

K – Nearest Neighbors and Classifiers Evaluation



Dr. Wedad Hussein


wedad.hussein@cis.asu.edu.eg



Dr. Mahmoud Mounir

mahmoud.mounir@cis.asu.edu.eg

Chapter 8. Classification: Basic Concepts

- Classification: Basic Concepts
- Decision Tree Induction
- Bayes Classification Methods
- K-Nearest Neighbors 
- Model Evaluation

K-Nearest Neighbors (KNN)

- **K-Nearest Neighbors (KNN)** is a supervised learning algorithm where the result of new instance query is classified based on majority of K-nearest neighbor category.
- The purpose of this algorithm is to classify a new object **based on attributes and training samples**.
- KNN used **neighborhood classification** as the prediction value of the new query instance.

K-Nearest Neighbors (KNN)

- Given data instance

$X1 = 3$ and $X2 = 7$

Determine the suitable class of this instance using KNN algorithm.

X1	X2	Class
7	7	Bad
7	4	Bad
3	4	Good
1	4	Good

K-Nearest Neighbors (KNN)

Here is step by step on how to compute K-nearest neighbors KNN algorithm:

- Determine **parameter K** = number of nearest neighbors.
- Calculate the distance between the query-instance and all the training samples.
- **Sort the distance** and determine nearest neighbors based on the K-th minimum distance.
- Gather the **category** of the nearest neighbors.
- Use **simple majority** of the category of nearest neighbors as the prediction value of the query instance

K-Nearest Neighbors (KNN)

Here is step by step on how to compute K-nearest neighbors KNN algorithm:

- Determine parameter K = number of nearest neighbors.
 - Suppose $k = 3$
- Calculate the distance between the query-instance and all the training samples.
 - We will use the Euclidean distance

X1	X2	Distance
7	7	$\sqrt{(7 - 3)^2 + (7 - 7)^2} = 4$
7	4	$\sqrt{(7 - 3)^2 + (4 - 7)^2} = 5$
3	4	$\sqrt{(3 - 3)^2 + (4 - 7)^2} = 3$
1	4	$\sqrt{(1 - 3)^2 + (4 - 7)^2} = \sqrt{13} = 3.6$

K-Nearest Neighbors (KNN)

- Sort the distance and determine nearest neighbors based on the K-th minimum distance.

X1	X2	Distance	Ranked distance	Is it included in the 3-Nearest Neighbors
7	7	4	3	Yes
7	4	5	4	No
3	4	3	1	Yes
1	4	3.6	2	Yes

K-Nearest Neighbors (KNN)

- Gather the category of the nearest neighbors.

X1	X2	Distance	Ranked distance	Is it included in the 3-Nearest Neighbors	Class
7	7	4	3	Yes	Bad
7	4	5	4	No	
3	4	3	1	Yes	Good
1	4	3.6	2	Yes	Good

- Use simple majority of the category of nearest neighbors as the prediction value of the query instance

K-Nearest Neighbors (KNN)

X1	X2	Distance	Ranked distance	Is it included in the 3-Nearest Neighbors	Class
7	7	4	3	Yes	Bad
7	4	5	4	No	
3	4	3	1	Yes	Good
1	4	3.6	2	Yes	Good

- Use simple majority of the category of nearest neighbors as the prediction value of the query instance
 - We have 2 good and 1 bad,
 - We conclude that data instance $X1 = 3$ and $X2 = 7$ is included in Good category.

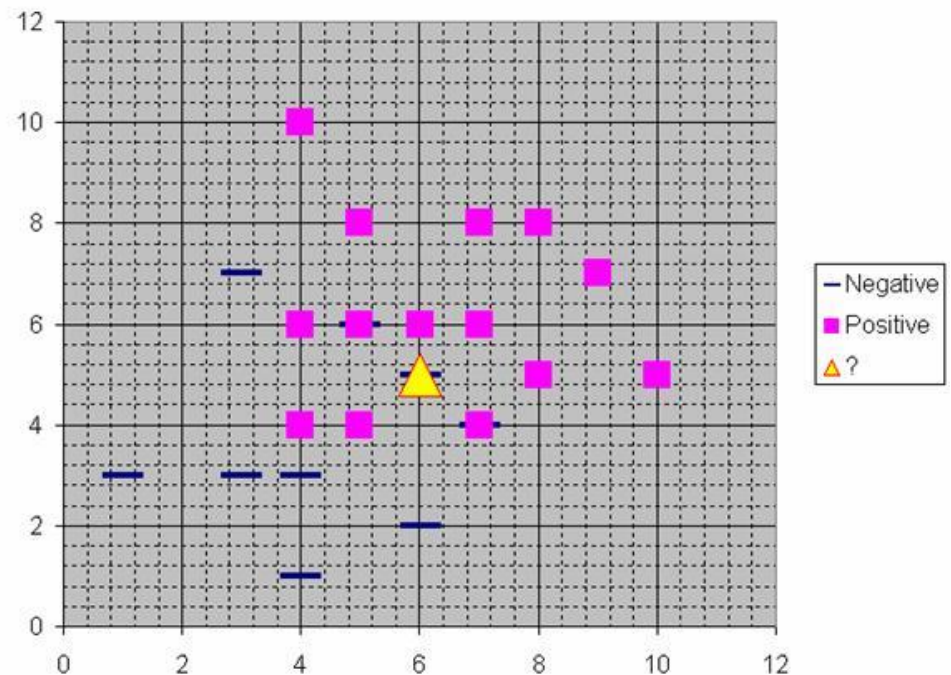
K-Nearest Neighbors (KNN)

