K-nearest Neighbor & Naïve Bayes

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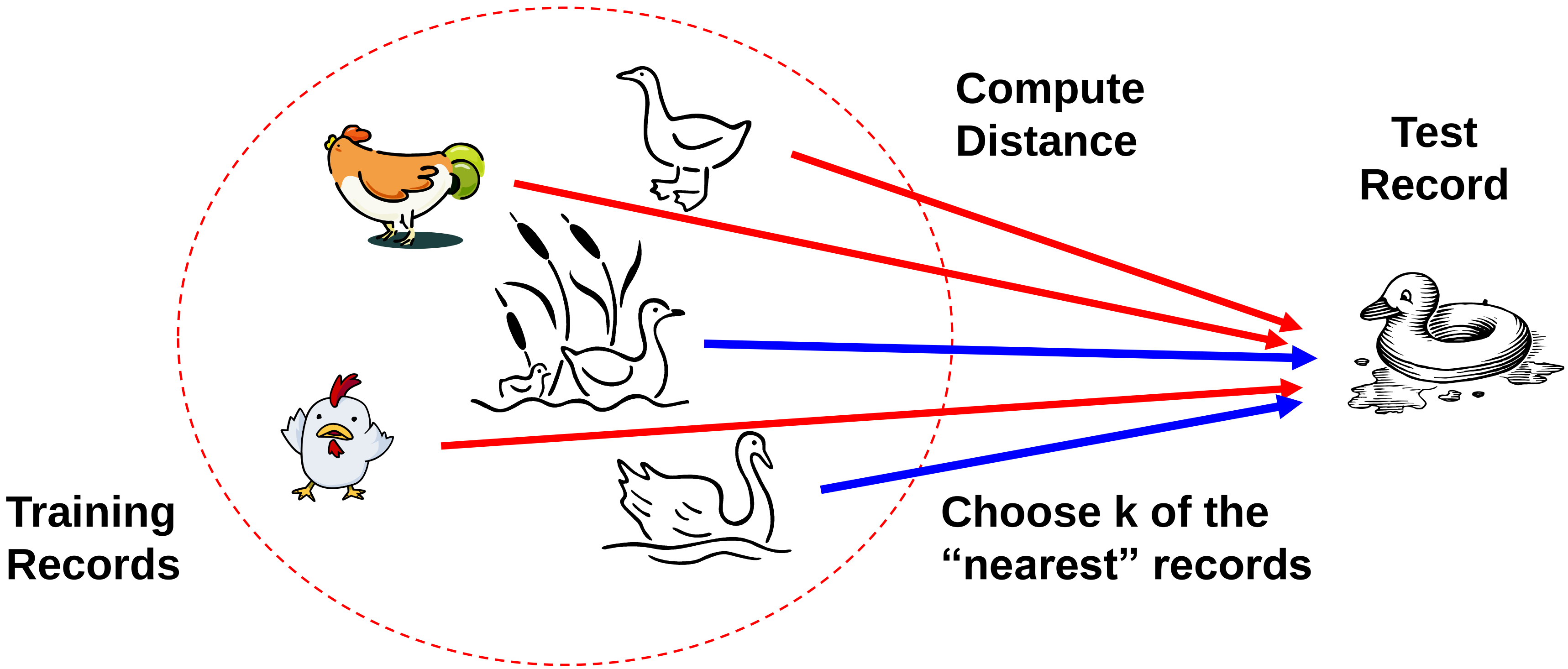
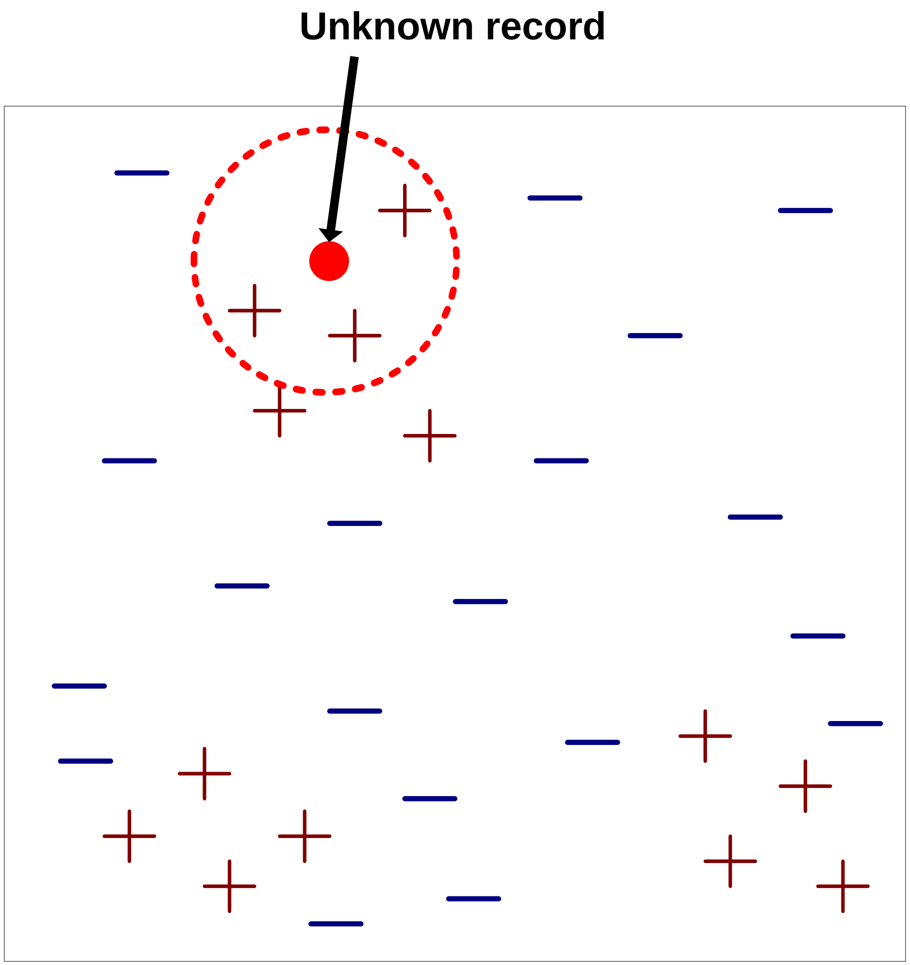
1. Nearest Neighbor Classifiers

