

DATA SCIENCE

CLUSTERING

I. SUPERVISED AND UNSUPERVISED LEARNING

II. K-MEANS CLUSTERING

III. DBSCAN CLUSTERING

I. SUPERVISED AND UNSUPERVISED LEARNING

One definition: “Machine learning is the semi-automatic extraction of knowledge from data.”

- **Knowledge from data:** Starts with a question that might be answerable using data
- **Automatic extraction:** A computer provides the insight
- **Semi-automatic:** Requires many smart decisions by a human

There are two main categories of machine learning: **supervised learning** and **unsupervised learning**.

Supervised learning (aka “predictive modeling”):

- Predict an outcome based on input data
- Example: predict whether an email is spam or ham
- Goal is “generalization”

There are two categories of supervised learning:

Regression

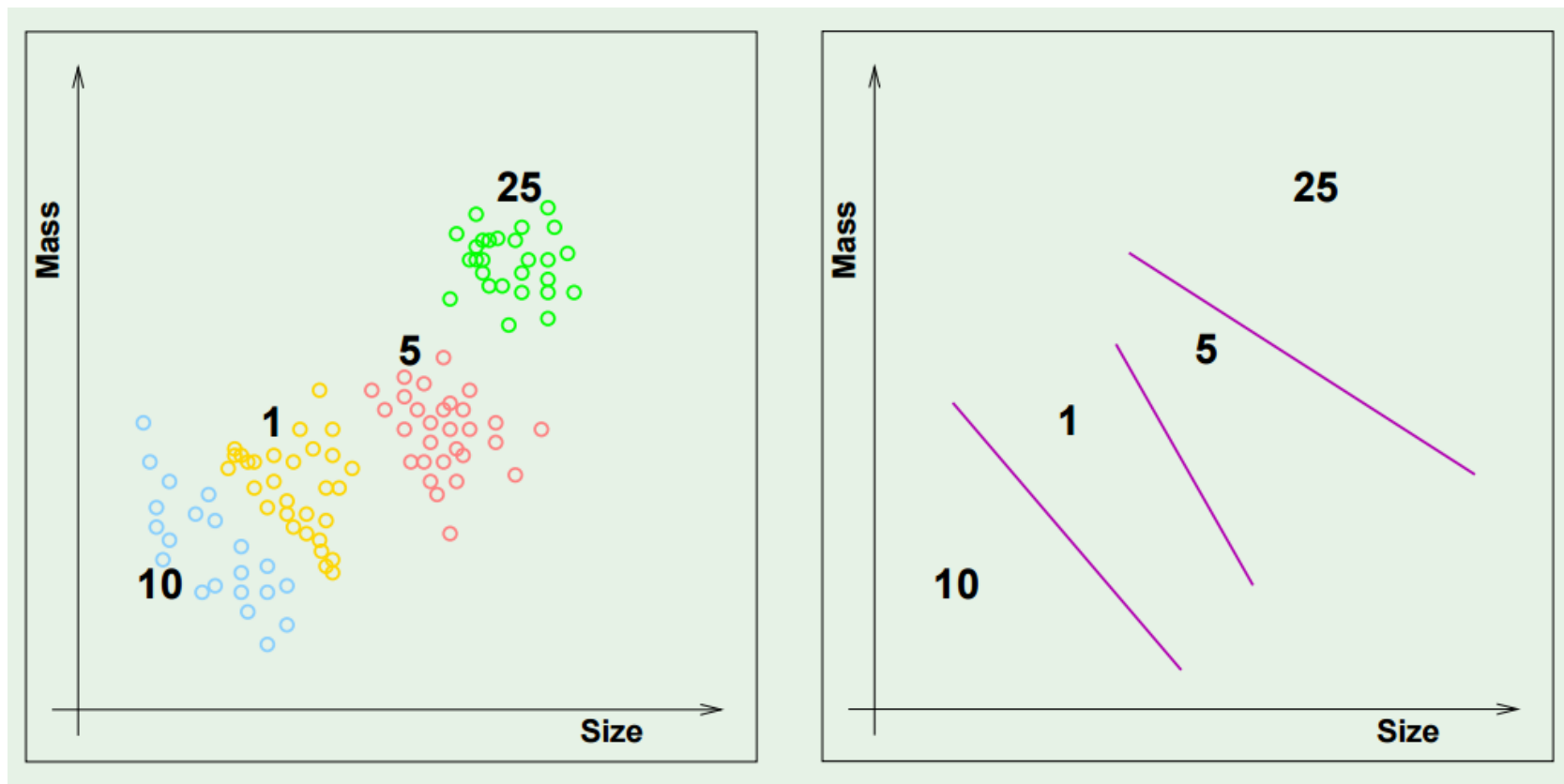
- Outcome we are trying to predict is continuous
- Examples: price, blood pressure

