Lecture 3: K-Nearest Neighbors

COMP90049
Introduction to Machine Learning

Semester 2, 2022

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Acknowledgement: Lea Frermann

Roadmap

Last time... Machine Learning concepts

- data, features, classes
- models, training
- practical considerations

Today... Our first machine learning algorithm

- K-nearest neighbors
- Application to classification
- Application to regression

Also: the topic of your **first assignment**!

- Released on Canvas on Wed 3rd August at 7pm!
- Questions: assignment1 discussion board (don't share solutions!)

Introduction

K-Nearest Neighbors: Example

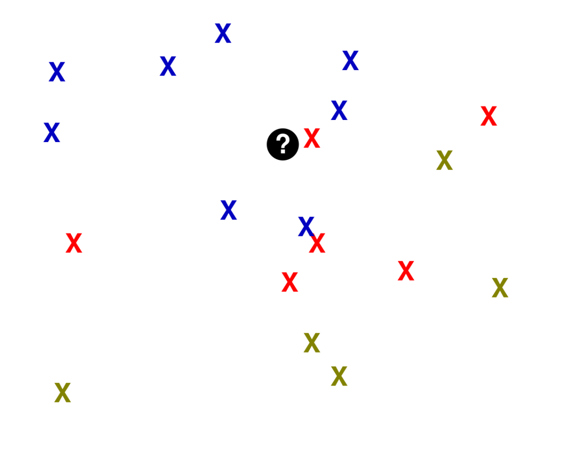
Your ’photographic memory’ of all handwritten digits you’ve ever seen:

K-Nearest Neighbors: Example

Your 'photographic memory' of all handwritten digits you've ever seen:

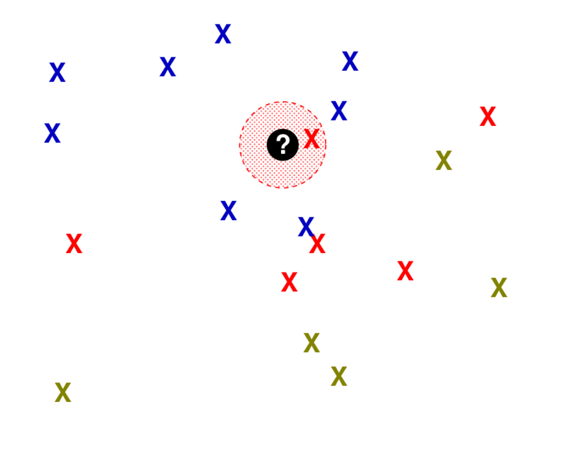
Given a new drawing, determine the digit by comparing it to all digits in your 'memory'.

K-Nearest Neighbors: Visualization



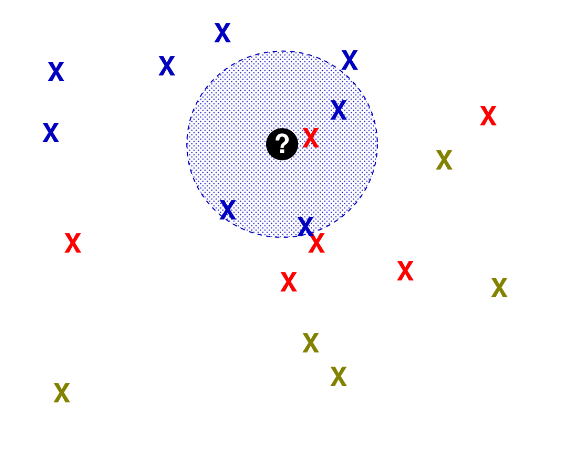
K nearest neighbors = K closest stored data points

K-Nearest Neighbors: Visualization



1 nearest neighbor = single closest stored data point

K-Nearest Neighbors: Visualization



4 nearest neighbors = 4 closest stored data points

K-Nearest Neighbors: Algorithm

Training

- Store all training examples

Testing

- Compute **distance** of test instance to all training data points
- Find the K closest training data points (*nearest neighbors*)
- Compute **target concept** of the test instance based on labels of the training instances

K-Nearest Neighbors: Target Concepts

KNN Classification

- Return the most common class label among neighbors
- Example: cat vs dog images; text classification; ...