Example


X1	X2	Y
4	3	+
1	3	+
3	3	+
3	7	+
7	4	+
4	1	+
6	5	+
5	6	+
3	7	+
6	2	+
4	6	-
4	4	-
5	8	-
7	8	-
5	6	-
10	5	-
7	6	-
4	10	-
9	7	-
5	4	-
8	5	-
6	6	-
7	4	-
8	8	-
6	5	?

training data

prediction



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Model Evaluation and Selection

- Evaluation metrics: How can we measure accuracy? Other metrics to consider?
- Use **validation test set** of class-labeled tuples instead of training set when assessing accuracy
- Methods for estimating a classifier's accuracy:
 - Holdout method, random subsampling
 - Cross-validation
 - Bootstrap
- Comparing classifiers:
 - Confidence intervals
 - Cost-benefit analysis and ROC Curves

Classifier Evaluation Metrics: Confusion Matrix

Confusion Matrix:

Actual class\Predicted class	C_1	$\neg C_1$
C_1	True Positives (TP)	False Negatives (FN)
$\neg C_1$	False Positives (FP)	True Negatives (TN)

Example of Confusion Matrix:

Actual class\Predicted class	buy_computer = yes	buy_computer = no	Total
buy_computer = yes	6954	46	7000
buy_computer = no	412	2588	3000
Total	7366	2634	10000

- Given m classes, an entry, $\mathbf{CM}_{i,j}$ in a **confusion matrix** indicates # of tuples in class i that were labeled by the classifier as class j
- May have extra rows/columns to provide totals

Classifier Evaluation Metrics: Accuracy, Error Rate, Sensitivity and Specificity

A\P	C	¬C	
C	TP	FN	P
¬C	FP	TN	N
	P'	N'	All

- **Classifier Accuracy**, or **recognition rate**:
percentage of test set tuples that are correctly classified

$$\text{Accuracy} = \frac{TP + TN}{ALL}$$

- **Error rate**:

$$\text{Error rate} = 1 - \text{accuracy}, \text{ or}$$

$$\text{Error rate} = \frac{FP + FN}{ALL}$$

Classifier Evaluation Metrics: Accuracy, Error Rate, Sensitivity and Specificity

A\P	C	¬C	
C	TP	FN	P
¬C	FP	TN	N
	P'	N'	All

■ Sensitivity (Recall):

- What % of positive tuples did the classifier label as positive?
- True Positive recognition rate

$$\text{Sensitivity} = \frac{TP}{P} = \frac{TP}{TP+FN}$$

■ Specificity:

- What % of negative tuples did the classifier label as negative?
- True Negative recognition rate

$$\text{Specificity} = \frac{TN}{N} = \frac{TN}{FP+TN}$$

Classifier Evaluation Metrics: Accuracy, Error Rate, Sensitivity and Specificity

A\P	C	¬C	
C	TP	FN	P
¬C	FP	TN	N
	P'	N'	All

■ Precision:

- what % of tuples that the classifier labeled as positive are actually positive

$$\text{Precision} = \frac{TP}{P'} = \frac{TP}{TP+FP}$$

Classifier Evaluation Metrics: Confusion Matrix

Confusion Matrix:

Actual class\Predicted class	Positive (H_0 is True)	Negative (H_0 is False)
Positive (Do not reject H_0)	(TP)	(FN) Type (II) Error
Negative (Reject H_0)	(FP) Type (I) Error	(TN)

Example of Confusion Matrix:

Actual class\Predicted class	buy_computer = yes	buy_computer = no	Total
buy_computer = yes	6954	46	7000
buy_computer = no	412	2588	3000
Total	7366	2634	10000

Classifier Evaluation Metrics: Example (1)

Actual Class\Predicted class	cancer = yes	cancer = no	Total	Recognition(%)
cancer = yes	90	210	300	30.00 (<i>sensitivity</i>)
cancer = no	140	9560	9700	98.56 (<i>specificity</i>)
Total	230	9770	10000	96.50 (<i>accuracy</i>)

- ***Precision*** = $TP/TP+FP = 90/230 = 39.13\%$
- ***Sensitivity (Recall)*** = $TP/P = 90/300 = 30.00\%$
- ***Specificity*** = $TN/N = 9560/9700 = 98.56\%$
- ***Accuracy*** = $TP+TN/ALL = 90+9560/10000 = 96.50\%$

A\P	C	¬C	
C	TP	FN	P
¬C	FP	TN	N
	P'	N'	All

Classifier Evaluation Metrics: Example (2)

		Predicted		
		A	B	C
Actual	A	95	3	2
	B	5	90	5
	C	15	0	85

- a) The recognition rate.
- b) The sensitivity of Class C.
- c) The error rate.

a) Recognition rate = $95+90+85/300 = 90\%$

b) Sensitivity (Recall) = $TP/P = 85/100 = 85\%$

c) Error rate = $1 - \text{recognition rate} = 1 - 0.9 = 0.1 = 10\%$