Classification

- Outcome we are trying to predict is categorical (values in a finite, unordered set)
- Examples: spam/ham, cancer class of tissue sample

Supervised learning example: Coin classifier

- Observations: Coins
 - Features: Size and mass
 - Response: Coin type, hand-labeled
1. Train a **machine learning model** using **labeled data**
 - Model learns the relationship between the features and the coin type
 2. Make predictions on **new data** for which the response is unknown
 - Give it a new coin, predicts the coin type automatically

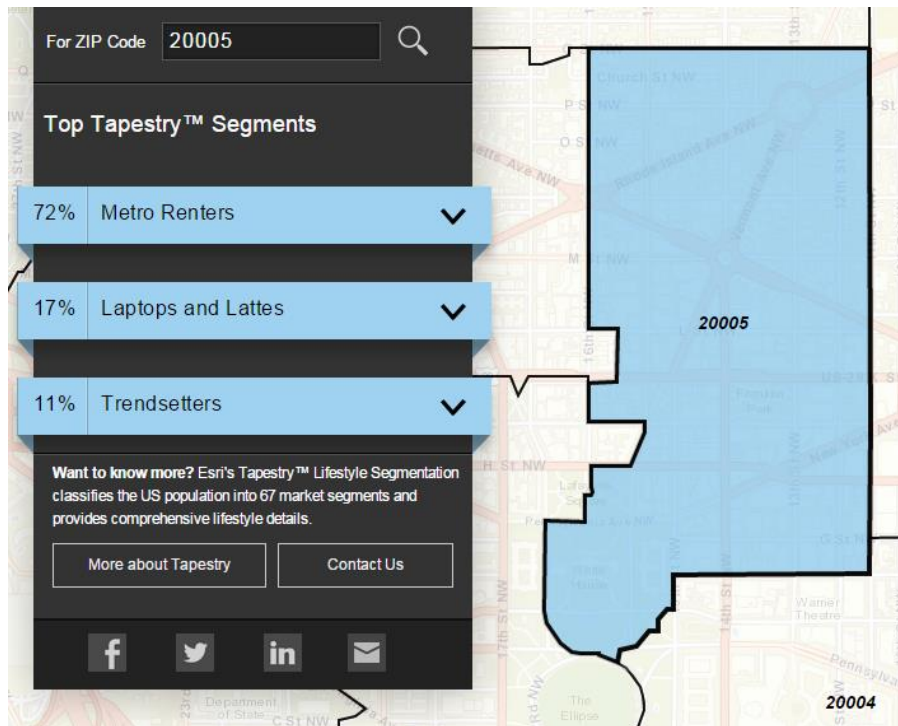


There are two main categories of machine learning: **supervised learning** and **unsupervised learning**.

Unsupervised learning:

- Extracting structure from data
- Example: segment grocery store shoppers into “clusters” that exhibit similar behaviors
- Goal is “representation”

Group US residential neighborhoods into 67 unique segments based on demographic and socioeconomic characteristics



Metro Renters:

Young, mobile, educated, or still in school, we live alone or with a roommate in rented apartments or condos in the center of the city. Long hours and hard work don't deter us; we're willing to take risks to get to the top of our professions... We buy groceries at Whole Foods and Trader Joe's and shop for clothes at Banana Republic, Nordstrom, and Gap. We practice yoga, go skiing, and attend Pilates sessions.

