Chapter 4 :Supervised Learning

Supervised vs. Unsupervised Learning

- Supervised learning (classification)
  - Supervision: The training data (observations, measurements, etc.) are accompanied by **labels** indicating the class of the observations
  - New data is classified based on the training set
- Unsupervised learning (clustering)
  - The class labels of training data is unknown
  - Given a set of measurements, observations, etc. with the aim of establishing the existence of classes or clusters in the data

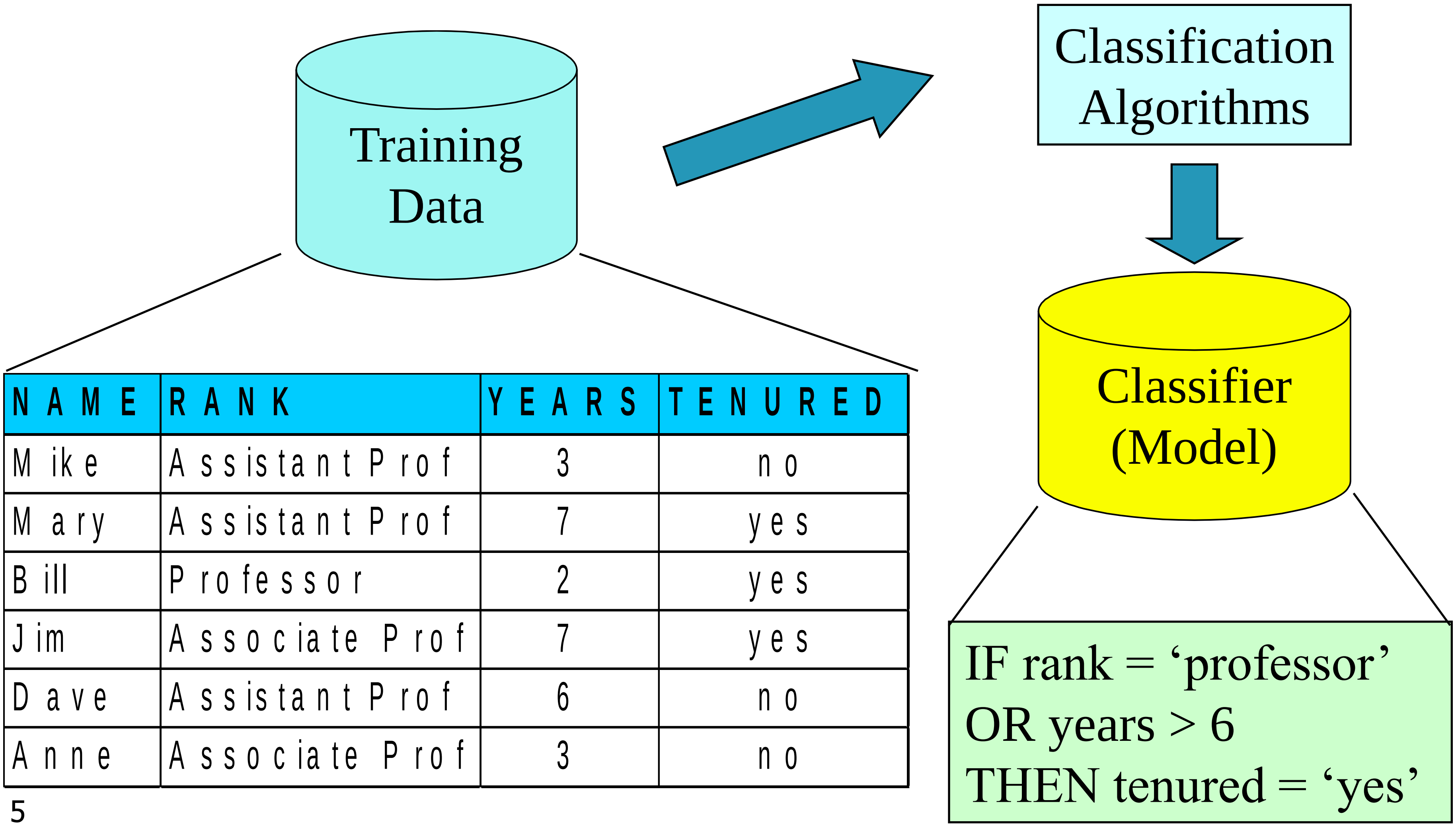
Prediction Problems: Classification vs. Numeric Prediction