KNN Regression

- Return the average value of among K nearest neighbors
- Example: housing price prediction;

Four problems

1. **How to represent each data point?**
2. How to measure the distance between data points?
3. What if the neighbors disagree?
4. How to select K?

Feature Vectors

A data set of 6 instances (a...f) with 4 features and a label

	Outlook	Temperature	Humidity	Windy	Play
a	sunny	hot	high	FALSE	no
b	sunny	hot	high	TRUE	no
c	overcast	hot	high	FALSE	yes
d	rainy	mild	high	FALSE	yes
e	rainy	cool	normal	FALSE	yes
f	rainy	cool	normal	TRUE	no

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Feature Vectors

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We can represent each instance as a feature vector

$$\text{feature vector} = \begin{bmatrix} \text{Outlook} \\ \text{Temperature} \\ \text{Humidity} \\ \text{Windy} \end{bmatrix}$$

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Feature (or attribute) Types

Recall, from last lecture?

1. Nominal
   - set of values with no intrinsic ordering
   - possibly *boolean*
2. Ordinal
   - explicitly ordered
3. Numerical
   - real-valued, often no upper bound, easily mathematical manipulatable
   - vector valued

Outline

1. How to represent each data point?
2. **How to measure the distance between data points?**
3. What if the neighbors disagree?
4. How to select K?

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Comparing Nominal Feature Vectors

First, we convert the nominal features into numeric features.

instance	features			
	color	shape	taste	size
apple	red	round	sweet	–
banana	yellow	curved	sweet	–
cherry	red	round	sweet	small

instance	features					
	red	yellow	round	sweet	curved	small
apple	1	0	1	1	0	?
banana	0	1	0	1	1	?
cherry	1	0	1	1	0	1

Comparing Nominal Features: Hamming Distance

instance	features					
	red	yellow	round	sweet	curved	small
apple	1	0	1	1	0	?
banana	0	1	0	1	1	?
cherry	1	0	1	1	0	1

The number of differing elements in two ‘strings’ of equal length.

Comparing Nominal Features: Hamming Distance

instance	features					
	red	yellow	round	sweet	curved	small
apple	1	0	1	1	0	?
banana	0	1	0	1	1	?
cherry	1	0	1	1	0	1

The number of differing elements in two ‘strings’ of equal length.

$d(apple, banana) = 4$

Comparing Nominal Features: Simple Matching Distance

instance	features					
	red	yellow	round	sweet	curved	small
apple	1	0	1	1	0	?
banana	0	1	0	1	1	?
cherry	1	0	1	1	0	1

The number of matching features divided by the number of all features in the sample

$$d = 1 - \frac{k}{m}$$

- d: distance
- k: number of matching features
- m: total number of features

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Comparing Nominal Features: Simple Matching Distance

instance	features					
	red	yellow	round	sweet	curved	small
apple	1	0	1	1	0	?
banana	0	1	0	1	1	?
cherry	1	0	1	1	0	1

The number of matching features divided by the number of all features in the sample

$$d = 1 - \frac{k}{m}$$

- d: distance
- k: number of matching features
- m: total number of features

$$d(apple, banana) = 1 - \frac{2}{6} = \frac{4}{6}$$

Comparing Nominal Feature Vectors: Jaccard Distance

instance	features					
	red	yellow	round	sweet	curved	small
apple	1	0	1	1	0	?
banana	0	1	0	1	1	?
cherry	1	0	1	1	0	1

Jaccard *similarity* J: intersection of two **sets** divided by their union.

$$
\begin{aligned}
d &= 1 - J \\
&= 1 - \frac{|A \cap B|}{|A \cup B|} \\
&= 1 - \frac{|A \cap B|}{|A| + |B| - |A \cap B|}
\end{aligned}
$$

