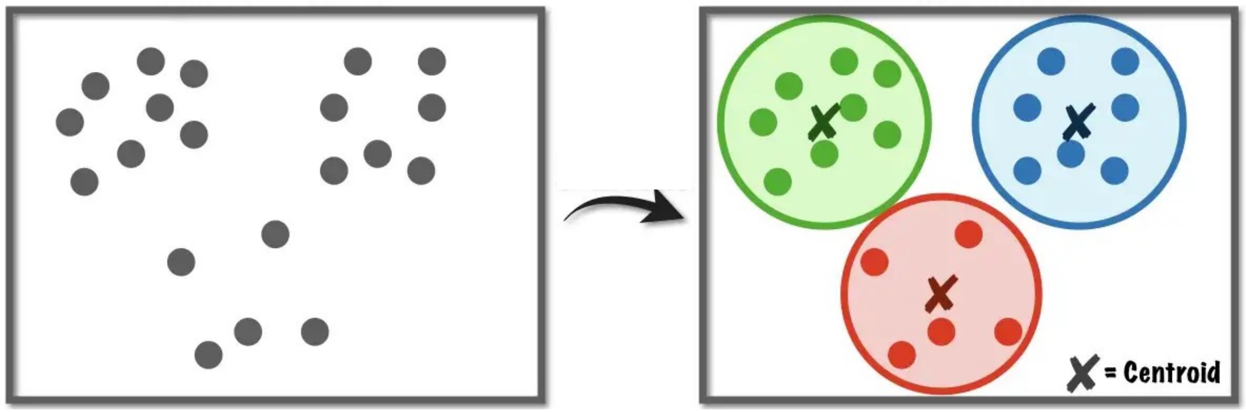
Clustering: K-Means & Nearest Neighbor

Foundation of Data Analysis

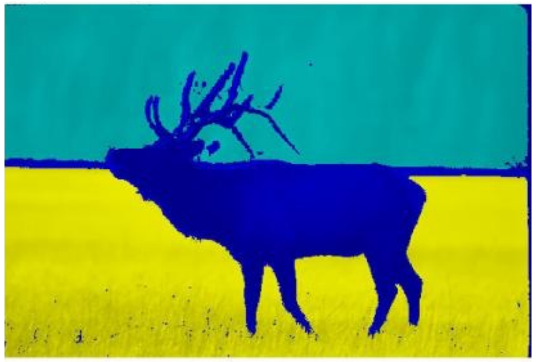
February 08, 2023

Clustering Example



Divide data into different groups

Original image

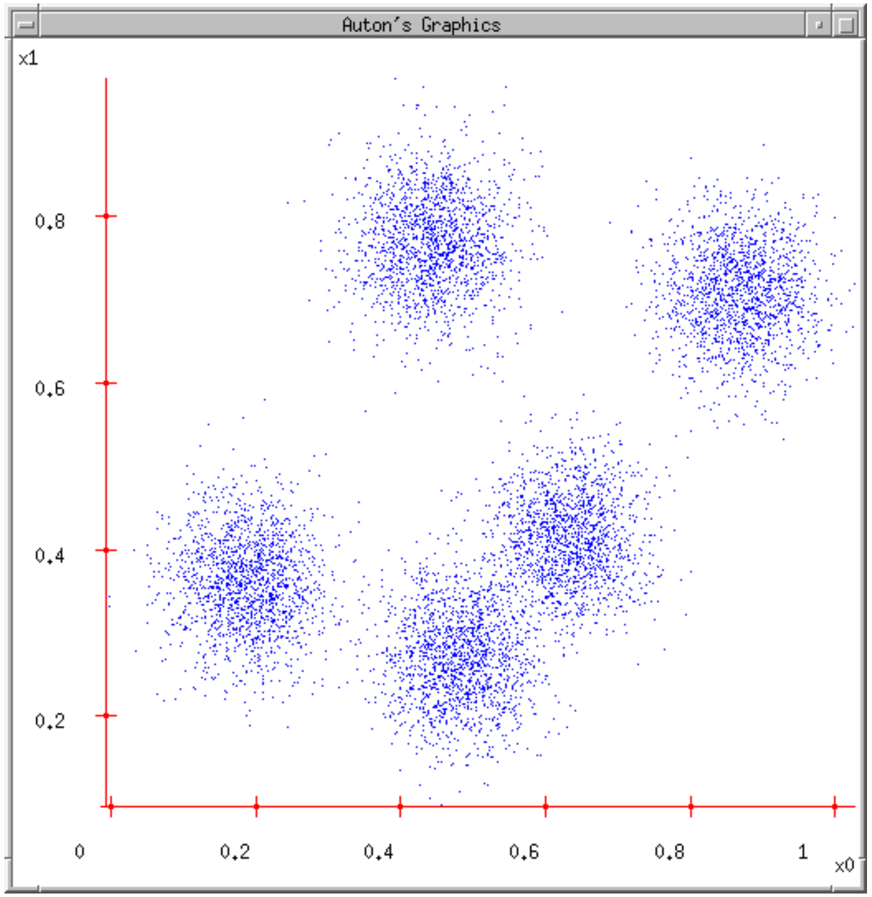

Segmented image

Types of Learning Algorithms

- **Supervised (inductive) learning**
  - Training data (observed examples) includes desired outputs
- **Unsupervised learning**