- Classification
  - predicts categorical class labels (discrete or nominal)
  - classifies data (constructs a model) based on the training set and the values (class labels) in a classifying attribute and uses it in classifying new data
- Numeric Prediction
  - models continuous-valued functions, i.e., predicts unknown or missing values
- Typical applications
  - Credit/loan approval:
  - Medical diagnosis: if a tumor is cancerous or benign
  - Fraud detection: if a transaction is fraudulent
  - Web page categorization: which category it is

Classification—A Two-Step Process

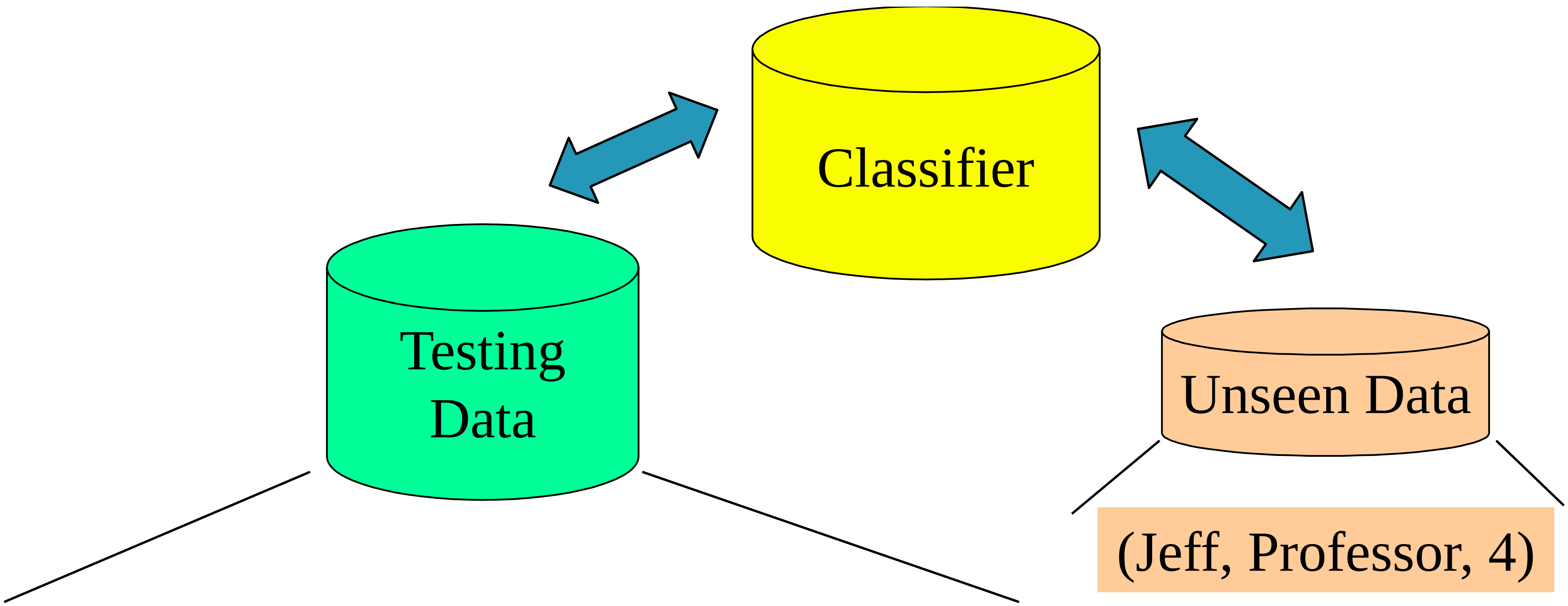
- Model construction: describing a set of predetermined classes
  - Each tuple/sample is assumed to belong to a predefined class, as determined by the class label attribute
  - The set of tuples used for model construction is training set
  - The model is represented as classification rules, decision trees, or mathematical formulae
- Model usage: for classifying future or unknown objects
  - Estimate accuracy of the model
    - The known label of test sample is compared with the classified result from the model
    - Accuracy rate is the percentage of test set samples that are correctly classified by the model
    - Test set is independent of training set (otherwise overfitting)
  - If the accuracy is acceptable, use the model to classify new data
- Note: If *the test set* is used to select models, it is called validation (test) set