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



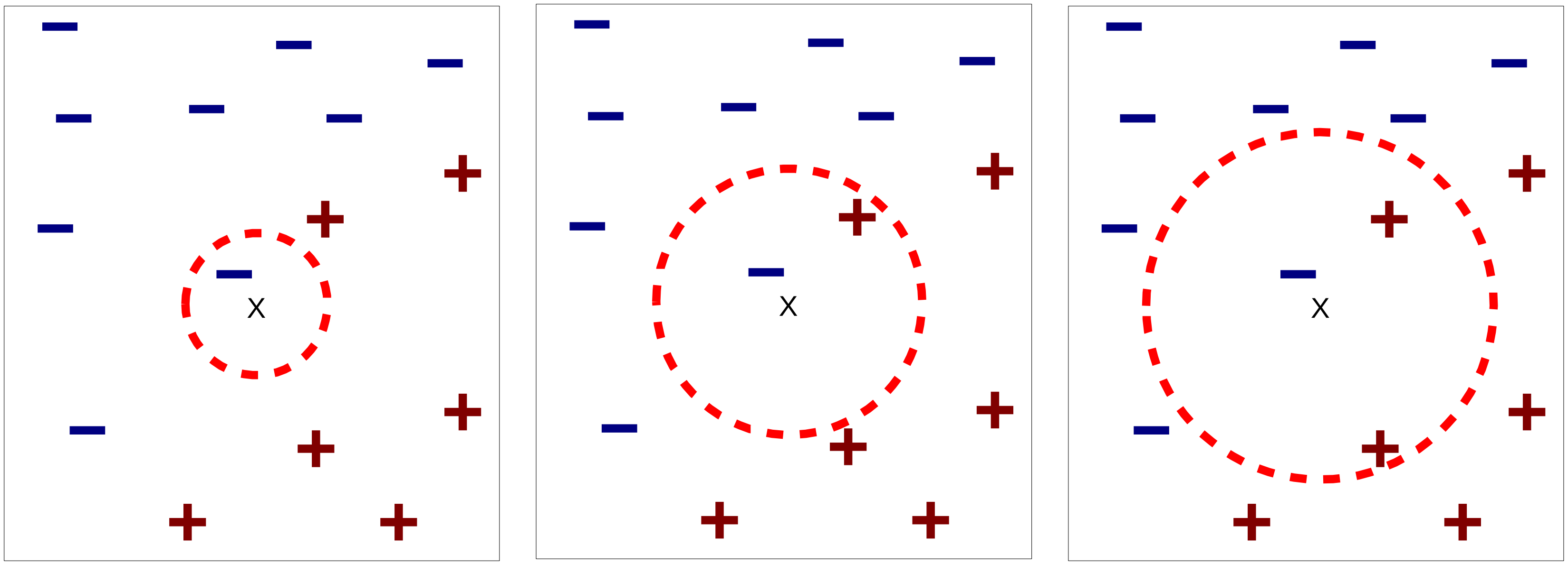
Nearest-Neighbor Classifiers



- Requires three things
  - The set of stored records
  - Distance Metric to compute distance 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 distance to x

Nearest Neighbor Classification

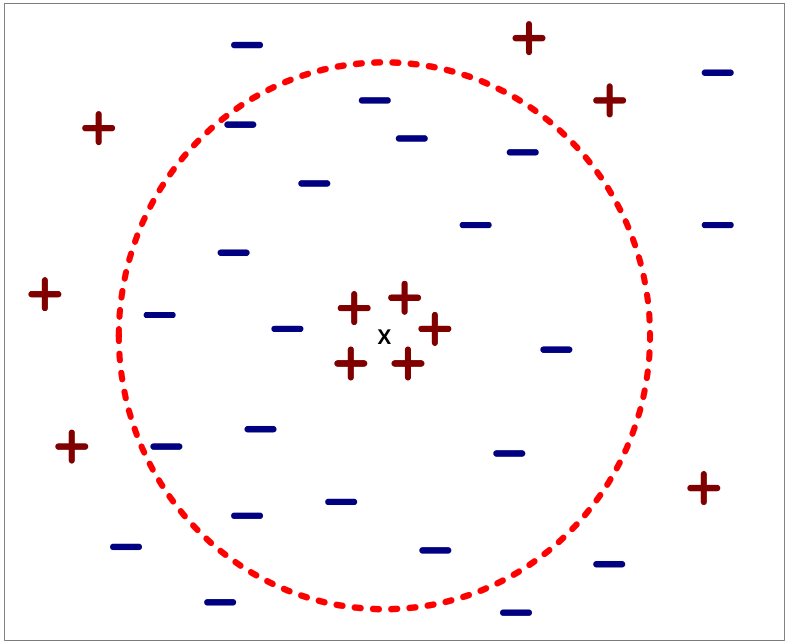
- Compute distance between two points:
  - Euclidean distance

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

- Determine the class from nearest neighbor list
  - take the majority vote of class labels among the k-nearest neighbors
  - Weigh 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 points
  - If k is too large, neighborhood may include points from other classes



Nearest Neighbor Classification…

- Scaling issues
  - Attributes 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

Nearest neighbor Classification…

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

Pros and Cons

- **Pros**
  - It is extremely easy to implement
  - As said earlier, it is lazy learning algorithm and therefore requires no training prior to making real time predictions. This makes the KNN algorithm much faster than other algorithms that require training e.g SVM, linear regression, etc.
  - Since the algorithm requires no training before making predictions, new data can be added seamlessly.
  - There are only two parameters required to implement KNN i.e. the value of K and the distance function (e.g. Euclidean or Manhattan etc.)

Pros and Cons

- **Cons**
  - The KNN algorithm doesn't work well with high dimensional data because with large number of dimensions, it becomes difficult for the algorithm to calculate distance in each dimension.
  - The KNN algorithm has a high prediction cost for large datasets. This is because in large datasets the cost of calculating distance between new point and each existing point becomes higher.
  - Finally, the KNN algorithm doesn't work well with categorical features since it is difficult to find the distance between dimensions with categorical features.

2. Bayes Classifier

- A probabilistic framework for solving classification problems
- Conditional Probability:

$$P(C \mid A) = \frac{P(A, C)}{P(A)}$$

$$P(A \mid C) = \frac{P(A, C)}{P(C)}$$

- Bayes theorem:

$$P(C \mid A) = \frac{P(A \mid C) P(C)}{P(A)}$$

Example of Bayes Theorem (1)

- P(Fire): how often there is fire
- P(Smoke): how often we see smoke
- P(Fire|Smoke) means how often there is fire when we see smoke.
- P(Smoke|Fire) means how often we see smoke when there is fire.

