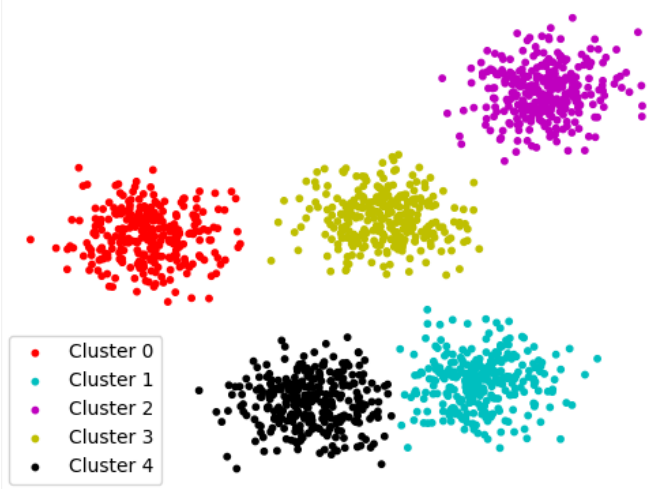
Clustering: K-Means, Nearest Neighbors

Foundation of Data Analysis

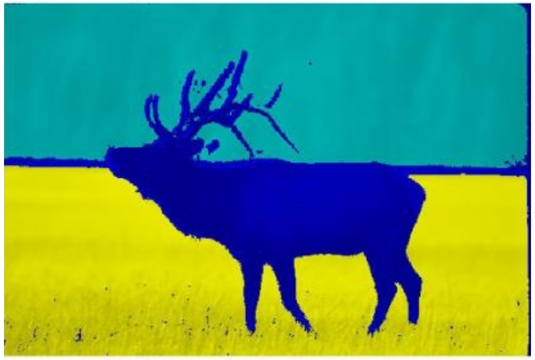
03/02/2021

Clustering Example



Divide data into different groups

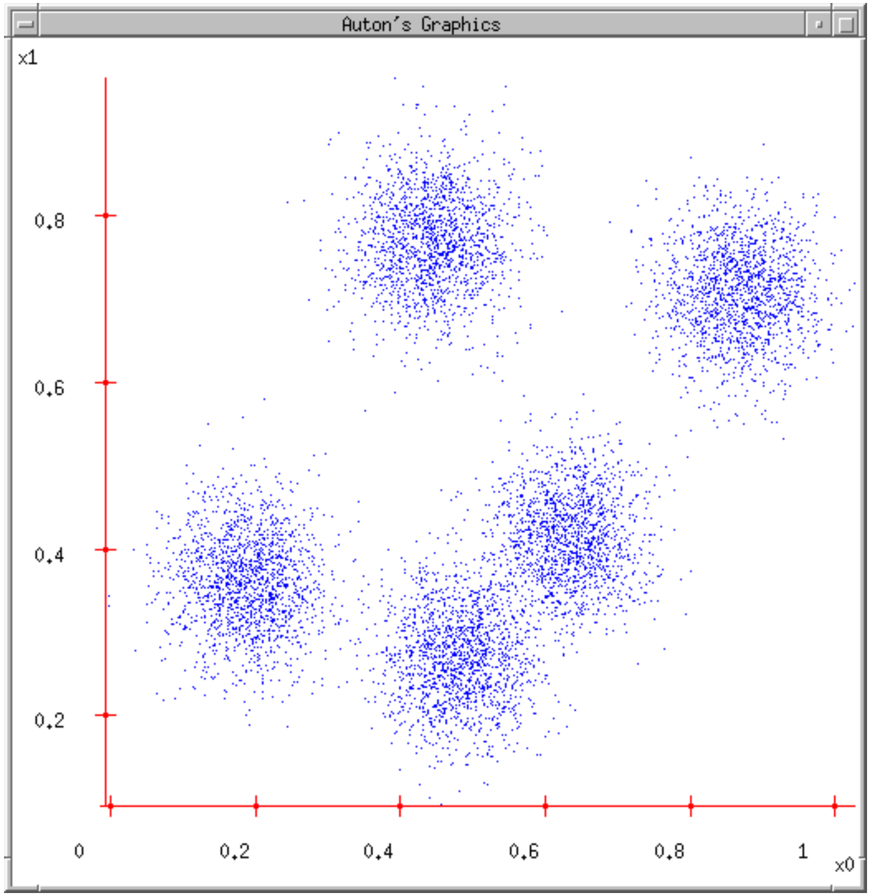
Original image