Process (1): Model Construction

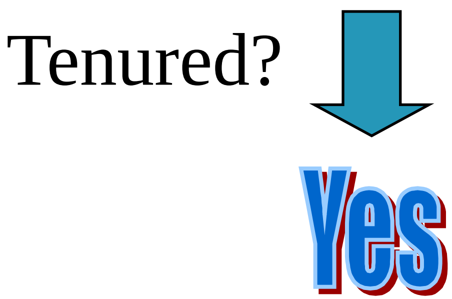


NAME	RANK	YEARS	TENURED
Mike	Assistant Prof	3	no
Mary	Assistant Prof	7	yes
Bill	Professor	2	yes
Jim	Associate Prof	7	yes
Dave	Assistant Prof	6	no
Anne	Associate Prof	3	no

Process (2): Using the Model in Prediction



NAME	RANK	YEARS	TENURED
Tom	Assistant Prof	2	no
Merlisa	Associate Prof	7	no
George	Professor	5	yes
Joseph	Assistant Prof	7	yes



Naïve Bayes

Bayes' Theorem: Basics

- Total probability Theorem: $P(B) = \sum_{i=1}^{M} P(B|A_i)P(A_i)$
- Bayes' Theorem: $P(H|\mathbf{X}) = \frac{P(\mathbf{X}|H)P(H)}{P(\mathbf{X})} = P(\mathbf{X}|H) \times P(H) / P(\mathbf{X})$
  - Let **X** be a data sample ("*evidence*"): class label is unknown
  - Let H be a *hypothesis* that X belongs to class C
  - Classification is to determine P(H|**X**), (i.e., *posteriori probability):* the probability that the hypothesis holds given the observed data sample **X**
  - P(H) (*prior probability*): the initial probability
    - E.g., **X** will buy computer, regardless of age, income, …
  - P(**X**): probability that sample data is observed
  - P(**X**|H) (likelihood): the probability of observing the sample **X**, given that the hypothesis holds
    - E.g., Given that **X** will buy computer, the prob. that X is 31..40, medium income

Prediction Based on Bayes' Theorem

- Given training data **X**, *posteriori probability of a hypothesis* H, P(H|**X**), follows the Bayes' theorem

$$P(H|\mathbf{X}) = \frac{P(\mathbf{X}|H)P(H)}{P(\mathbf{X})} = P(\mathbf{X}|H) \times P(H) / P(\mathbf{X})$$

- Informally, this can be viewed as

  posteriori = likelihood x prior/evidence

- Predicts **X** belongs to C_i iff the probability $P(C_i|\mathbf{X})$ is the highest among all the $P(C_k|X)$ for all the *k* classes
- Practical difficulty: It requires initial knowledge of many probabilities, involving significant computational cost

