Nearest Neighbor Methods

CS 584 Data Mining (Spring 2022)

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Slides are adapted from the available book slides developed by Tan, Steinbach and Kumar, with additional input from Prof. Huzefa Rangwala

Instance-Based Classifiers

Set of Stored Cases

Atr1	………	AtrN	Class
			A
			B
			B
			C
			A
			C
			B

- Store the training records
- Use training records to predict the class label of unseen cases

Unseen Case

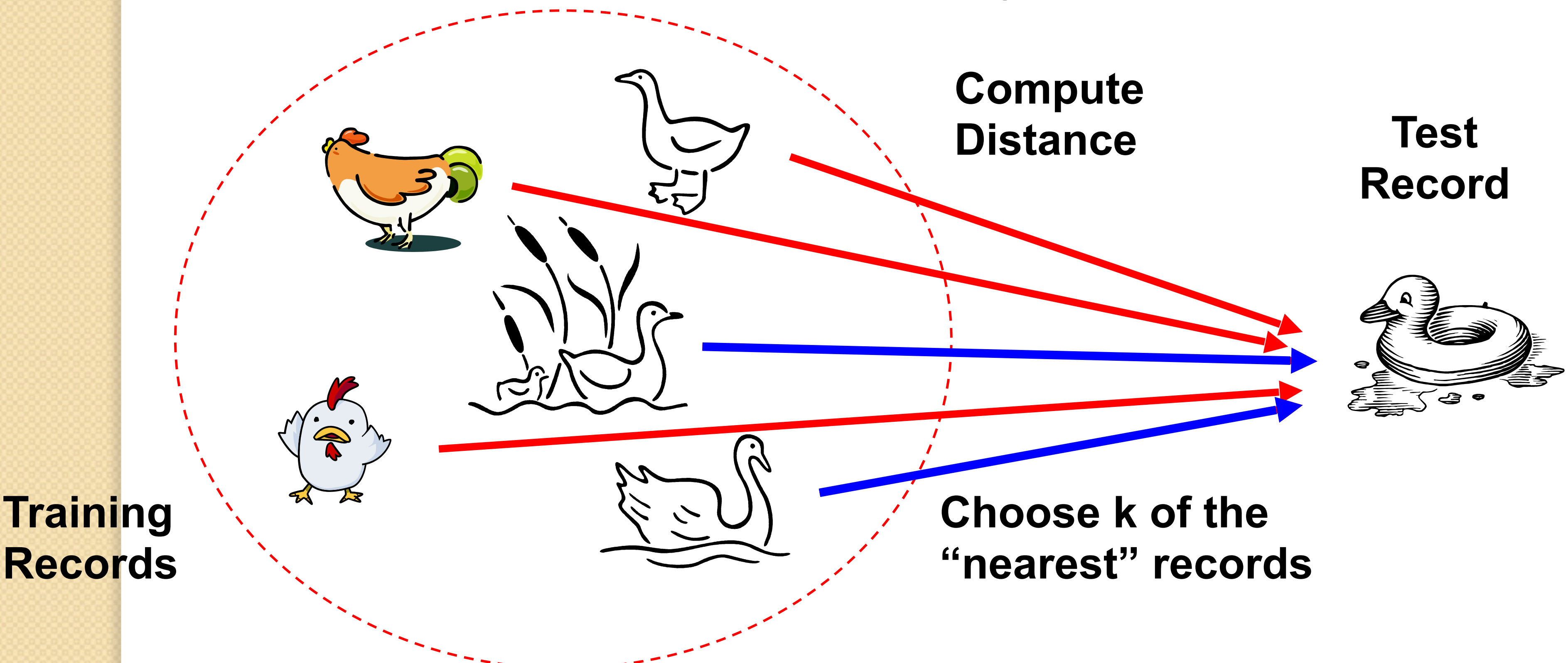