Segmented image

Clustering: K-means

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



Sides credit to Andrew W. Moore, CMU

Clustering: K-means

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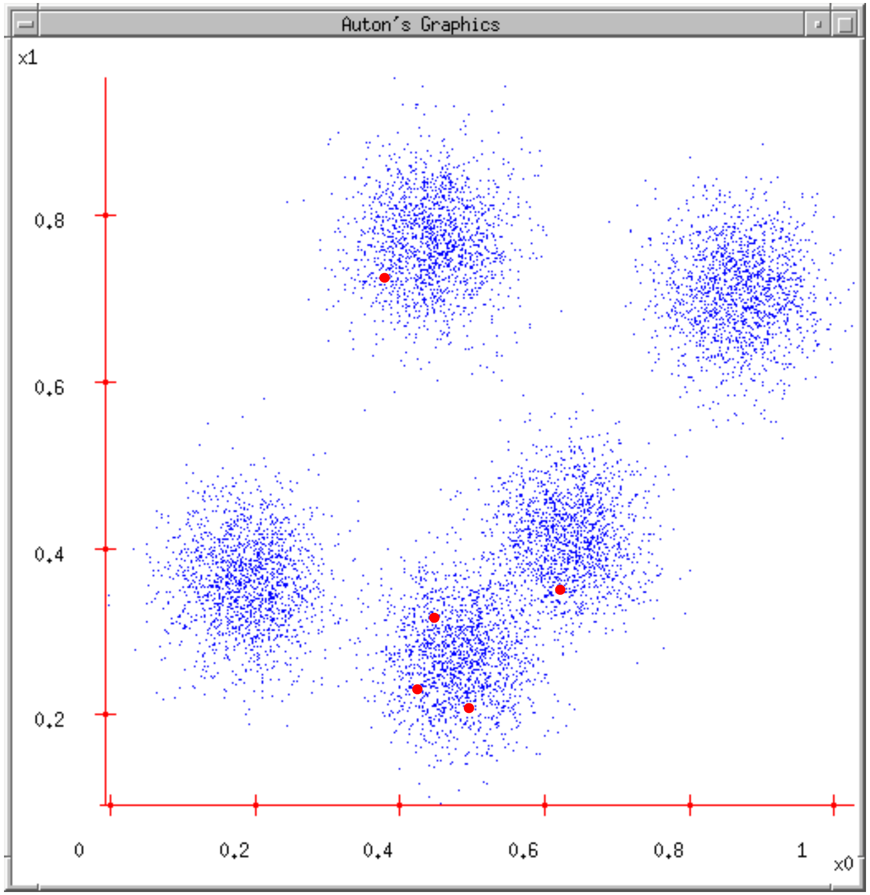
2. Randomly guess k cluster Center locations