Source: <http://www.esri.com/landing-pages/tapestry/>

Common types of unsupervised learning:

- **Clustering:** group “similar” data points together
- **Dimensionality Reduction:** reduce the dimensionality of a dataset by extracting features that capture most of the variance in the data

Unsupervised learning has some clear differences from supervised learning. With **unsupervised learning**:

- There is no clear objective
- There is no “right answer” (hard to tell how well you are doing)
- There is no response variable, just observations with features
- Labeled data is not required

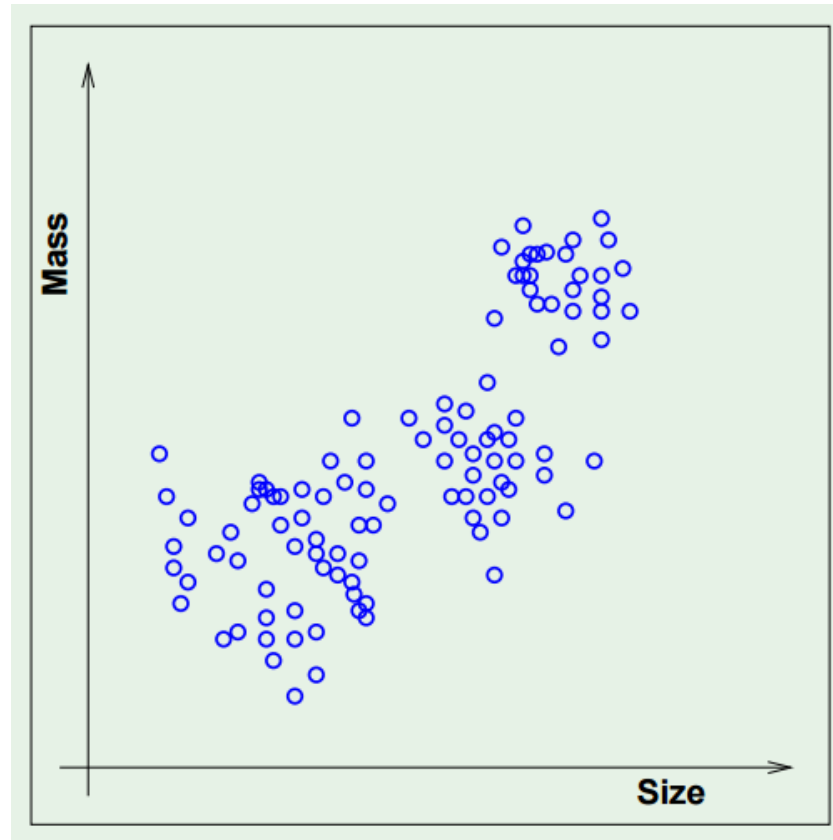
Unsupervised learning example: Coin clustering

- Observations: Coins
- Features: Size and mass
- Response: There isn't one (no hand-labeling required!)

1. Perform **unsupervised learning**

- Cluster the coins based on “similarity”
- You're done!

Sometimes, unsupervised learning is used as a “preprocessing” step for supervised learning. (How?)



II. K-MEANS CLUSTERING

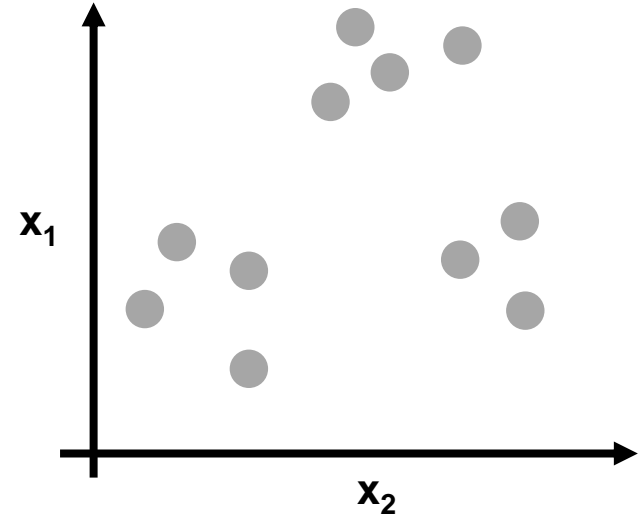
1) *choose k initial centroids (note that k is an input)*