  - Training data does not include desired outputs
- **Semi-supervised learning**
  - Training data includes a few desired outputs
- **Reinforcement learning**
  - Rewards from sequence of actions

Clustering I: K-means

1. Ask user how many clusters they'd like (e.g. k=5)



Clustering I: K-means

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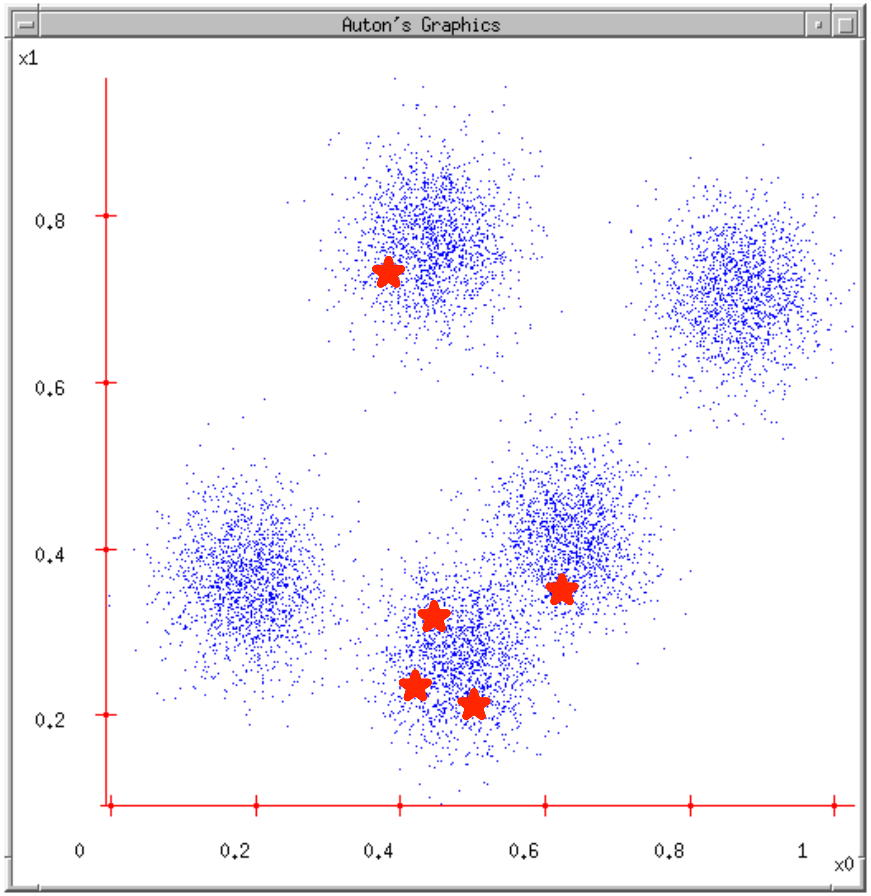
2. Randomly guess k cluster Center locations