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Clustering: K-means

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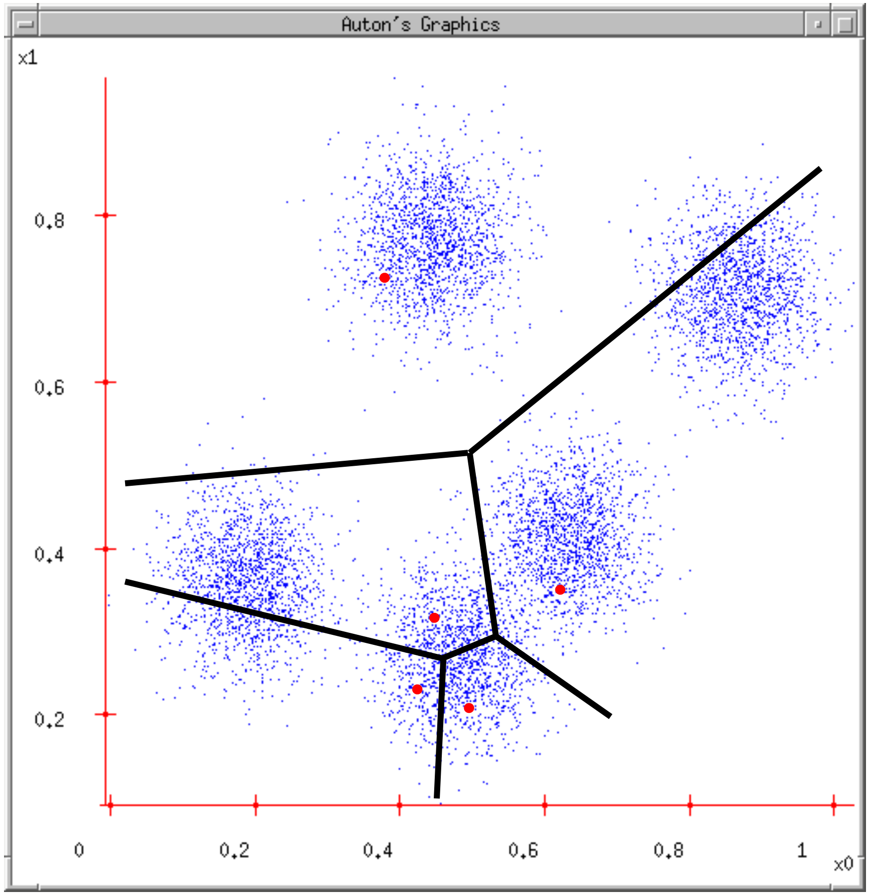

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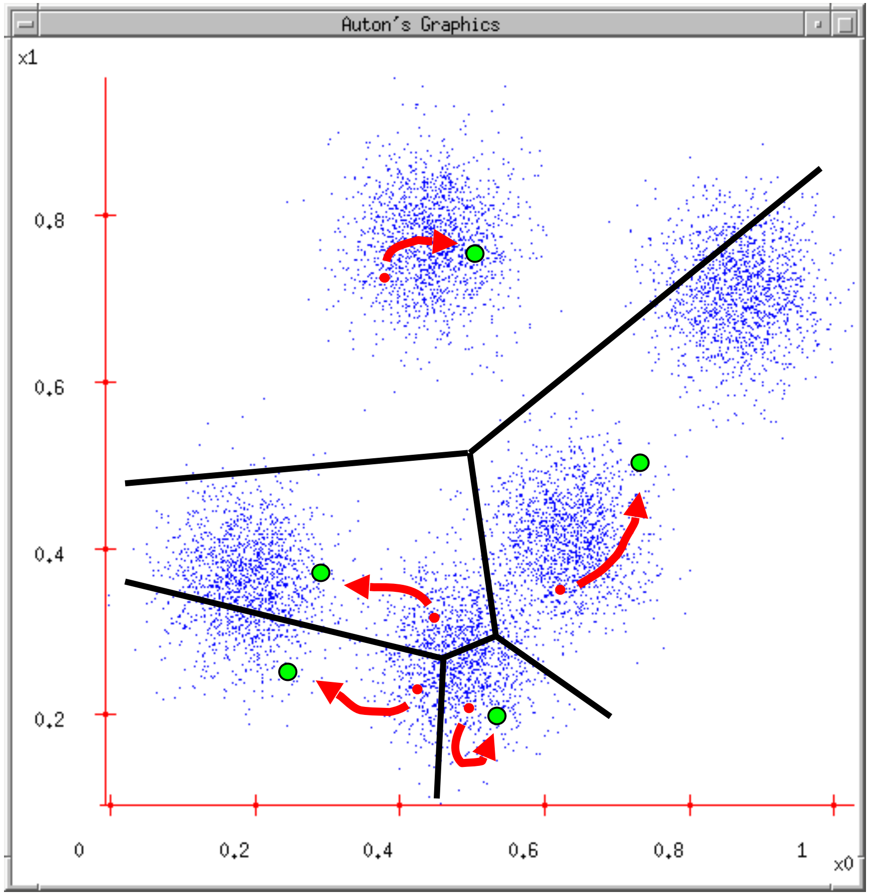