Classification Is to Derive the Maximum Posteriori

- Let D be a training set of tuples and their associated class labels, and each tuple is represented by an n-D attribute vector $\mathbf{X} = (x_1, x_2, \ldots, x_n)$
- Suppose there are *m* classes $C_1, C_2, \ldots, C_m$.
- Classification is to derive the maximum posteriori, i.e., the maximal $P(C_i|\mathbf{X})$
- This can be derived from Bayes' theorem

$$P(C_i|\mathbf{X}) = \frac{P(\mathbf{X}|C_i)P(C_i)}{P(\mathbf{X})}$$

- Since P(X) is constant for all classes, only

needs to be maximized $$P(C_i|\mathbf{X}) = P(\mathbf{X}|C_i)P(C_i)$$

Naïve Bayes Classifier

- A simplified assumption: attributes are conditionally independent (i.e., no dependence relation between attributes):

$$P(\mathbf{X}|C_i) = \prod_{k=1}^{n} P(x_k|C_i) = P(x_1|C_i) \times P(x_2|C_i) \times \ldots \times P(x_n|C_i)$$

- This greatly reduces the computation cost: Only counts the class distribution
- If A_k is categorical, $P(x_k|C_i)$ is the # of tuples in C_i having value x_k for A_k divided by $|C_{i,D}|$ (# of tuples of C_i in D)
- If A_k is continous-valued, $P(x_k|C_i)$ is usually computed based on Gaussian distribution with a mean μ and standard deviation σ

$$g(x,\mu,\sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

and $P(x_k|C_i)$ is

$$P(\mathbf{X}|C_i) = g(x_k, \mu_{C_i}, \sigma_{C_i})$$

Naïve Bayes Classifier: Training Dataset

Class:

C1:buys_computer = ‘yes’

C2:buys_computer = ‘no’

Data to be classified:

X = (age <=30,

Income = medium,

Student = yes

Credit_rating = Fair)

age	income	student	credit_rating	_comp
<=30	high	no	fair	no
<=30	high	no	excellent	no
31…40	high	no	fair	yes
>40	medium	no	fair	yes
>40	low	yes	fair	yes
>40	low	yes	excellent	no
31…40	low	yes	excellent	yes
<=30	medium	no	fair	no
<=30	low	yes	fair	yes
>40	medium	yes	fair	yes
<=30	medium	yes	excellent	yes
31…40	medium	no	excellent	yes
31…40	high	yes	fair	yes
>40	medium	no	excellent	no

Naïve Bayes Classifier: An Example

age	income	student	credit_rating	comp
<=30	high	no	fair	no
<=30	high	no	excellent	no
31…40	high	no	fair	yes
>40	medium	no	fair	yes
>40	low	yes	fair	yes
>40	low	yes	excellent	no
31…40	low	yes	excellent	yes
<=30	medium	no	fair	no
<=30	low	yes	fair	yes
>40	medium	yes	fair	yes
<=30	medium	yes	excellent	yes
31…40	medium	no	excellent	yes
31…40	high	yes	fair	yes
>40	medium	no	excellent	no

- $P(C_i)$: P(buys_computer = "yes") = 9/14 = 0.643
  P(buys_computer = "no") = 5/14= 0.357
- Compute $P(X|C_i)$ for each class
  P(age = "<=30" | buys_computer = "yes") = 2/9 = 0.222
  P(age = "<= 30" | buys_computer = "no") = 3/5 = 0.6
  P(income = "medium" | buys_computer = "yes") = 4/9 = 0.444
  P(income = "medium" | buys_computer = "no") = 2/5 = 0.4
  P(student = "yes" | buys_computer = "yes) = 6/9 = 0.667
  P(student = "yes" | buys_computer = "no") = 1/5 = 0.2
  P(credit_rating = "fair" | buys_computer = "yes") = 6/9 = 0.667
  P(credit_rating = "fair" | buys_computer = "no") = 2/5 = 0.4
- **X = (age <= 30 , income = medium, student = yes, credit_rating = fair)**

$P(X|C_i)$: P(X|buys_computer = "yes") = 0.222 x 0.444 x 0.667 x 0.667 = 0.044
P(X|buys_computer = "no") = 0.6 x 0.4 x 0.2 x 0.4 = 0.019