Atr1	………	AtrN

Instance Based Classifiers

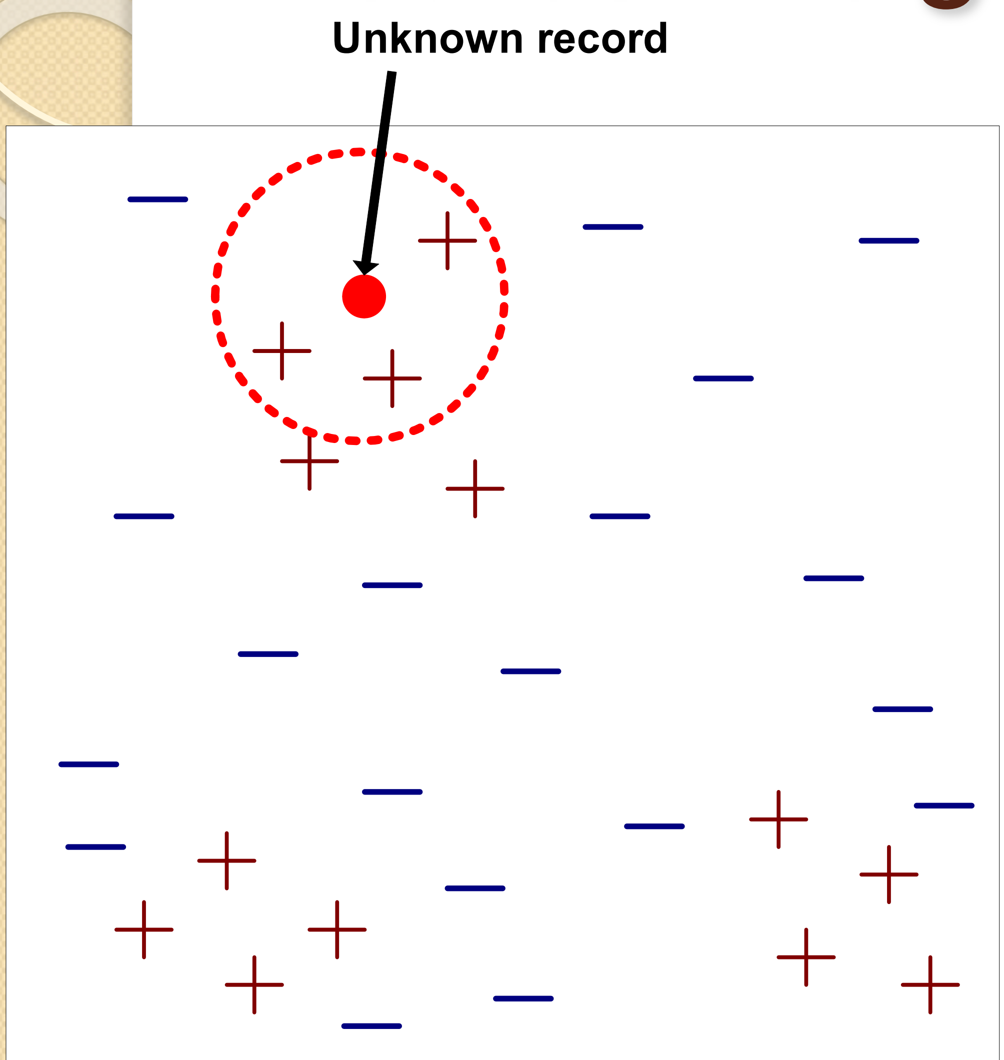
- Examples:
  - Rote-learner
    - Memorizes entire training data and performs classification only if attributes of record match one of the training examples exactly
  - Nearest neighbor
    - Uses k “closest” points (nearest neighbors) for performing classification

Nearest Neighbor Classifiers

- The simplest way of learning:
  - If it walks like a duck and quacks like a duck, then it's probably a duck