Comparing Nominal Feature Vectors: Jaccard Distance

instance	features					
	red	yellow	round	sweet	curved	small
apple	1	0	1	1	0	?
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&= 1 - \frac{|A \cap B|}{|A| + |B| - |A \cap B|}
\end{aligned}
$$

$$d(apple, banana) = 1 - \frac{1}{5} = \frac{4}{5}$$

Comparing Numerical Feature Vectors: Manhattan Distance

Manhattan Distance (or: L1 distance)

- Given two instances a and b, each with a set of numerical features, e.g.,
  $a = [2.0,\ 1.4,\ 4.6,\ 5.5]$
  $b = [1.0,\ 2.4,\ 6.6,\ 2.5]$
- Their distance d is the sum of absolute differences of each feature

$$d(a, b) = \sum_{i=1}^{m} |a_i - b_i| \tag{1}$$

Example

$$\begin{aligned} d(a, b) &= |2.0 - 1.0| + |1.4 - 2.4| + |4.6 - 6.6| + |5.5 - 2.5| \\ &= 1 + 1 + 2 + 3 \\ &= 7 \end{aligned}$$

Comparing Numerical Feature Vectors: Euclidean Distance

Euclidean Distance (or: L2 distance)

- Given two instances a and b, each with a set of numerical features, e.g.,
  $a = [2.0,\ 1.4,\ 4.6,\ 5.5]$
  $b = [1.0,\ 2.4,\ 6.6,\ 2.5]$
- Their distance d is the distance in Euclidean space (2-dimensional space). Defined as the squared root of the sum of squared differences of each feature

$$d(a,b) = \sqrt{\sum_{i=1}^{m}(a_i - b_i)^2} \tag{2}$$

Example

$$\begin{aligned} d(a,b) &= \sqrt{(2.0-1.0)^2 + (1.4-2.4)^2 + (4.6-6.6)^2 + (5.5-2.5)^2} \\ &= \sqrt{1+1+4+9} = \sqrt{15} \\ &= 3.87 \end{aligned}$$

Comparing Numerical Feature Vectors: Cosine distance

Cosine Distance

- Cosine similarity = cosine of angle between two vectors (= inner product of the *normalized* vectors)
- Cosine distance d: one minus cosine similarity

$$cos(a, b) = \frac{a \cdot b}{|a||b|} = \frac{\sum_i a_i b_i}{\sqrt{\sum_i a_i^2}\sqrt{\sum_i b_i^2}}$$

$$d(a, b) = 1 - cos(a, b)$$

- Cosine distance is **normalized by the magnitude** of both feature vectors, i.e., we can compare instances of different magnitude

$\rightarrow$ word counts: compare long vs short documents
$\rightarrow$ pixels: compare high vs low resolution images

Comparing Numerical Feature Vectors: Cosine distance

Example

$$cos(a,b) = \frac{a \cdot b}{|a||b|} = \frac{\sum_i a_i b_i}{\sqrt{\sum_i a_i^2}\sqrt{\sum_i b_i^2}}$$

$$d(a,b) = 1 - cos(a,b)$$

feature	doc1	doc2	doc3
word1	200	300	50
word2	300	200	40
word3	200	100	25

$$cos(doc1, doc2) = \frac{200 \times 300 + 300 \times 200 + 200 \times 100}{\sqrt{200^2 + 300^2 + 200^2}\sqrt{300^2 + 200^2 + 100^2}} = 0.93$$

$$d(doc1, doc2) = 0.07$$

$$cos(doc2, doc3) = \frac{300 \times 50 + 200 \times 40 + 100 \times 25}{\sqrt{300^2 + 200^2 + 100^2}\sqrt{50^2 + 40^2 + 25^2}} = 0.99$$

$$d(doc2, doc3) = 0.01$$

Comparing Ordinal Feature Vectors

Normalized Ranks

- sort values, and return a rank $r \in \{0 \ldots m\}$
- map ranks to evenly spaced values between 0 and 1

$$z = \frac{r}{m}$$

- compute a distance function for numeric features (e.g., Euclidean distance)

