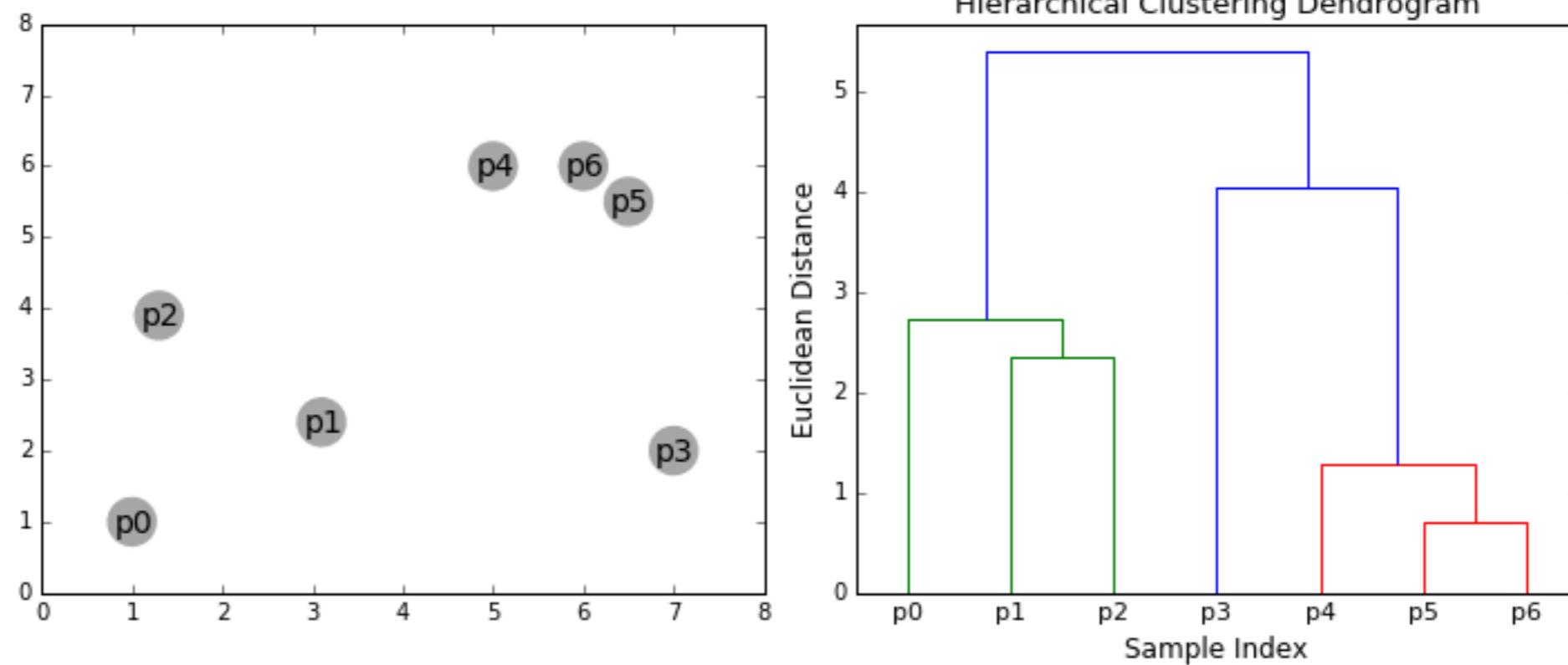
- Hierarchy of clusters is represented as a **tree**,
- **Root** is a unique cluster that gathers all samples,
- **Leaves** are clusters with only one sample.



Dendrogram is your friend



Source: Practical Guide to Cluster Analysis in R



Source: George Seif's blogpost on Towards Data Science

Agglomerative

Each observation starts in its own cluster, and pairs of clusters are merged as one moves up the hierarchy.

Divisive

All observations start in one cluster, and splits are performed recursively as one moves down the hierarchy.

Agglomerative Clustering Algorithm

1. Create separate cluster for each example in the dataset,
2. Find two closest clusters.
3. Merge them into one cluster.
4. Move to Step 2 if you have more than one cluster.