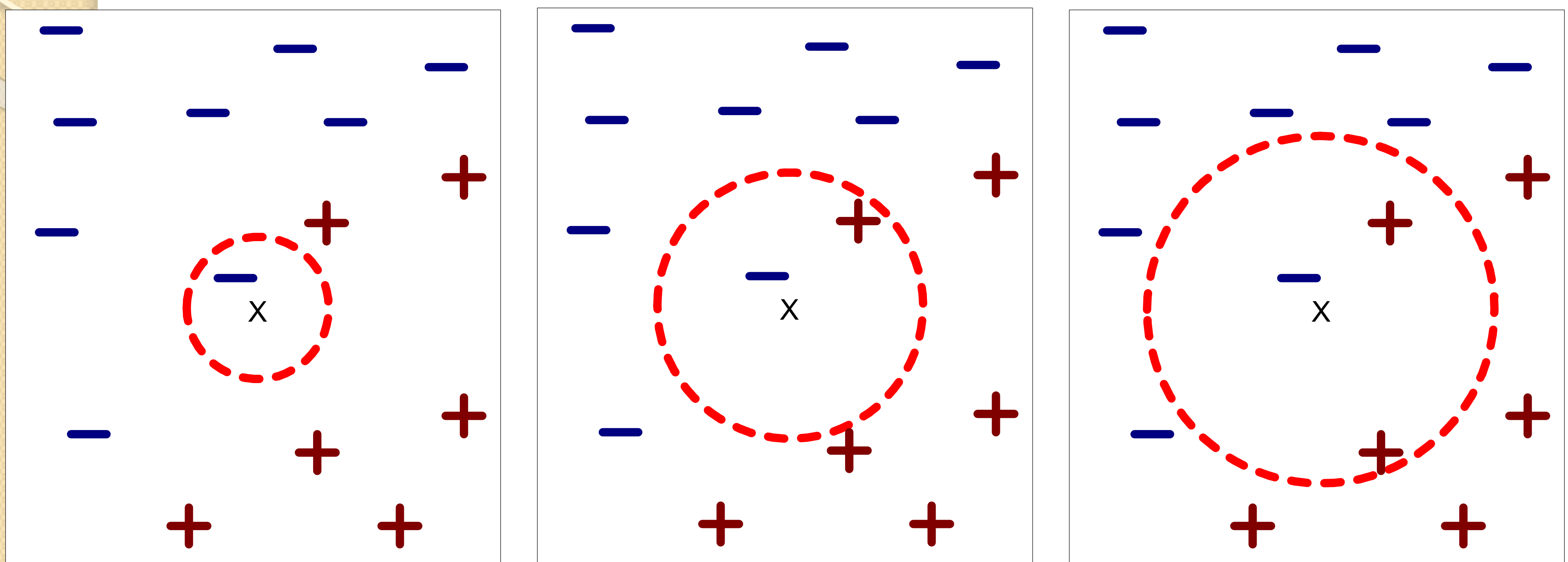
Nearest-Neighbor Classifiers



- Requires three things
  - The set of stored records
  - Distance Metric (Sim) to compute distance (Sim) between records
  - The value of *k*, the number of nearest neighbors to retrieve