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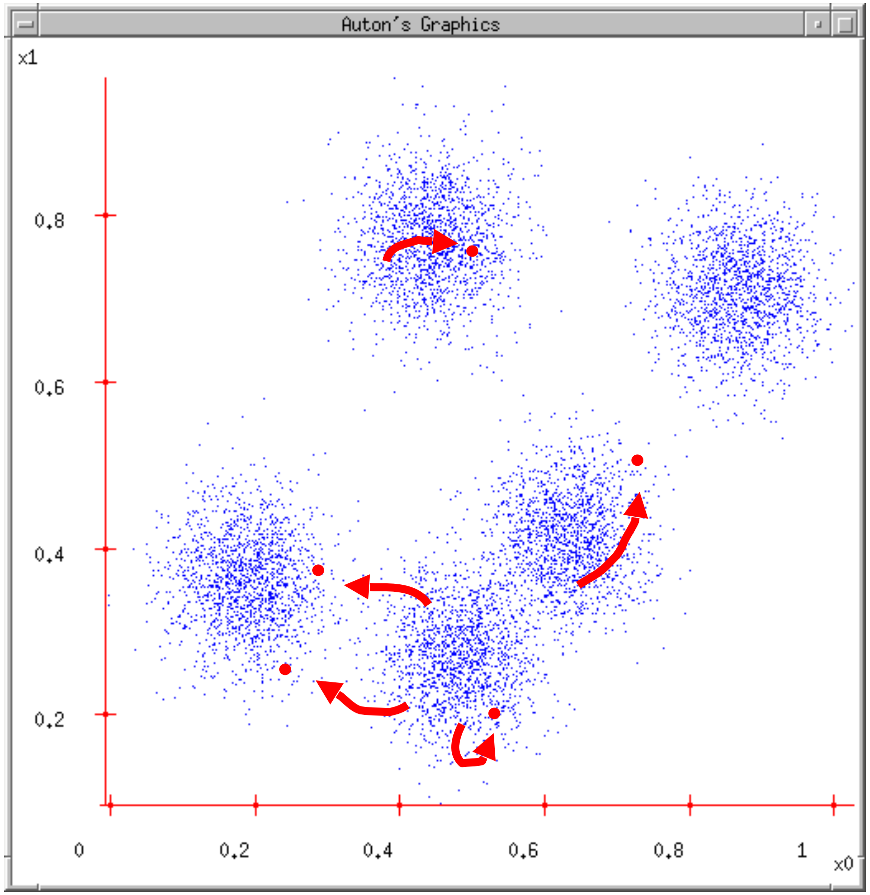
5. …and jumps there
6. …Repeat until terminated!