Why/Why not to use Hierarchical Clustering?

Advantages:

- No need to specify number of clusters a'priori,
- Works well with different metrics,
- The best for hierarchical data structures.

Disdvantages:

- Very low efficiency...

<http://bit.ly/2VxeyZw>

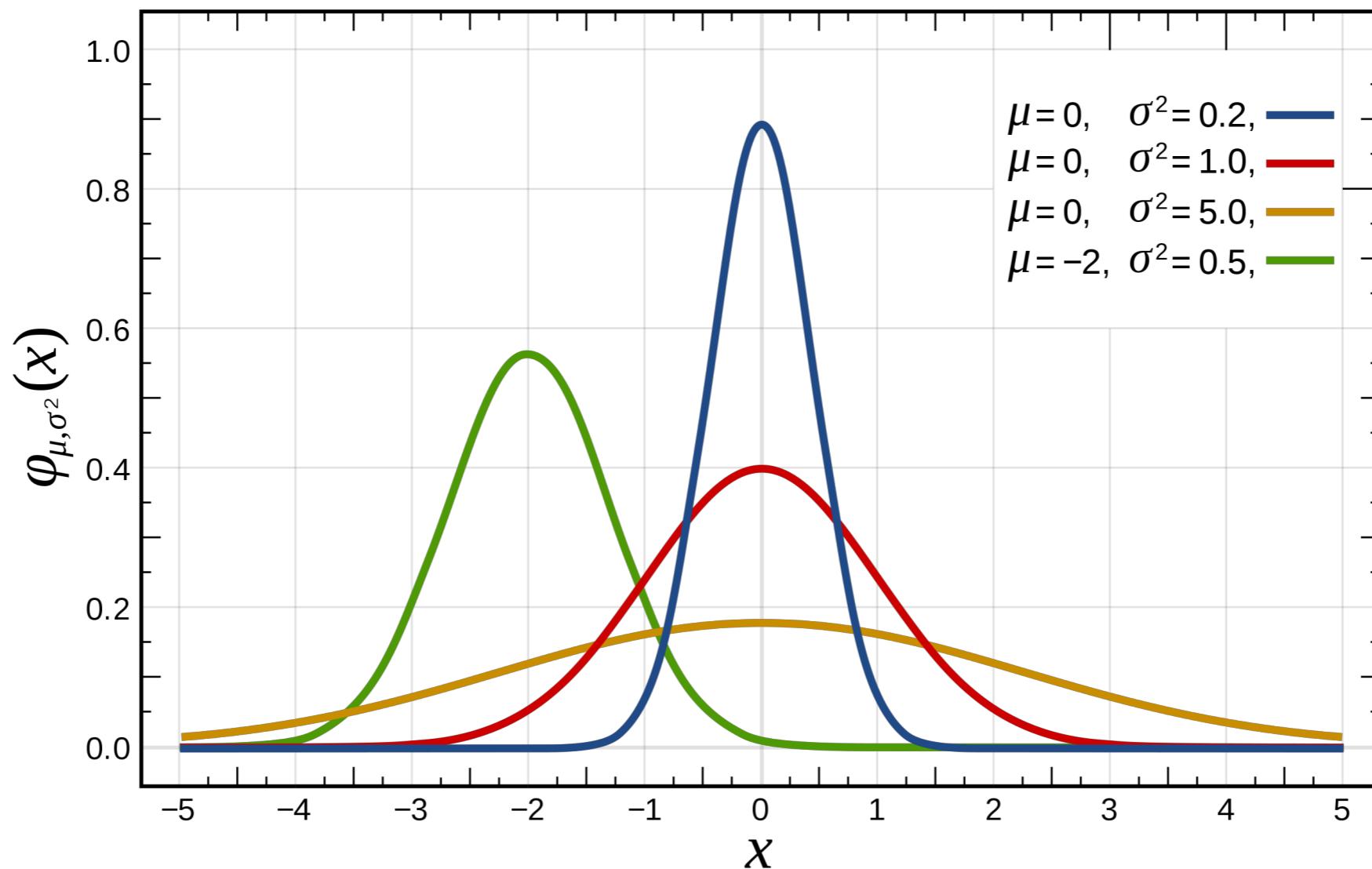
Let's use it in practice! 