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

Definition of Nearest Neighbor

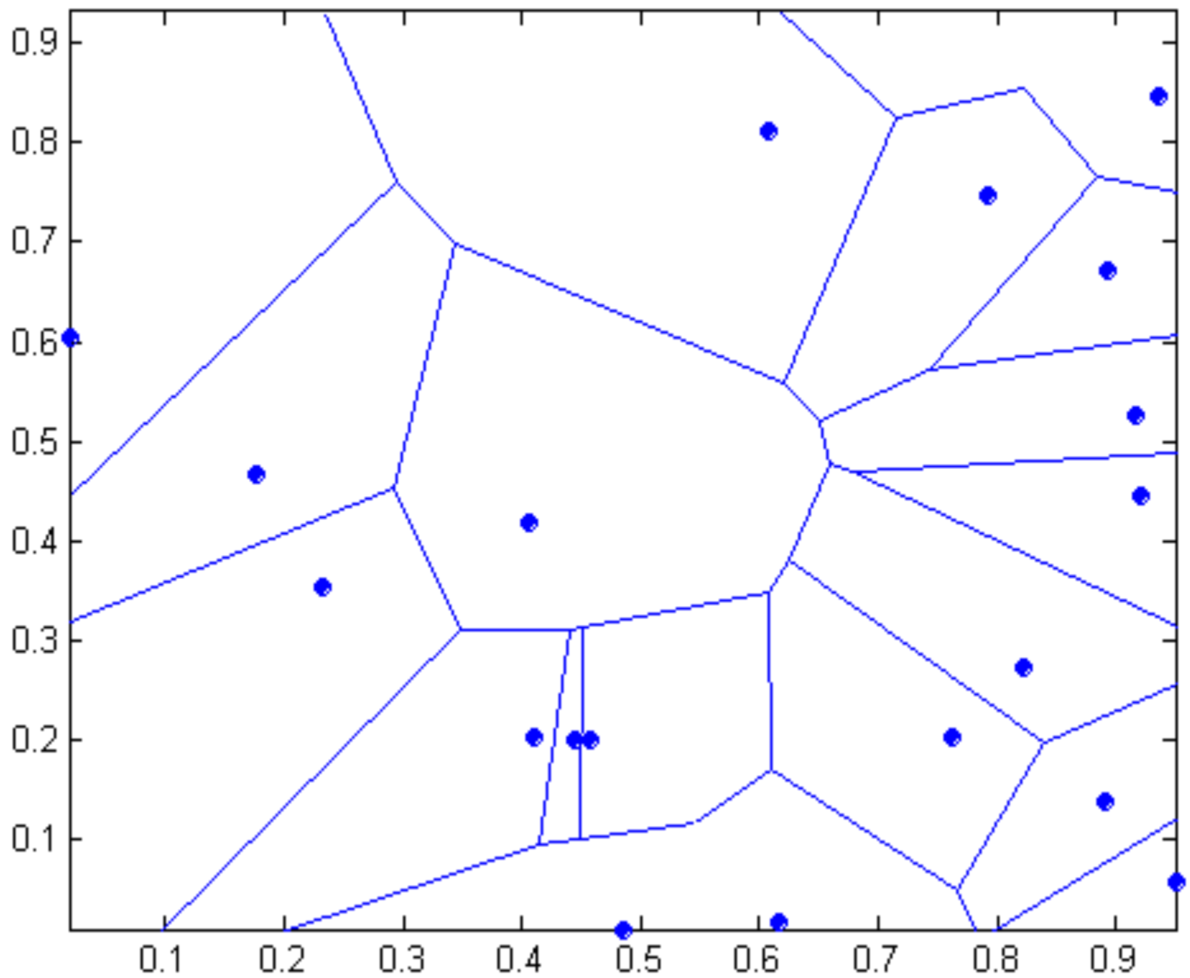


(a) 1-nearest neighbor (b) 2-nearest neighbor (c) 3-nearest neighbor

k-nearest neighbors of a record x are data points that have the k smallest distances to x

Hypothesis space: k=1

Voronoi Diagram



Nearest Neighbor Classification

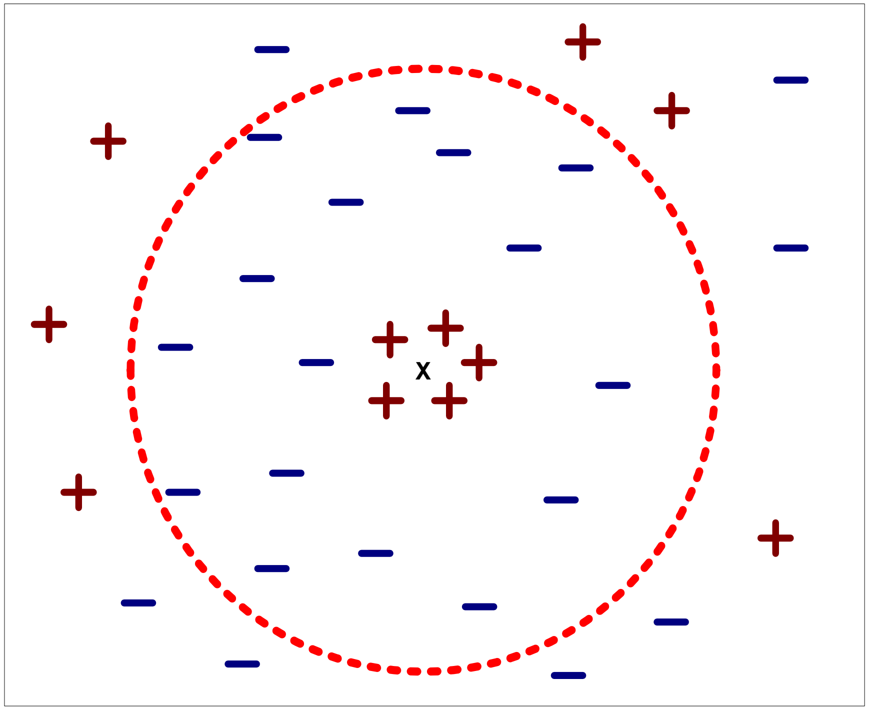
- Compute distance between two points:
  - Euclidean distance