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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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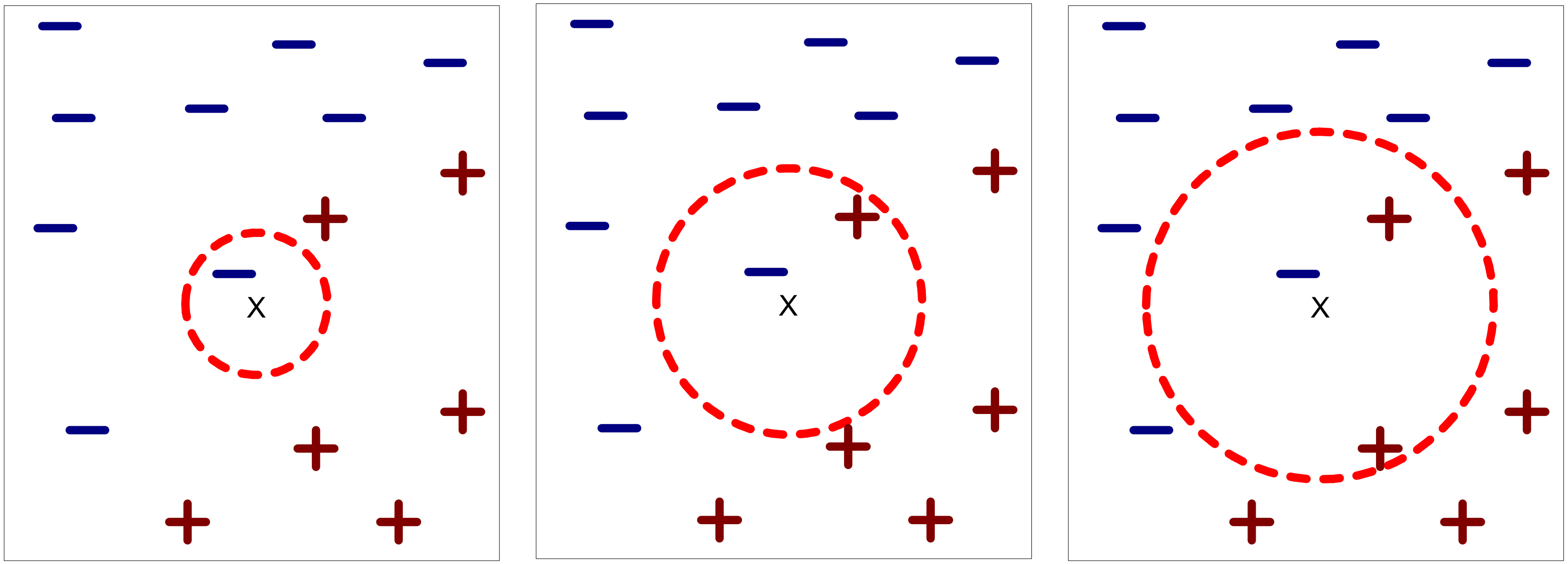
- Nearest Neighbors: (Un)supervised Learning (non-parametric model)