Questions? 😊

Anomaly Detection

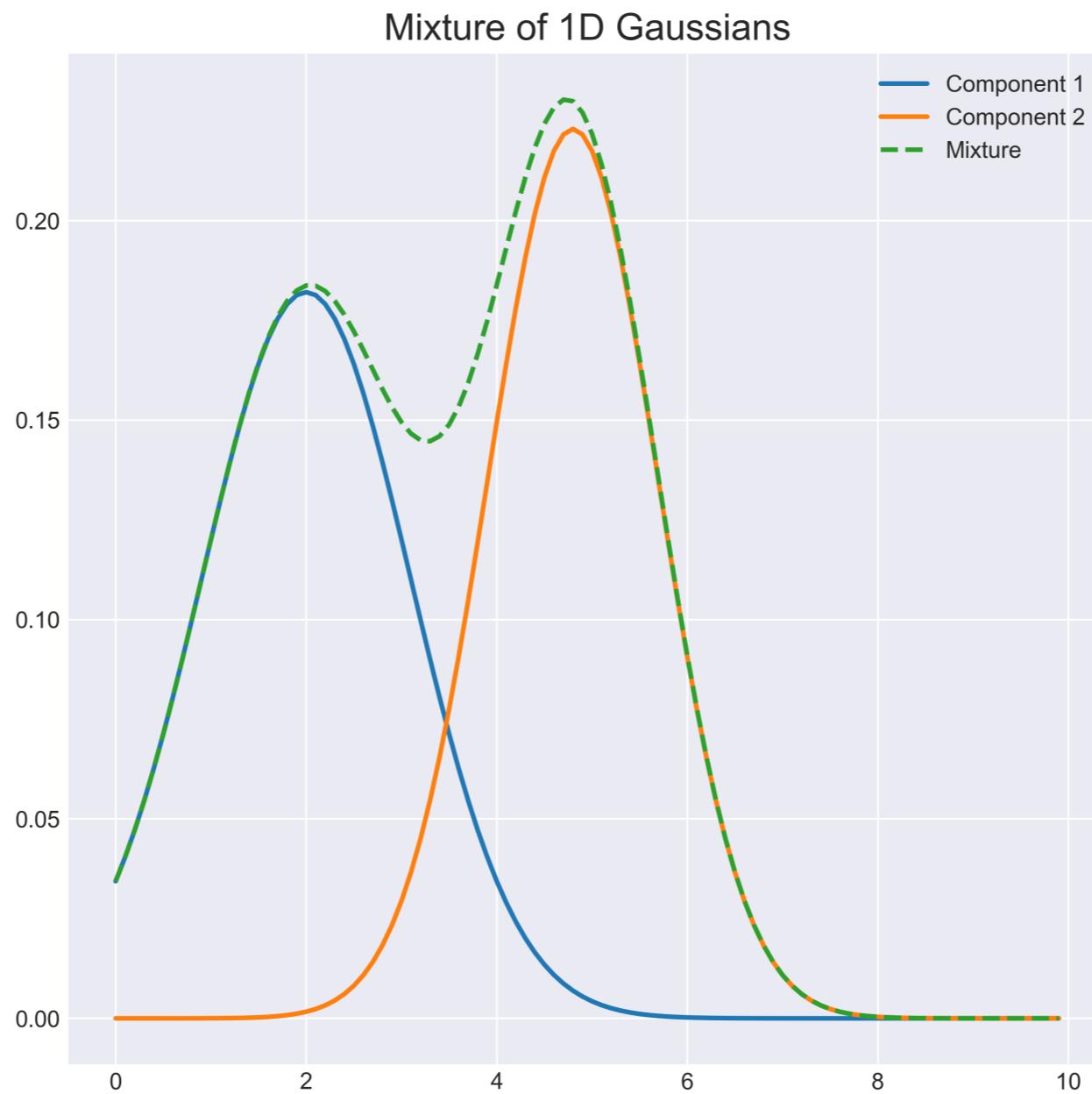
Gaussian Mixture Models

Gaussian Distribution as a base



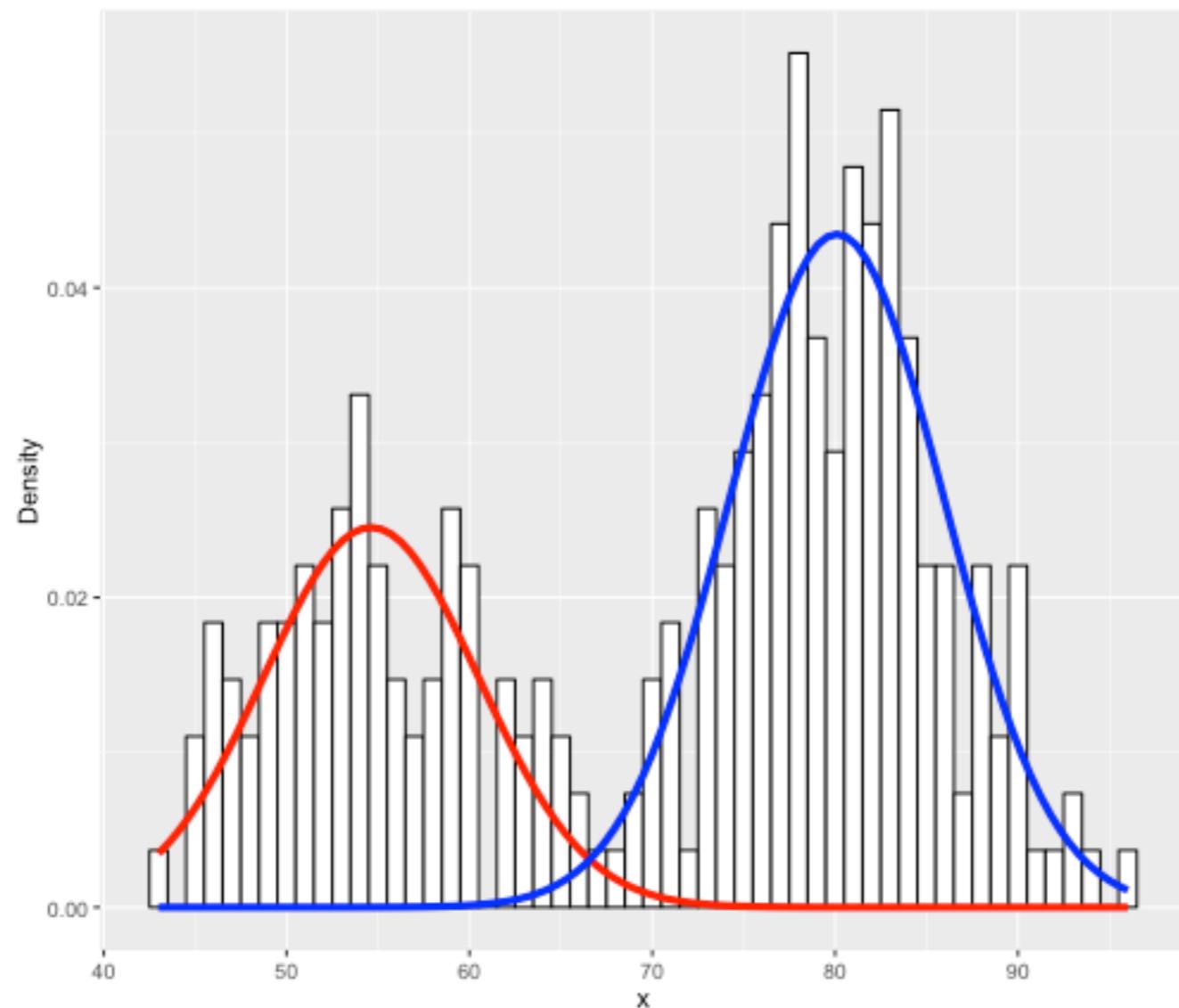
Source: Wikipedia

Mixture of Gaussians



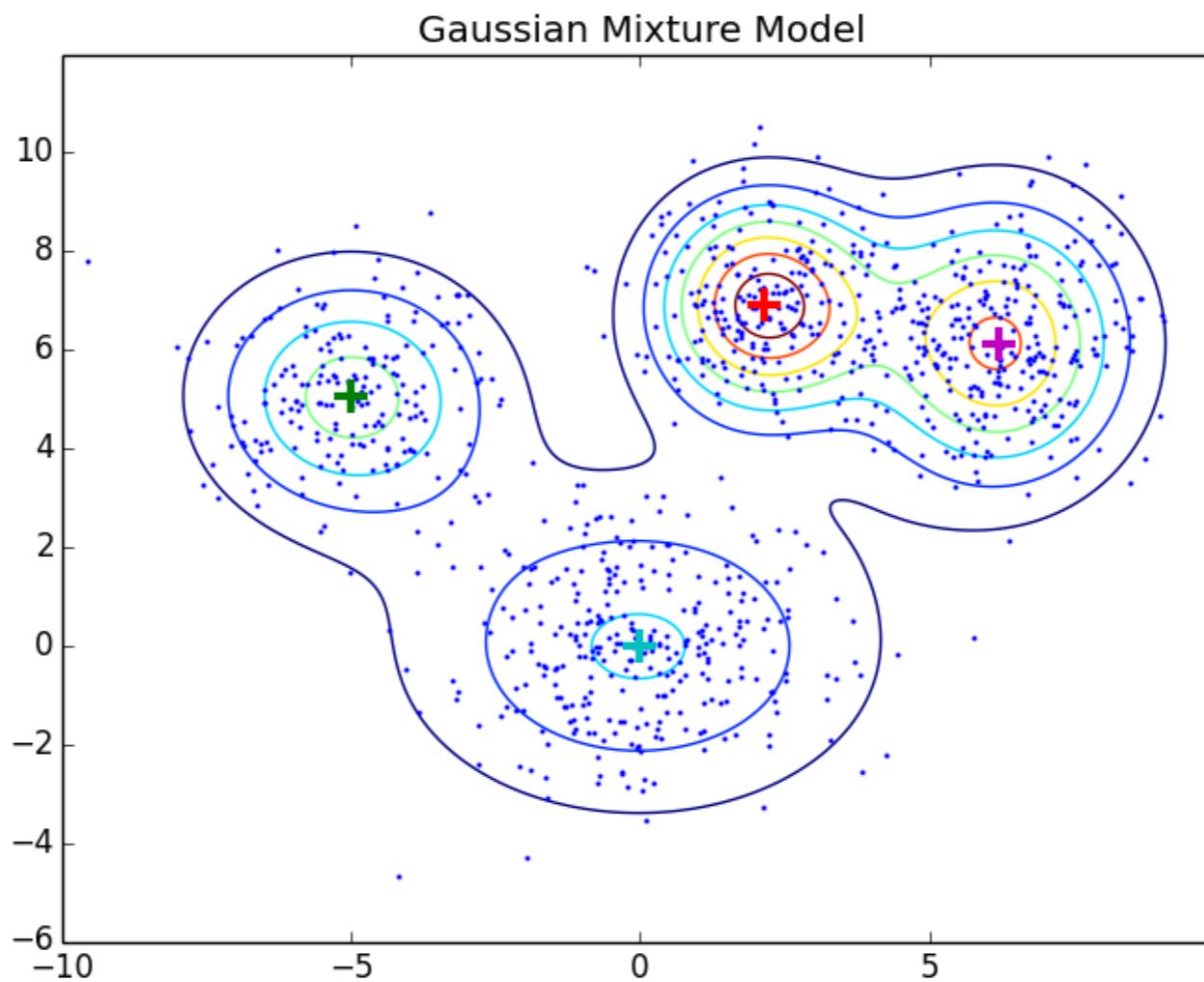
Source: Angus Turner's blog

Mixture of Gaussians

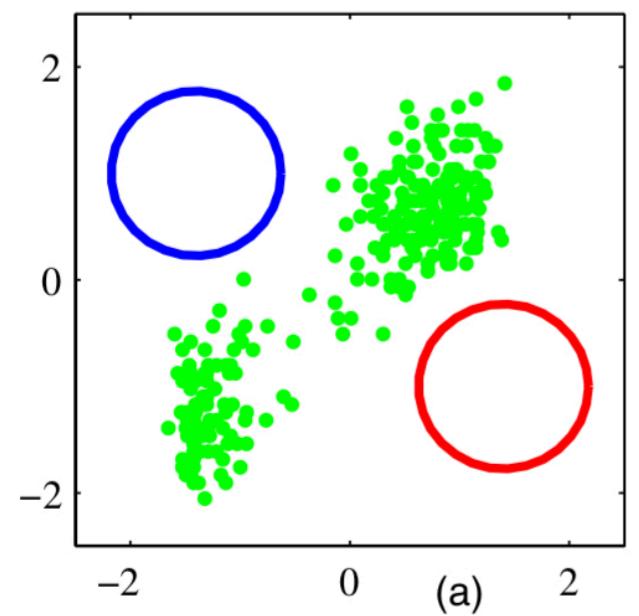


Source: Fong Chun Chan's blog

Mixture of Gaussians



Source: Yu's Machine Learning Garden blog



Source: *Pattern Recognition and Machine Learning*

Gaussian Mixture Models Algorithm