2) *for each point:*

- find distance to each centroid*
- assign point to nearest centroid*

3) *recalculate centroid positions*

4) *repeat steps 2-3 until stopping criteria met*



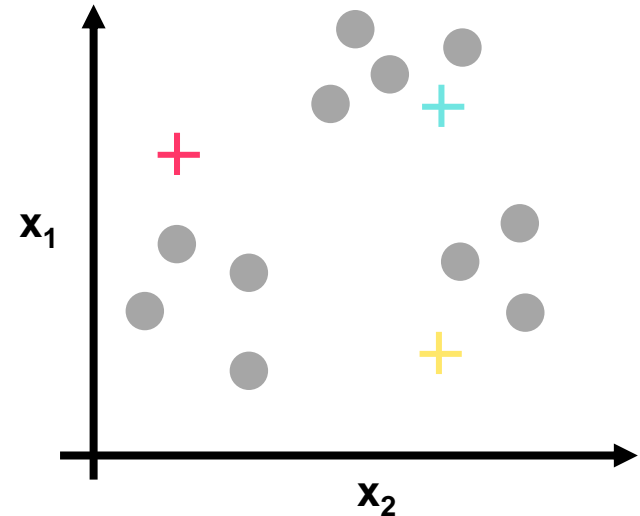
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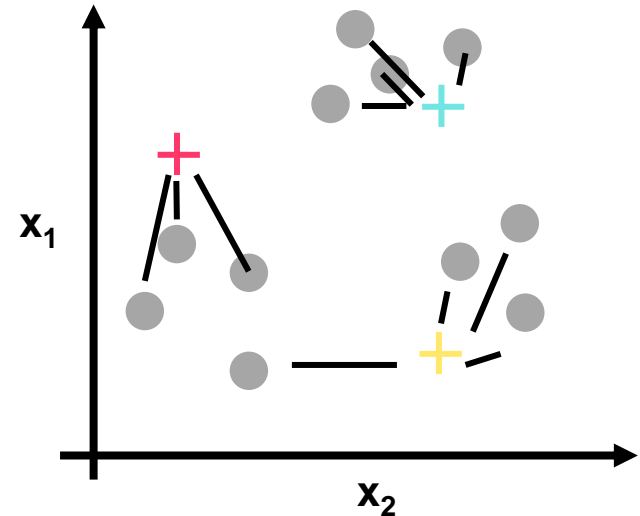
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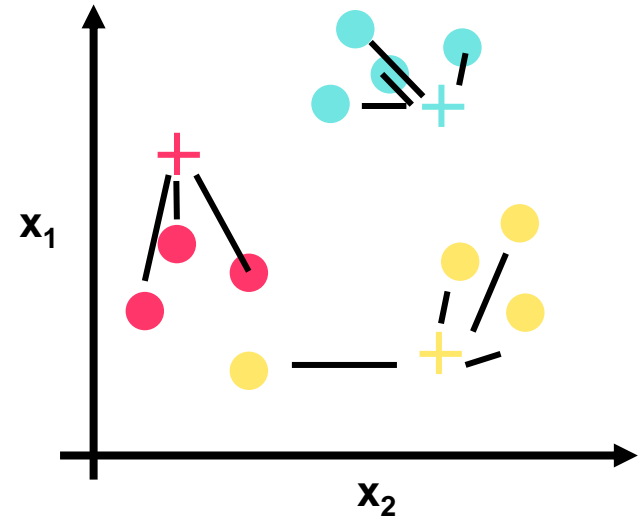
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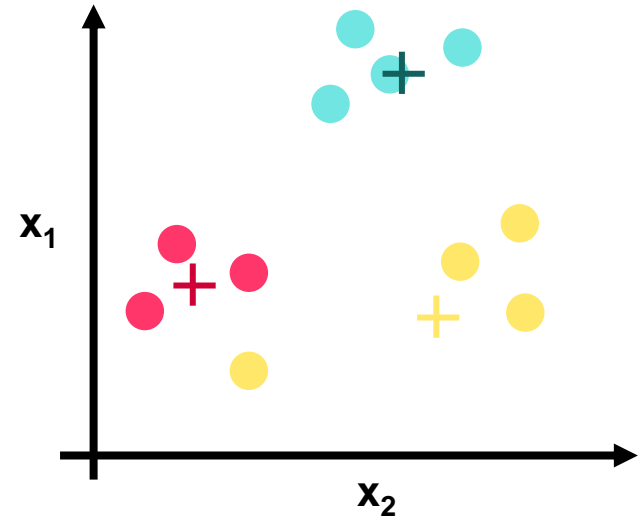
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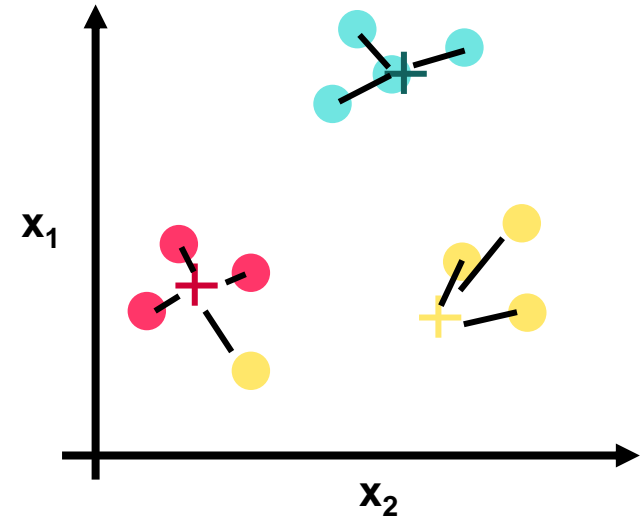
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3) *recalculate centroid positions*