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

- Determine the class from nearest neighbor list
  - take the majority vote of class labels among the k-nearest neighbors
  - may or may not weigh 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 points
  - If k is too large, neighborhood may include points from other classes



Nearest neighbor Classification…

- k-NN classifiers are lazy learners
  - It does not build models explicitly
  - Unlike eager learners such as decision tree induction.
  - Classifying unknown records is relatively expensive

What is Similarity?

The quality or state of being similar; likeness; resemblance; as, a similarity of features. **Webster's Dictionary**

Similarity is hard to define, but…
"*We know it when we see it*"

The real meaning of similarity is a philosophical question.

We will take a more pragmatic approach.

Similarity and Dissimilarity

- Similarity
  - Numerical measure of how alike two data objects are.
  - Is higher when objects are more alike.
  - Often falls in the range [0,1]
- Dissimilarity
  - Numerical measure of how different are two data objects
  - Lower when objects are more alike
  - Minimum dissimilarity is often 0
  - Upper limit varies
- Proximity refers to a similarity or dissimilarity

Similarity/Dissimilarity for Simple Attributes

p and *q* are the attribute values for two data objects.

Attribute Type	Dissimilarity	Similarity
Nominal	$d = \begin{cases} 0 & \text{if } p = q \\ 1 & \text{if } p \neq q \end{cases}$	$s = \begin{cases} 1 & \text{if } p = q \\ 0 & \text{if } p \neq q \end{cases}$
Ordinal	$d = \frac{\lvert p-q \rvert}{n-1}$ (values mapped to integers 0 to $n-1$, where n is the number of values)	$s = 1 - \frac{\lvert p-q \rvert}{n-1}$
Interval or Ratio	$d = \lvert p - q \rvert$	$s = -d$, $s = \frac{1}{1+d}$ or $s = 1 - \frac{d - min\_d}{max\_d - min\_d}$

Table 5.1. Similarity and dissimilarity for simple attributes

Defining Distance Measures

Definition: Let O_1 and O_2 be two objects from the universe of possible objects. The distance (dissimilarity) is denoted by $D(O_1,O_2)$

What properties should a distance measure have?

- $D(A,B) = D(B,A)$ *Symmetry*
- $D(A,A) = 0$ *Constancy of Self-Similarity*
- $D(A,B) = 0$ iff $A = B$ *Identity of Indiscernibles*
- $D(A,B) \leq D(A,C) + D(B,C)$ *Triangle Inequality*

When the last one holds, we call the measure a metric

Euclidean Distance

$$dist = \sqrt{\sum_{k=1}^{n} (p_k - q_k)^2}$$

Minkowski Distance

- Minkowski Distance is a generalization of Euclidean Distance

$$dist = \left(\sum_{k=1}^{n} | p_k - q_k |^r \right)^{\frac{1}{r}}$$

Where r is a parameter, n is the number of dimensions (attributes) and p_k and q_k are, respectively, the kth attributes (components) or data objects p and q.

Minkowski Distance: Examples

- $r = 1$. City block (Manhattan, taxicab, L1 norm) distance.
  - A common example of this is the Hamming distance, which is just the number of bits that are different between two binary vectors
- $r = 2$. Euclidean distance
- $r \to \infty$. "supremum" (L_{max} norm, L_∞ norm) distance.
  - This is the maximum difference between any component of the vectors
- Do not confuse r with n, i.e., all these distances are defined for all numbers of dimensions.