Repeat till
convergence

E Step

$$w_{ik} = \frac{\omega_k N(x_i | \mu_k, \Sigma_k^2)}{\sum_{m=1}^K \omega_m N(x_i | \mu_m, \Sigma_m^2)}$$

M Step

$$N_k = \sum_{n=1}^N w_{ik}$$

$$\mu_k = \frac{1}{N_k} \sum_{i=1}^N w_{ik} x_i$$

$$\Sigma_k = \frac{1}{N_k} \sum_{i=1}^N w_{ik} (x_i - \mu_k)(x_i - \mu_k)^T$$

$$\omega_k = \frac{N_k}{N}$$

Why/Why not to use GMMs?

Advantages:

- Mixed membership based on probability,
- More flexible in terms of covariance.

Disdvantages:

- Optimization is not so trivial...
- May not work for datasets that doesn't have “hidden” Gaussian distribution.

<http://bit.ly/2D6xA1y>

Let's use it in practice! 

Questions? 😊

Resources

- Machine Learning Course by Andrew Ng - [Coursera](#),
- “Pattern Recognition and Machine Learning”, Christopher M. Bishop,
- [Machine Learning for Everyone](#),
- Andrew Ng about [Anomaly Detection Problem](#),
- Fong Chun Chan’s blog [about Mixture Models](#),
- Yu’s Machine Learning Garden [about Gaussian Mixture Models](#),
- Angus Turner’s blogpost [about Gaussian Mixture Models in PyTorch](#).

Resources

- Iris Dataset - [Kaggle](#),
- Credit Card Fraud Detection Dataset - [Kaggle](#),
- Clustering - [Scikit-Learn User Guide](#),
- K-Means - [Scikit-Learn Documentation](#),
- Agglomerative Clustering - [Scikit-Learn Documentation](#),
- Gaussian Mixture Models - [Scikit-Learn User Guide](#),
- Gaussian Mixture Models - [Scikit-Learn Documentation](#).

Thanks

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[https://github.com/jpowie01/
UnsupervisedLearningWorkshop_BeIT](https://github.com/jpowie01/UnsupervisedLearningWorkshop_BeIT)