Nearest Neighbors

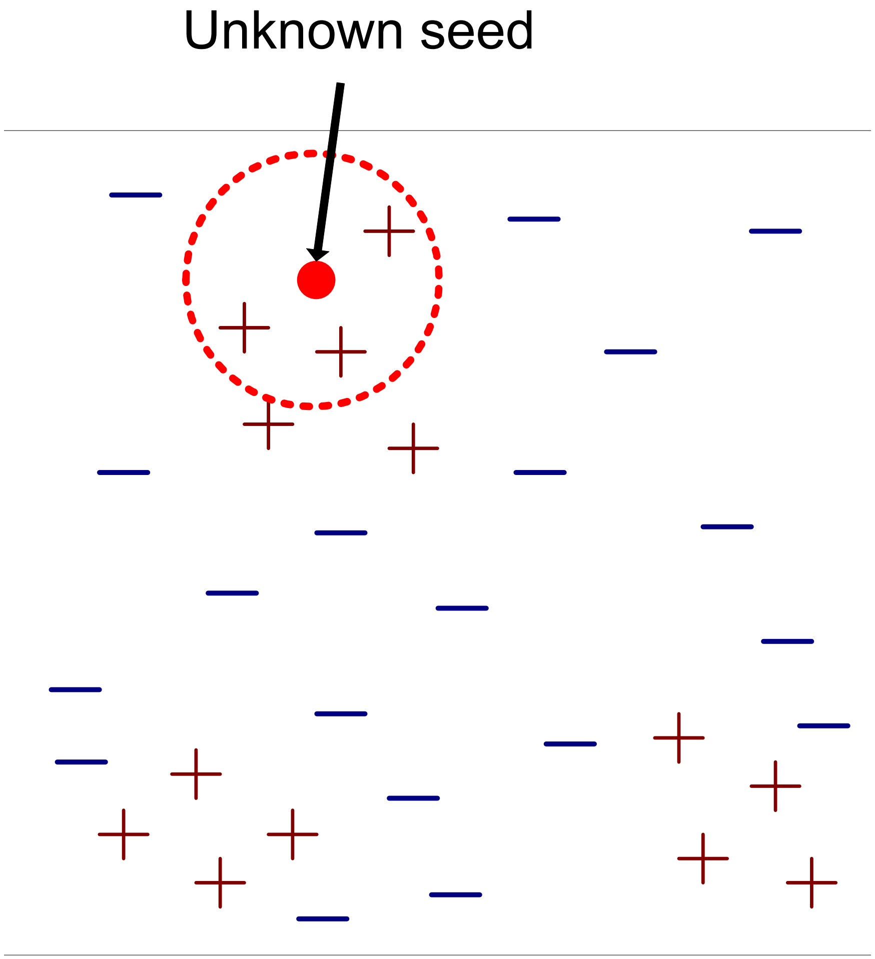


(a) 1-nearest neighbor (b) 2-nearest neighbor (c) 3-nearest neighbor

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

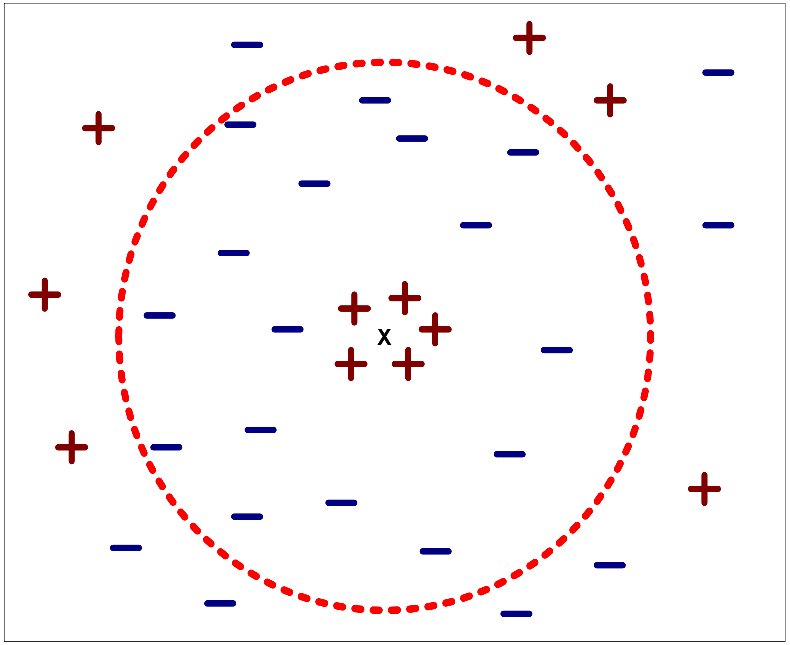
- Compute distance between two points:
  - Euclidean distance

$$d(p, q) = \sqrt{\sum_{i=1}^{d} (p^i - q^i)^2}$$

- Determine the class from nearest neighbor list
  - take the majority vote of class labels among the k-nearest neighbors
  - optionally 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

- At prediction:
  - Find the *k* training examples $(x_1,y_1),\dots(x_k,y_k)$ 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

K-means using r-NN

1. Pick k points c_1=x_1,…..,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….