4) *repeat steps 2-3 until stopping criteria met*



- 1) *choose k initial centroids (note that k is an input)*
- 2) *for each point:*
 - *find distance to each centroid*
 - *assign point to nearest centroid*
- 3) *recalculate centroid positions*
- 4) *repeat steps 2-3 until stopping criteria met*



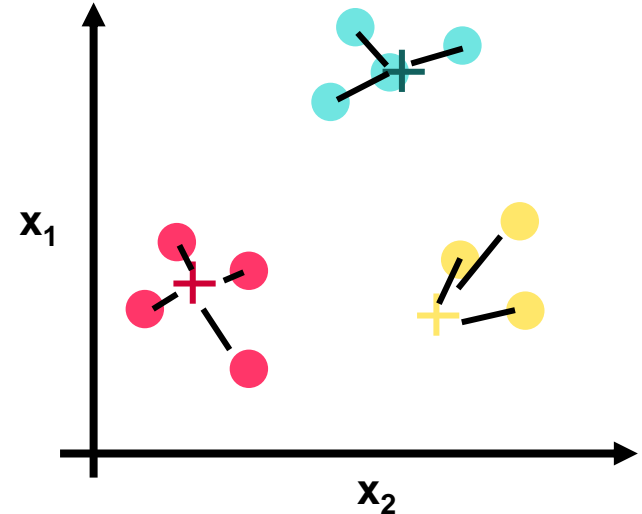
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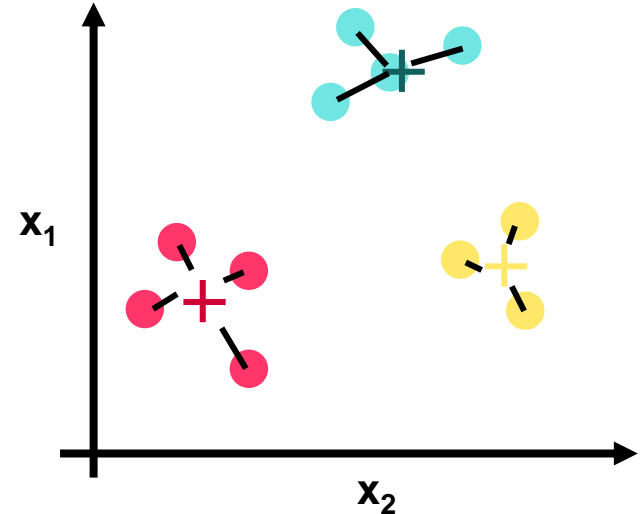
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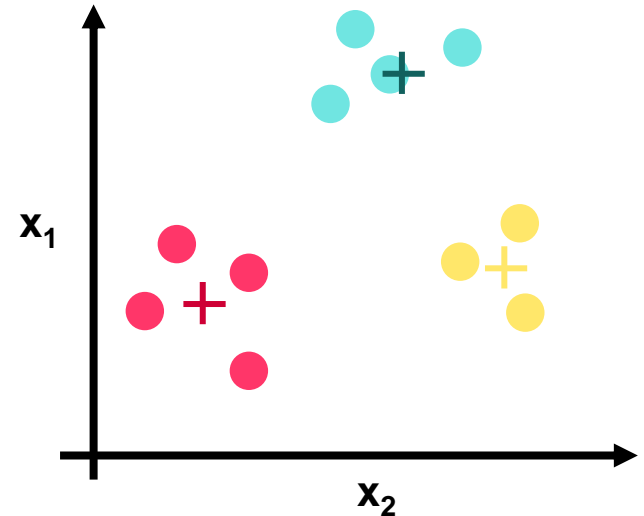
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Questions:

- What if no clusters exist?
- How to choose K ?
- How to choose the initial centroid positions?
- When to stop the algorithm?
- When might it produce poor results?

What if no clusters exist?

- It will still find clusters!
 - Visualization: I'll Choose, Uniform Points

How to choose K?

- It will find the number of clusters specified
 - Visualization: I'll Choose, Gaussian Mixture, $K=2/3/4$
- Try different values for K and pick the “best”

How to choose the initial centroid positions?

- Randomly
 - Doesn't tend to work well
 - Visualization: <http://asa.1gb.ru/kmeans/1.html>
- Farthest point
 - Visualization: Farthest Point, Packed Circles, K=7
- K-means++
 - Similar to farthest point, but adds some randomness
 - Used by default in scikit-learn
- In all cases: Run it several times and pick the best result to avoid local minima