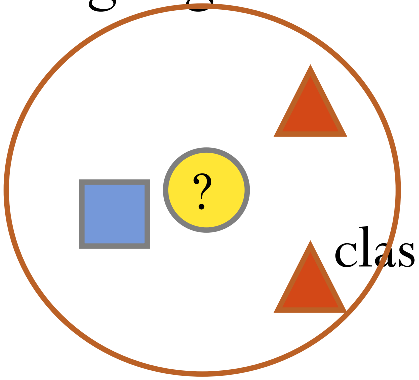
$P(X|C_i)*P(C_i)$: P(X|buys_computer = "yes") * P(buys_computer = "yes") = 0.028
P(X|buys_computer = "no") * P(buys_computer = "no") = 0.007

Therefore, X belongs to class ("buys_computer = yes")

KNN

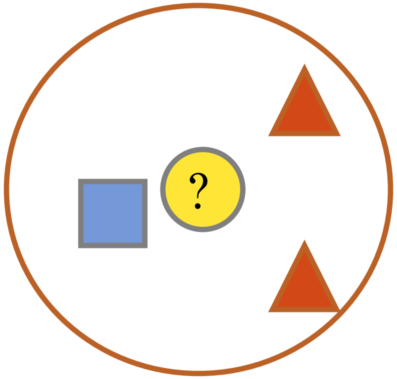
WHY NEAREST NEIGHBOR?

- Used to classify objects based on closest training examples in the feature space
  - Feature space: raw data transformed into sample vectors of fixed length using feature extraction (Training Data)
- Top 10 Data Mining Algorithm
  - ICDM paper – December 2007
- Among the simplest of all Data Mining Algorithms
  - Classification Method
- Implementation of lazy learner
  - All computation deferred until classification

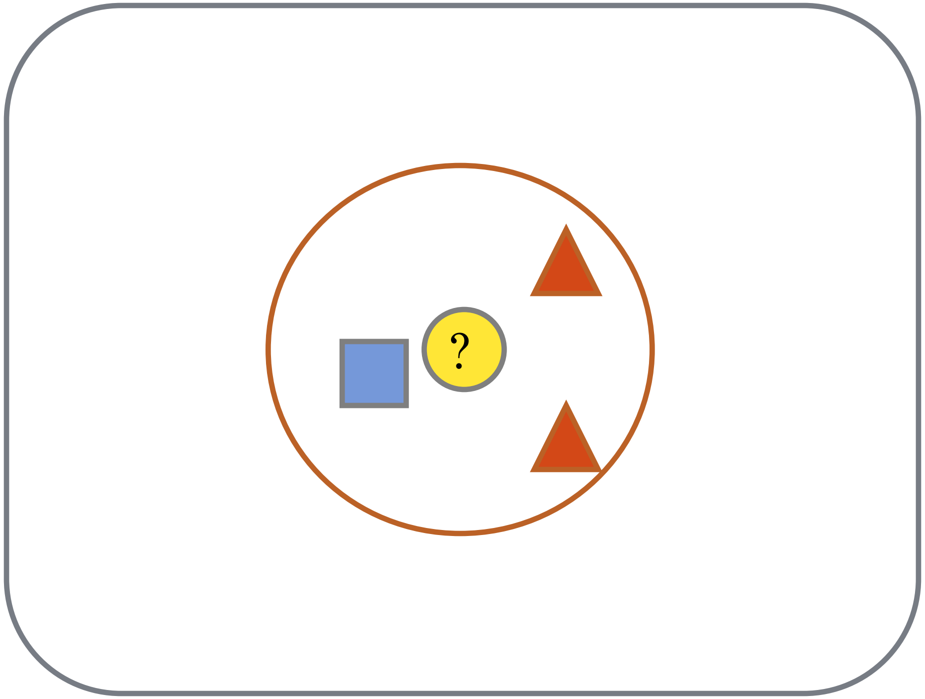


NEAREST NEIGHBOR CLASSIFICATION

- Nearest Neighbor Overview
- *k* Nearest Neighbor



k NEAREST NEIGHBOR



- Requires 3 things:
  - Feature Space(Training Data)
  - Distance metric
    - to compute distance between records
  - The value of *k*
    - the number of nearest neighbors to retrieve from which to get majority class
- 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

k NEAREST NEIGHBOR

- Common Distance Metrics:
  - Euclidean distance(continuos distribution)