Example: Customer ratings

1. Sorted ratings: { -2: 😭, -1: ☹️, 0: 😐, 1: 🙂, 2: 😀 }
2. Ranks: { 0, 1, 2, 3, 4 }

feature	A	B
safety	0	2
comfortable	-2	1
convenient	-1	2

Comparing Ordinal Feature Vectors

Normalized Ranks

- sort values, and return a rank $r \in \{0...m\}$
- map ranks to evenly spaced values between 0 and 1

$$z = \frac{r}{m}$$

- compute a distance function for numeric features (e.g., Euclidean distance)

Example: Customer ratings

1. Sorted ratings: { -2: 😭, -1: 😢, 0: 😐, 1: 🙂, 2: 😃 }
2. Ranks: { 0, 1, 2, 3, 4 }

feature	A	B
safety	0	2
comfortable	-2	1
convenient	-1	2

→

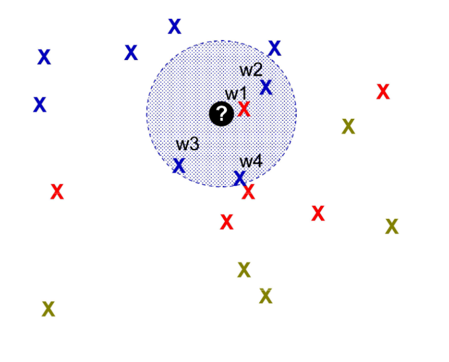
feature	A	B
safety	2/4	4/4
comfortable	0	3/4
convenient	1/4	4/4

Four problems

1. How to represent each data point?
2. How to measure the distance between data points?
3. **What if the neighbors disagree?**
4. How to select K?

Majority Voting

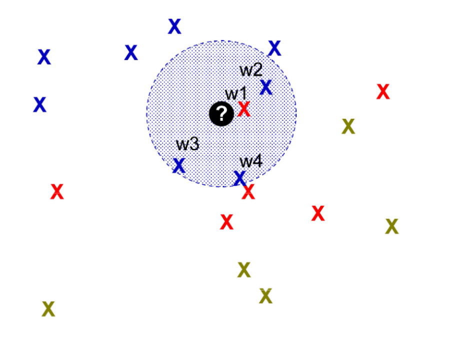
Equal weights (=majority vote)



Voting Example (k=4)

- $w_1 = w_2 = w_3 = w_4 = 1$

Equal weights (=majority vote)



Voting Example (k=4)

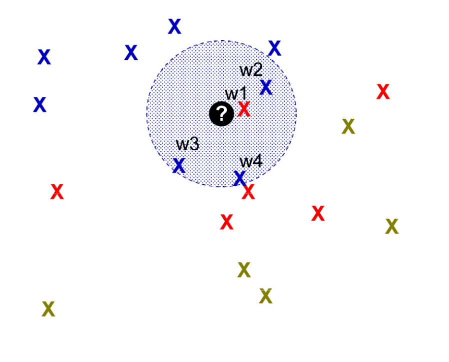
- $w_1 = w_2 = w_3 = w_4 = 1$
- red: 1
  blue: 1+1+1=3

Weighted KNN: Inverse Distance

Inverse Distance

$$w_j = \frac{1}{d_j + \epsilon}$$

with $\epsilon \approx 0$, e.g., $1e-10$



Voting Example (k=4)

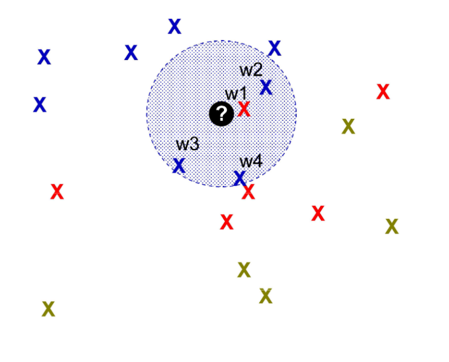
- $d_1 = 0$; $d_2 = 1$; $d_3 = d_4 = 1.5$
- $\epsilon = 1e-5$