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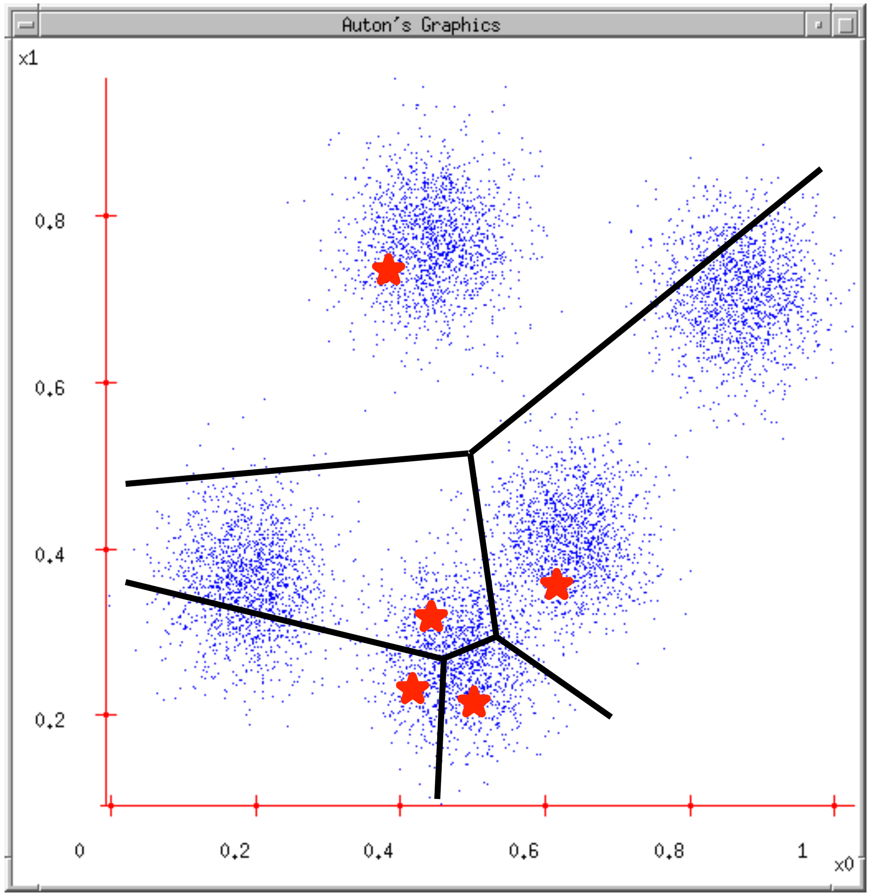
3. Each datapoint finds out which Center it's closest to.



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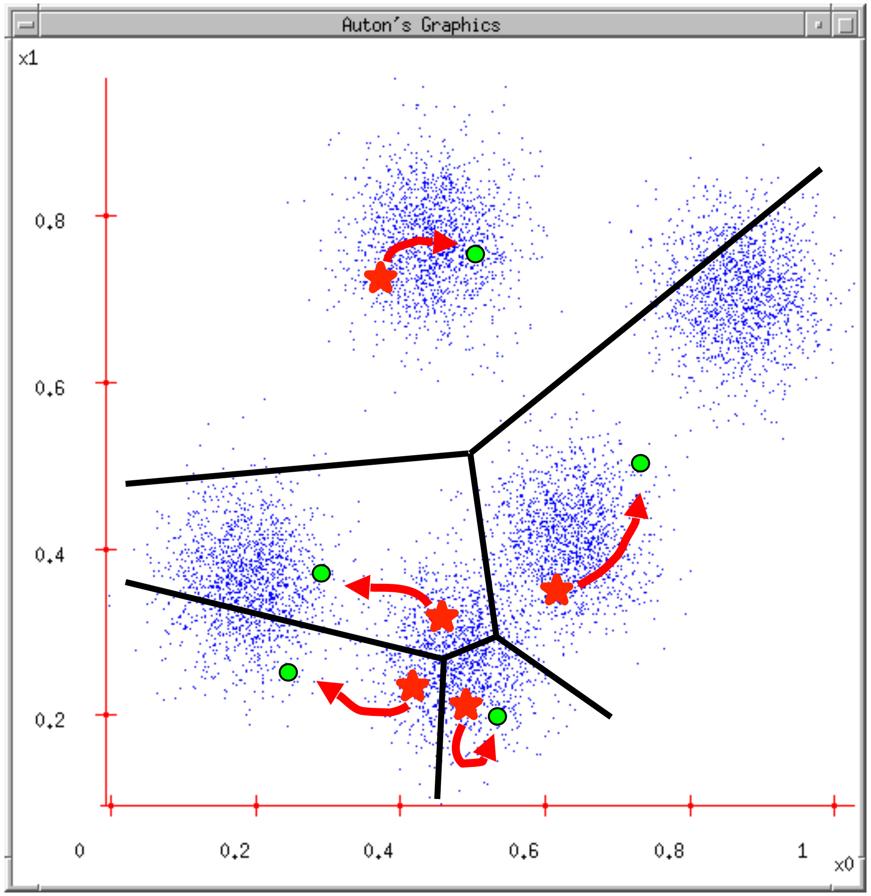