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

  - Hamming distance (overlap metric)

bat (distance = 1) **t**o**n**e**d** (distance = 3)
cat **r**o**s**e**s**

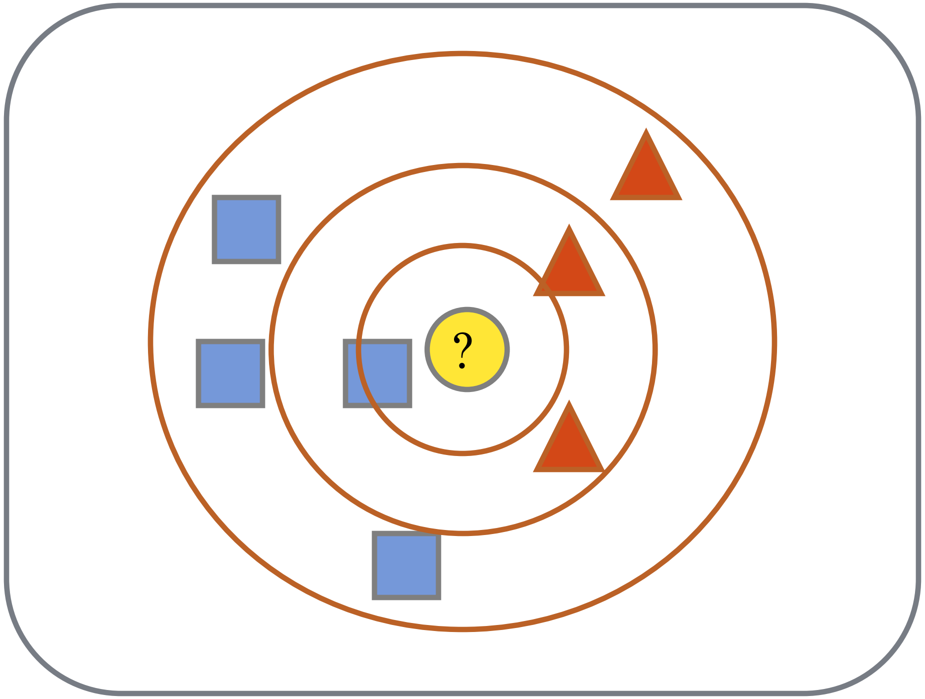
  - Discrete Metric(boolean metric)

if $x = y$ then $d(x,y) = 0$. Otherwise, $d(x,y) = 1$

- Determine the class from k nearest neighbor list
  - Take the majority vote of class labels among the k-nearest neighbors
  - Weighted factor

$w = 1/d$(generalized linear interpolation) or $1/d^2$

k NEAREST NEIGHBOR



- $k = 1$:
  - Belongs to square class
- $k = 3$:
  - Belongs to triangle class
- $k = 7$:
  - Belongs to square class

- 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
  - Choose an odd value for *k*, to eliminate ties

k NEAREST NEIGHBOR

- Accuracy of **all** NN based classification, prediction, or recommendations depends solely on a data model, no matter what specific NN algorithm is used.
- Scaling issues
  - Attributes may have to be scaled to prevent distance measures from being dominated by one of the attributes.
  - Examples
    - Height of a person may vary from 4' to 6'
    - Weight of a person may vary from 100lbs to 300lbs
    - Income of a person may vary from $10k to $500k
- Nearest Neighbor classifiers are lazy learners
  - No pre-constructed models for classification