- *Given:*
  - *If dangerous fires are rare (1%) but smoke is fairly common (10%) due to factories, and 90% of dangerous fires make smoke*
- *What is the probability of dangerous Fire when there is Smoke?*

P(Fire|Smoke) =P(Fire)*P(Smoke|Fire)/P(Smoke) =1% x 90%10% =9%

Example of Bayes Theorem (2)

- Given:
  - A doctor knows that meningitis causes stiff neck 50% of the time
  - Prior probability of any patient having meningitis is 1/50,000
  - Prior probability of any patient having stiff neck is 1/20

- If a patient has stiff neck, what's the probability he/she has meningitis?

$$P(M \mid S) = \frac{P(S \mid M)P(M)}{P(S)} = \frac{0.5 \times 1/50000}{1/20} = 0.0002$$

Bayesian Classifiers

- Consider each attribute and class label as random variables

- Given a record with attributes $(A_1, A_2, \ldots, A_n)$
  - Goal is to predict class C
  - Specifically, we want to find the value of C that maximizes $P(C| A_1, A_2, \ldots, A_n)$

- Can we estimate $P(C| A_1, A_2, \ldots, A_n)$ directly from data?

Bayesian Classifiers

- Approach:
  - compute the posterior probability $P(C \mid A_1, A_2, \ldots, A_n)$ for all values of C using the Bayes theorem

$$\boxed{P(C \mid A_1 A_2 \ldots A_n) = \frac{P(A_1 A_2 \ldots A_n \mid C) P(C)}{P(A_1 A_2 \ldots A_n)}}$$

  - Choose value of C that maximizes
    $P(C \mid A_1, A_2, \ldots, A_n)$

  - Equivalent to choosing value of C that maximizes
    $P(A_1, A_2, \ldots, A_n|C)\ P(C)$

- How to estimate $P(A_1, A_2, \ldots, A_n \mid C)$?

Naïve Bayes Classifier

- Assume independence among attributes A_i when class is given:
  - $P(A_1, A_2, \ldots, A_n | C) = P(A_1| C_j)\, P(A_2| C_j) \ldots P(A_n| C_j)$
  - Can estimate $P(A_i| C_j)$ for all A_i and C_j.
  - New point is classified to C_j if $P(C_j) \prod P(A_i| C_j)$ is maximal.

How to Estimate Probabilities from Data?

Tid	Refund	Marital Status	Taxable Income	Evade
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

- Class: $P(C) = N_c/N$
  - e.g., P(No) = 7/10, P(Yes) = 3/10
- For discrete attributes:

$$P(A_i \mid C_k) = |A_{ik}| / N_{c_k}$$

  - where $|A_{ik}|$ is number of instances having attribute A_i and belongs to class C_k
  - Examples:

P(Status=Married|No) = 4/7
P(Refund=Yes|Yes)=0

How to Estimate Probabilities from Data?

- For continuous attributes:
  - Discretize the range into bins
    - one ordinal attribute per bin
    - violates independence assumption k
  - Two-way split: (A < v) or (A > v)
    - choose only one of the two splits as new attribute
  - Probability density estimation:
    - Assume attribute follows a normal distribution
    - Use data to estimate parameters of distribution (e.g., mean and standard deviation)
    - Once probability distribution is known, can use it to estimate the conditional probability $P(A_i|c)$

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- Normal distribution:

$$P(A_i \mid c_j) = \frac{1}{\sqrt{2\pi\sigma_{ij}^2}} e^{-\frac{(A_i-\mu_{ij})^2}{2\sigma_{ij}^2}}$$

  – One for each (A_i, c_j) pair

- For (Income, Class=No):
  – If Class=No
    - sample mean = 110
    - sample variance = 2975

$$P(Income=120 \mid No) = \frac{1}{\sqrt{2\pi}(54.54)} e^{-\frac{(120-110)^2}{2(2975)}} = 0.0072$$

Example of Naïve Bayes Classifier

Given a Test Record:

$$X = (\text{Refund} = \text{No}, \text{Married}, \text{Income} = 120\text{K})$$

naive Bayes Classifier:

P(Refund=Yes|No) = 3/7
P(Refund=No|No) = 4/7
P(Refund=Yes|Yes) = 0
P(Refund=No|Yes) = 1
P(Marital Status=Single|No) = 2/7
P(Marital Status=Divorced|No)=1/7
P(Marital Status=Married|No) = 4/7
P(Marital Status=Single|Yes) = 2/7
P(Marital Status=Divorced|Yes)=1/7
P(Marital Status=Married|Yes) = 0

For taxable income:
If class=No: sample mean=110
sample variance=2975
If class=Yes: sample mean=90
sample variance=25

- P(X|Class=No) = P(Refund=No|Class=No) $\times$ P(Married| Class=No) $\times$ P(Income=120K| Class=No)
  = 4/7 $\times$ 4/7 $\times$ 0.0072 = 0.0024

- P(X|Class=Yes) = P(Refund=No| Class=Yes) $\times$ P(Married| Class=Yes) $\times$ P(Income=120K| Class=Yes)
  = 1 $\times$ 0 $\times$ 1.2 $\times$ 10^{-9} = 0

Since P(X|No)P(No) > P(X|Yes)P(Yes)

Therefore P(No|X) > P(Yes|X)
=> Class = No

Naïve Bayes Classifier

- If one of the conditional probability is zero, then the entire expression becomes zero
- Probability estimation:

$$\text{Original}: P(A_i \mid C) = \frac{N_{ic}}{N_c}$$

$$\text{Laplace}: P(A_i \mid C) = \frac{N_{ic} + 1}{N_c + c}$$

$$\text{m - estimate}: P(A_i \mid C) = \frac{N_{ic} + mp}{N_c + m}$$

c: number of classes

p: prior probability

m: parameter

Example of Naïve Bayes Classifier

Name	Give Birth	Can Fly	Live in Water	Have Legs	Class
human	yes	no	no	yes	mammals
python	no	no	no	no	non-mammals
salmon	no	no	yes	no	non-mammals
whale	yes	no	yes	no	mammals
frog	no	no	sometimes	yes	non-mammals
komodo	no	no	no	yes	non-mammals
bat	yes	yes	no	yes	mammals
pigeon	no	yes	no	yes	non-mammals
cat	yes	no	no	yes	mammals
leopard shark	yes	no	yes	no	non-mammals
turtle	no	no	sometimes	yes	non-mammals
penguin	no	no	sometimes	yes	non-mammals
porcupine	yes	no	no	yes	mammals
eel	no	no	yes	no	non-mammals
salamander	no	no	sometimes	yes	non-mammals
gila monster	no	no	no	yes	non-mammals
platypus	no	no	no	yes	mammals
owl	no	yes	no	yes	non-mammals
dolphin	yes	no	yes	no	mammals
eagle	no	yes	no	yes	non-mammals

A: attributes

M: mammals

N: non-mammals

$$P(A|M) = \frac{6}{7} \times \frac{6}{7} \times \frac{2}{7} \times \frac{2}{7} = 0.06$$

$$P(A|N) = \frac{1}{13} \times \frac{10}{13} \times \frac{3}{13} \times \frac{4}{13} = 0.0042$$

$$P(A|M)P(M) = 0.06 \times \frac{7}{20} = 0.021$$

$$P(A|N)P(N) = 0.004 \times \frac{13}{20} = 0.0027$$

Give Birth	Can Fly	Live in Water	Have Legs	Class
yes	no	yes	no	?

P(A|M)P(M) > P(A|N)P(N)

=> Mammals

Naïve Bayes (Summary)

- Robust to isolated noise points

- Handle missing values by ignoring the instance during probability estimate calculations

- Robust to irrelevant attributes

- Independence assumption may not hold for some attributes
  - Use other techniques such as Bayesian Belief Networks (BBN)

Python Code

```
from sklearn.neighbors import KNeighborsClassifier
knn1 = KNeighborsClassifier(n_neighbors=5)
knn1.fit(X_train, y_train)
y_pred_knn1 = knn1.predict(X_test)


from sklearn.naive_bayes import GaussianNB
nb1 = GaussianNB()
nb1.fit(X_train, y_train)
y_pred_nb1 = nb1.predict(X_test)
```

Reference

- James, Witten, Hastie, and Tibshirani. "*Introduction to Statistical Learning*". Chapter 4.
- Tan, Pang-Ning et al. Introduction to Data Mining. 2018. Chapter 4.3 and 4.4