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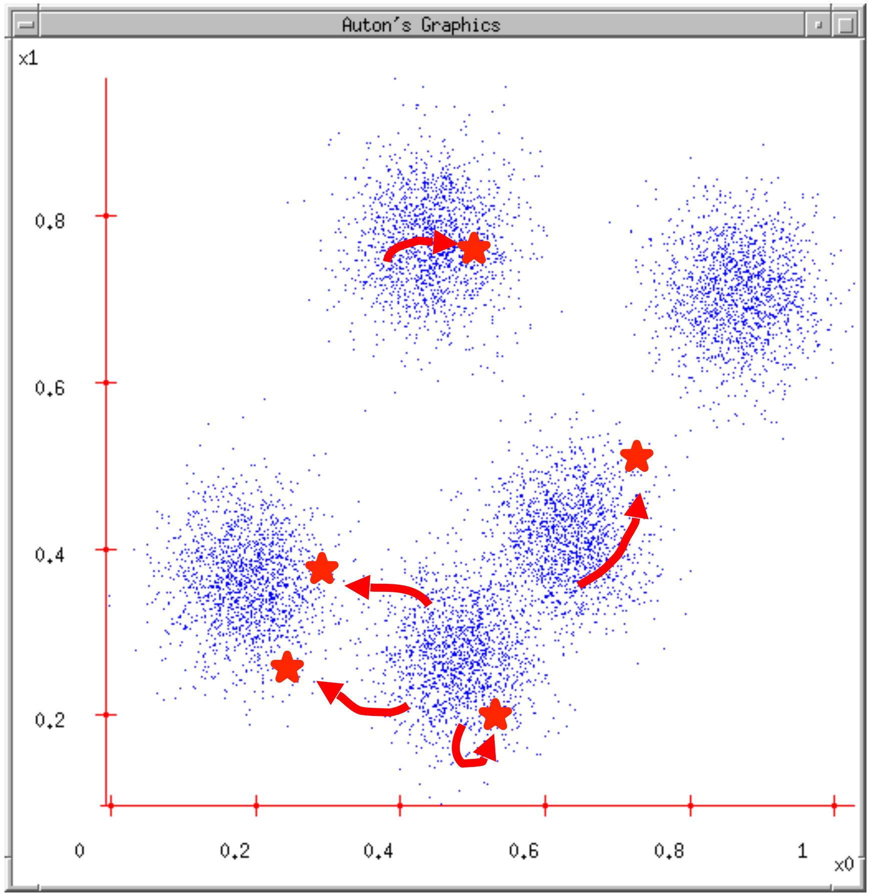
5. …and jumps there
6. …Repeat until terminated!



Disadvantages of K-means

- Does not work efficiently with complex geometrical shaped data (mostly non-linear)