K NEAREST NEIGHBOR ADVANTAGES

- Simple technique that is easily implemented
- Building model is inexpensive
- Extremely flexible classification scheme
  - does not involve preprocessing
- Well suited for
  - Multi-modal classes (classes of multiple forms)
  - Records with multiple class labels
- Asymptotic Error rate at most twice Bayes rate
  - Cover & Hart paper (1967)
- Can sometimes be the best method
  - Michihiro Kuramochi and George Karypis, Gene Classification using Expression Profiles: A Feasibility Study, International Journal on Artificial Intelligence Tools. Vol. 14, No. 4, pp. 641-660, 2005
  - K nearest neighbor outperformed SVM for protein function prediction using expression profiles

k NEAREST NEIGHBOR DISADVANTAGES

- Classifying unknown records are relatively expensive
  - Requires distance computation of k-nearest neighbors
  - Computationally intensive, especially when the size of the training set grows
- Accuracy can be severely degraded by the presence of noisy or irrelevant features

Height (in cms)	Weight (in kgs)	T Shirt Size
158	58	M
158	59	M
158	63	M
160	59	M
160	60	M
163	60	M
163	61	M
160	64	L
163	64	L
165	61	L
165	62	L
165	65	L
168	62	L
168	63	L
168	66	L
170	63	L
170	64	L
170	68	L

- **Step 1 : Calculate Similarity based on distance function**
- **New customer named 'Monica' has height 161cm and weight 61kg.**

Euclidean :

$$d(x, y) = \sqrt{\sum_{i=1}^{m} (x_i - y_i)^2}$$

Manhattan / city - block :

$$d(x, y) = \sum_{i=1}^{m} |x_i - y_i|$$

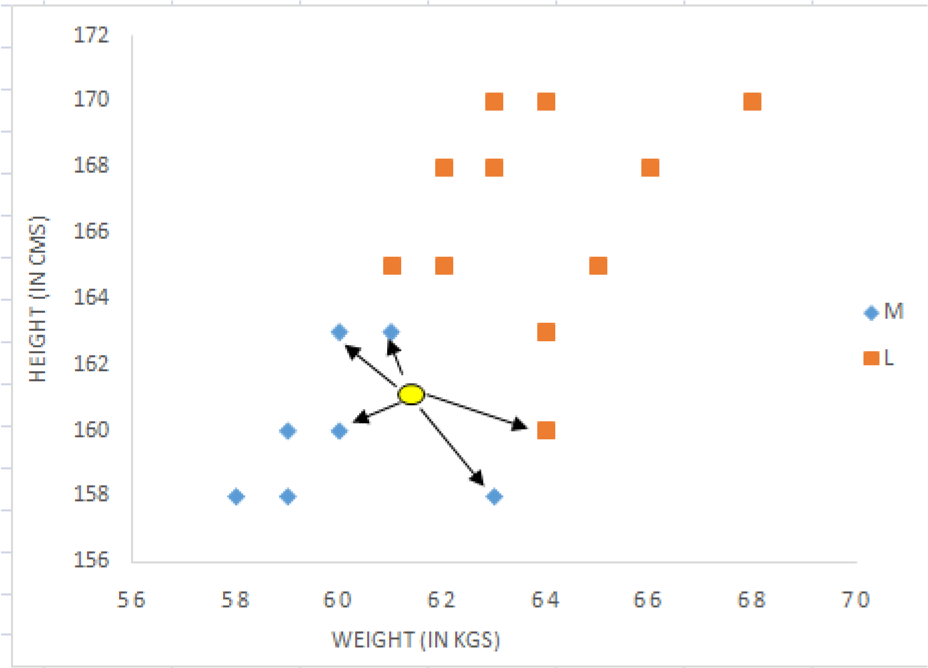
- =SQRT((161-158)^2+(61-58)^2)

- Similarly, we will calculate distance of all the training cases with new case and calculates the rank in terms of distance. The smallest distance value will be ranked 1 and considered as nearest neighbor.