Weighted KNN: Inverse Distance

Inverse Distance

$$w_j = \frac{1}{d_j + \epsilon}$$

with $\epsilon \approx 0$, e.g., $1e - 10$



Voting Example (k=4)

- $d_1 = 0$; $d_2 = 1$; $d_3 = d_4 = 1.5$
- $\epsilon = 1e - 5$

red: $\frac{1}{0+\epsilon} = 100000$

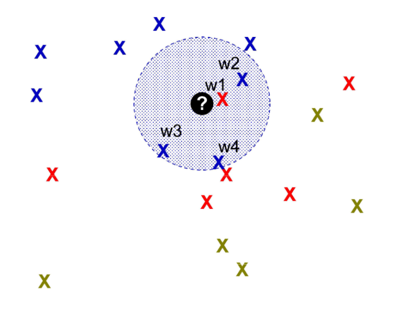
blue: $\frac{1}{1+\epsilon} + \frac{1}{1.5+\epsilon} + \frac{1}{1.5+\epsilon} = 1.0 + 0.67 + 0.67 = 2.34$

Weighted K-NN: Inverse Linear Distance

Inverse Linear distance

$$w_j = \frac{d_k - d_j}{d_k - d_1}$$

d_1 = min d among neighbors
d_k = max d among neighbors
d_j = distance of jth neighbor



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Weighted K-NN: Inverse Linear Distance

Inverse Linear distance

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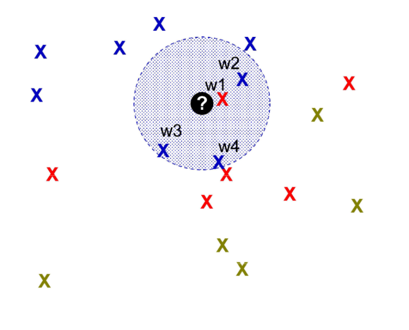

Voting Example (k=4)

- $d_1 = 0$; $d_2 = 1$; $d_3 = d_4 = 1.5$

red: $\frac{1.5-0}{1.5-0} = 1$

blue: $\frac{1.5-1}{1.5-0} + \frac{1.5-1.5}{1.5-0} + \frac{1.5-1.5}{1.5-0} = 0.3 + 0 + 0 = 0.3$

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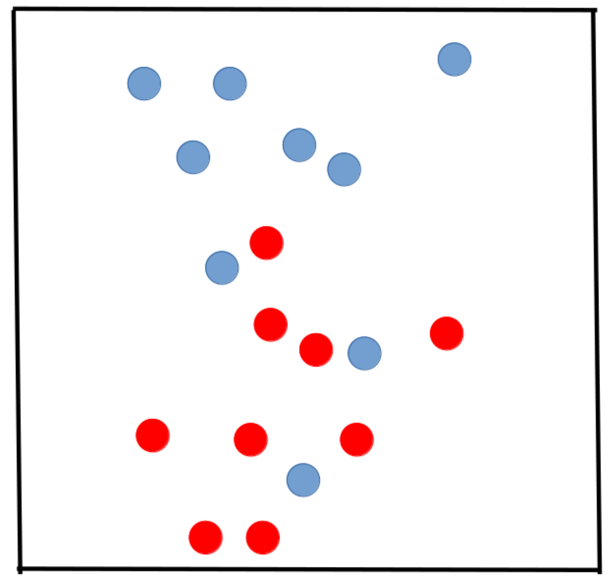
Four problems

1. How to represent each data point?
2. How to measure the distance between data points?
3. What if the neighbors disagree?
4. **How to select K?**