- Hard assignment for labels might lead to misgrouping

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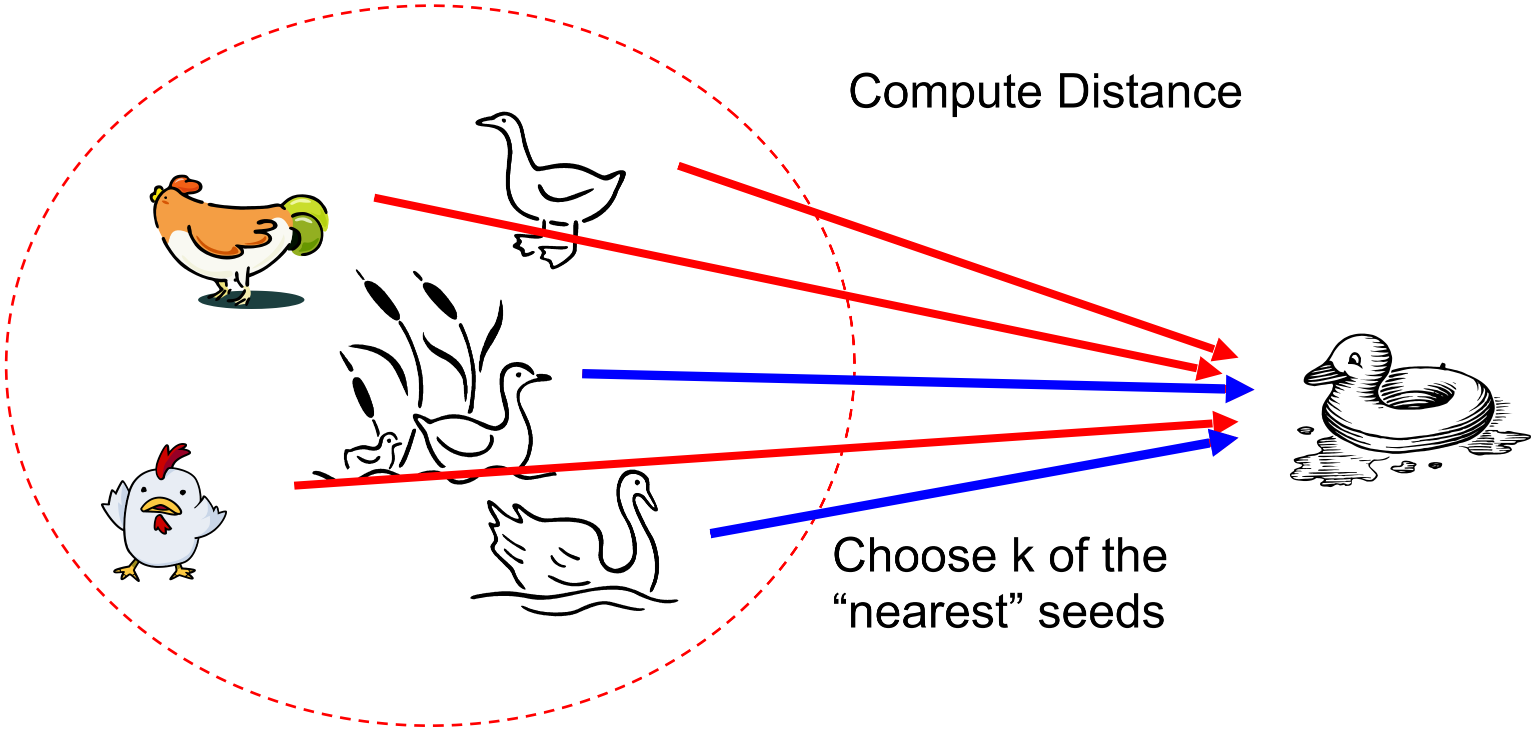
Clustering II: Nearest Neighbors