- **Step 2 : Find K-Nearest Neighbors**

fx =SQRT((A21-A6)^2+(B21-B6)^2)

	A	B	C	D	E
1	Height (in cms)	Weight (in kgs)	T Shirt Size	Distance	
2	158	58	M	4.2	
3	158	59	M	3.6	
4	158	63	M	3.6	
5	160	59	M	2.2	3
6	160	60	M	1.4	1
7	163	60	M	2.2	3
8	163	61	M	2.0	2
9	160	64	L	3.2	5
10	163	64	L	3.6	
11	165	61	L	4.0	
12	165	62	L	4.1	
13	165	65	L	5.7	
14	168	62	L	7.1	
15	168	63	L	7.3	
16	168	66	L	8.6	
17	170	63	L	9.2	
18	170	64	L	9.5	
19	170	68	L	11.4	
20					
21	161	61			



172
170
168
166
164
162
160
158
156
HEIGHT (IN CMS)
56
58
60
62
64
66
68
70
WEIGHT (IN KGS)
M
L

- **Assumptions of KNN**

- **1. Standardization**

When independent variables in training data are measured in different units, it is important to standardize variables before calculating distance

$$Xs = \frac{X - mean}{s.d.}$$

$$Xs = \frac{X - mean}{max - min}$$

$$Xs = \frac{X - min}{\max - min}$$

	A	B	C	D	E
1	**Height (in cms)**	**Weight (in kgs)**	**T Shirt Size**	**Distance**	
2	-1.39	-1.64	M	1.3	
3	-1.39	-1.27	M	1.0	
4	-1.39	0.25	M	1.0	
5	-0.92	-1.27	**M**	0.8	**4**
6	-0.92	-0.89	**M**	0.4	**1**
7	-0.23	-0.89	**M**	0.6	**3**
8	-0.23	-0.51	**M**	0.5	**2**
9	-0.92	0.63	L	1.2	
10	-0.23	0.63	L	1.2	
11	0.23	-0.51	**L**	0.9	**5**
12	0.23	-0.13	L	1.0	
13	0.23	1.01	L	1.8	
14	0.92	-0.13	L	1.7	
15	0.92	0.25	L	1.8	
16	0.92	1.39	L	2.5	
17	1.39	0.25	L	2.2	
18	1.39	0.63	L	2.4	
19	1.39	2.15	L	3.4	
20					
21	**-0.7**	**-0.5**			

- **Outlier**
- Low k-value is sensitive to outliers and a higher K-value is more resilient to outliers as it considers more voters to decide prediction

KNN Exercise

- We have a data from questionnaires survey and objective testing with two attributes(acid durability and strength) to classify whether a special paper tissue is good or not. Here are four training samples .

X1= Acid durability (seconds)	X2=Strength (kg/m2)	Y=Classification
7	7	Bad
7	4	Bad
3	4	Good
1	4	Good

- Now the factory produces a new paper tissue that pass laboratory test with X1=3 and X2=7, without another expensive survey can we guess what the classification of new tissue is

Step 1:Determine parameter k= number of nearest neighbors.

Suppose K=3

Step 2: Calculate the distance between query instance and all the training samples.

X1= Acid durability (seconds)	X2=Strength (kg/m2)	Distance
7	7	4
7	4	5
3	4	3
1	4	3.6

- Step3: Sort the distance and determine the nearest neighbor based on the Kth minimum distance.

X1= Acid durability (seconds)	X2=Strength (kg/m2)	Distance	Rank	is it included in 3NN?
7	7	4	3	YES
7	4	5	4	No
3	4	3	1	YES
1	4	3.6	2	YES

- Step 4: Use simple majority of the category of nearest neighbour as the prediction value for query instance.

- Therefore we have 2 good and one bad . Since 2>1.

a new paper tissue that pass laboratory test with $X1=3$ and $X2=7$ is included in Good category