When to stop the algorithm?

- Tends to converge quickly
- Set stopping criteria:
 - Maximum number of iterations
 - Once centroids move less than a threshold amount
 - Once fewer points than a threshold amount change clusters
 - Visualization: Randomly, Pimpled Smiley, $K=6$

When might it produce poor results?

- Data with varying shapes
 - Visualization: I'll Choose, Smiley Face, $K=4$
 - Visualization: I'll Choose, Density Bars, $K=1$
- Data with different scales
- Still the most popular clustering algorithm, used for a wide range of applications

III. DBSCAN CLUSTERING

DBSCAN: Density-Based Spatial Clustering of Applications with Noise

For DBSCAN, clusters are areas of **high density** separated by areas of **low density**.

DBSCAN Algorithm:

1. Choose “epsilon” and “min_samples”
2. Pick an arbitrary point, and check if there are at least “min_samples” points within the distance “epsilon”
 - If yes, add those points to the cluster and check each of the new points
 - If no, choose another arbitrary point to start a new cluster
3. Stop once all points have been checked

Visualization: Uniform Points

DBSCAN Advantages:

- Clusters can be any shape or size
- No need to choose the number of clusters

DBSCAN Disadvantages:

- More parameters to tune
- Doesn't work with clusters of varying density

Note: Not every point is necessarily assigned to a cluster!