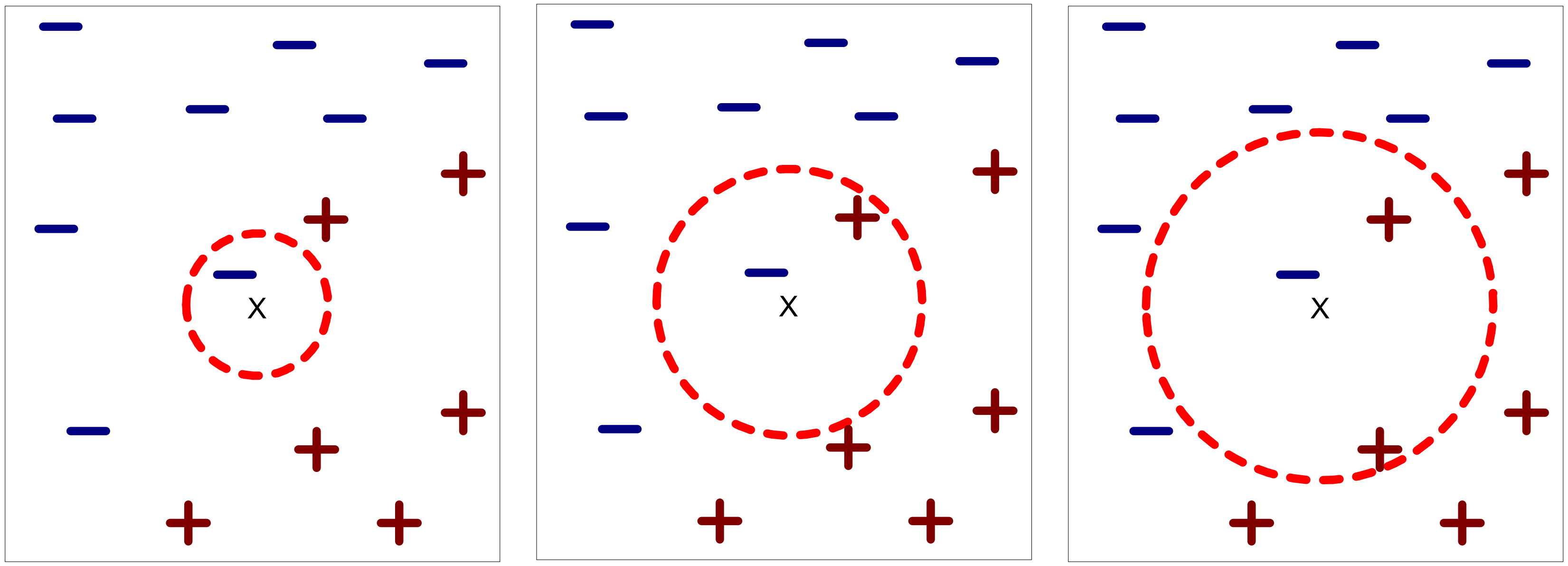
- Can be either supervised Learning or unsupervised learning

Nearest Neighbors: Unsupervised Learning

- Basic idea:
  - If it walks like a duck, quacks like a duck, then it's probably a duck



Nearest Neighbors

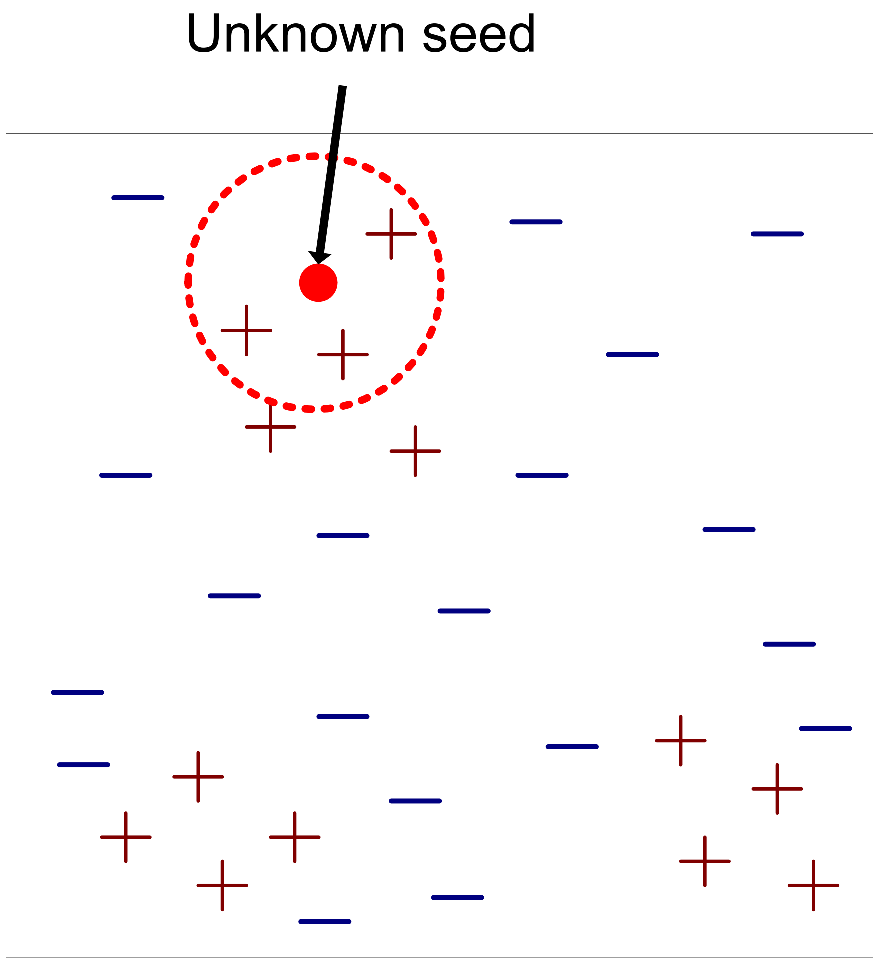


(a) 1-nearest neighbor (b) 2-nearest neighbor (c) 3-nearest neighbor

- K-nearest neighbors of seed x: data points that have the k smallest distance to x.