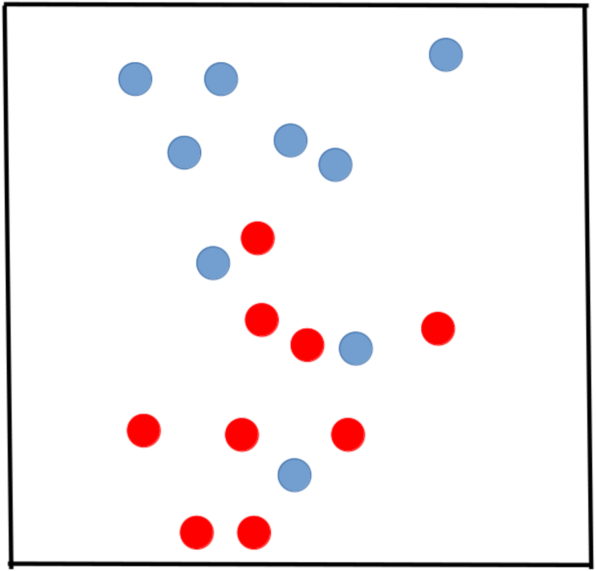
Selecting the value of K

K=1



Selecting the value of K

K=3



Selecting the value of K

Small K

- jagged decision boundary
- we capture noise
- lower classifier performance

Large K

- smooth decision boundary
- danger of grouping together unrelated classes
- also: lower classifier performance!
- what if $K == N$? (N=number of training instances)

Draw validation error:

Breaking Ties

What if more than K neighbors have the same (smallest) distance?

- select at random
- change the distance metric

What if two classes are equally likely given the current neighborhood?

- avoid an even K
- random tie breaking
- include $K + 1$th neighbor
- use class with highest prior probability

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Quiz!

`pollev.com/comp90049`

Why K-NN?

Pros

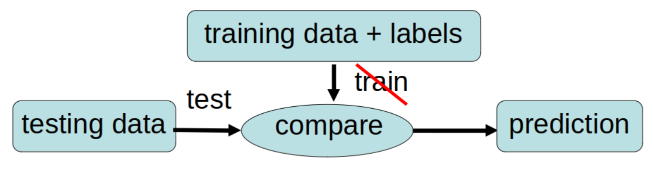
- Intuitive and simple
- No assumptions
- Supports classification and regression
- **No training**: new data $\rightarrow$ evolve and adapt immediately

Cons

- How to decide on best distance functions?
- How to combine multiple neighbors?
- How to select K?
- Expensive with large (or growing) data sets

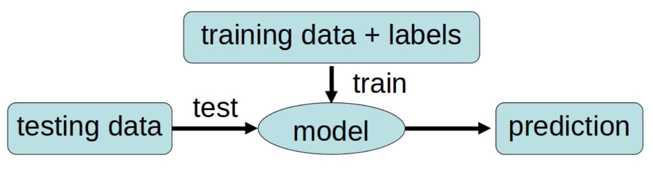
Lazy vs Eager Learning

Lazy Learning (also known as **Instance-based Learning**)



- **store** the training data
- **fixed** distance function
- **fixed** prediction rule (majority, weighting, ...)
- **compare** test instances with stored instances
- **no learning**

Eager Learning



- **train** a **model** using labelled training instances
- the model will **generalize** from seen data to unseen data
- use the model to **predict** labels for test instances
- we will look at a variety of **eager** models and their learning algorithms over the next couple of weeks

Summary

Today... Our first machine learning algorithm

- K-nearest neighbors
- Application to classification
- Application to regression

Also: the topic of your **first assignment**!

Next: Probabilities (recap) and probabilistic modeling

Further Reading

- *Data Mining: Concepts and Techniques*, 2nd ed., Jiawei Han and Micheline Kamber, Morgan Kaufmann, 2006. Chapter 2, Chapter 9.5.
- *The elements of statistical learning*, 2nd ed., Trevor Hastie, Jerome Friedman and Robert Tibshirani. New York: Springer series in statistics, 2001. Chapter 2.3.2

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