- K-Nearest Neighbor (KNN) classification - supervised learning

KNN Classifiers



- Requires three things
  - The set of stored records
  - Distance metric
  - The value of *k*, the number of nearest neighbors to retrieve

- To classify an unknown seed:
  - Compute distance to other training seeds
  - Identify *k* nearest neighbors
  - Use class labels of nearest neighbors to determine the class label of unknown seed (e.g., by taking majority vote)

Nearest Neighbor Classification

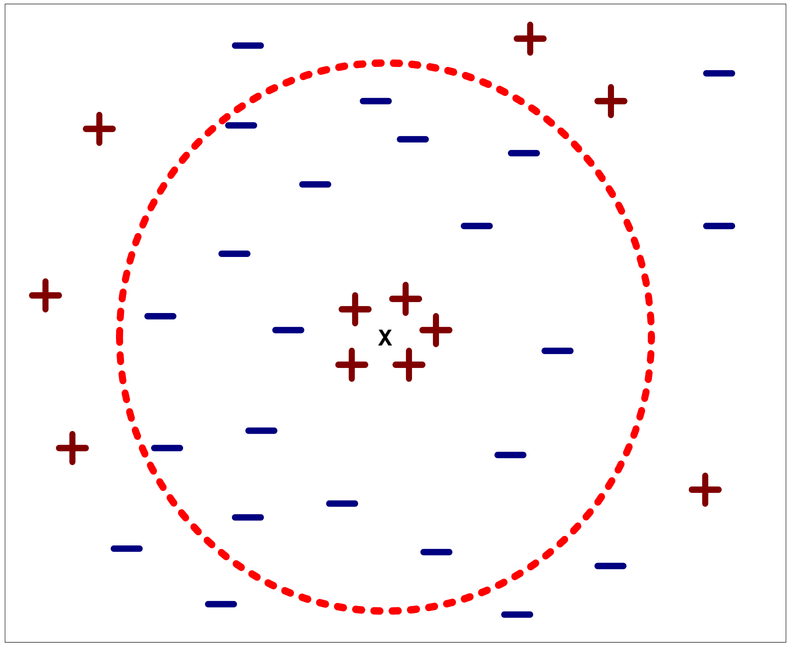
- Compute distance between two points:
  - Euclidean distance

$$d(p,q) = \sqrt{\sum_i (p_i - q_i)^2}$$

- Determine the class from nearest neighbor list
  - take the majority vote of class labels among the k-nearest neighbors
  - Weight the vote according to distance
    - weight factor, w = $1/d^2$

Nearest Neighbor Classification…

- Choosing the value of k:
  - If k is too small, sensitive to noise
  - If k is too large, neighborhood may include points from other classes



Issues of Nearest Neighbor Classification

- Scaling issues
  - Attributes (features) may have to be scaled to prevent distance measures from being dominated by one of the attributes
  - Example:
    - height of a person may vary from 1.5m to 1.8m
    - weight of a person may vary from 90lb to 300lb
    - income of a person may vary from $10K to $1M

K-NN Algorithm

- Training:
  - Save the training examples (a lazy learner; does not build training model explicitly).
- At prediction:
  - Find the k training examples $(x_1,y_1),\ldots(x_k,y_k)$ that are closest to the test example x
  - Predict the most frequent class among those y_i's.

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- Improvements:
  - Weighting examples from the neighborhood
  - Measuring “closeness”
  - Finding “close” examples in a large training set quickly

Tricks with Fast k-NN

Anyway to speed up the KNN?

Tricks with Fast k-NN

K-means using r-NN

1. Pick k points $c_1=x_1,\ldots.,c_k=x_k$ as centers
2. For each x_i, find D_i=Neighborhood(x_i)
3. For each x_i, let c_i=mean(D_i)
4. Go to step 2….