Lecture outline

- Introduction to classification
- Evaluating classifiers
- k-NN

Some of the material presented here is from the supplementary material of the book: Introduction to Data Mining by Tan, Steinbach and Kumar

What is classification?

	binary	categorical	continuous	class
Tid	**Home Owner**	**Marital Status**	**Annual Income**	**Defaulted Borrower**
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

Figure 4.6. Training set for predicting borrowers who will default on loan payments.

Figure from Introduction to Data Mining (Tan, Steinbach and Kumar)

What is classification?

- **Classification** is the task of **learning a target function f** that maps attribute set **x** to one of the predefined class labels **y**

	binary	categorical	continuous	class
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Figure 4.6. Training set for predicting borrowers who will default on loan payments.

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What is classification?

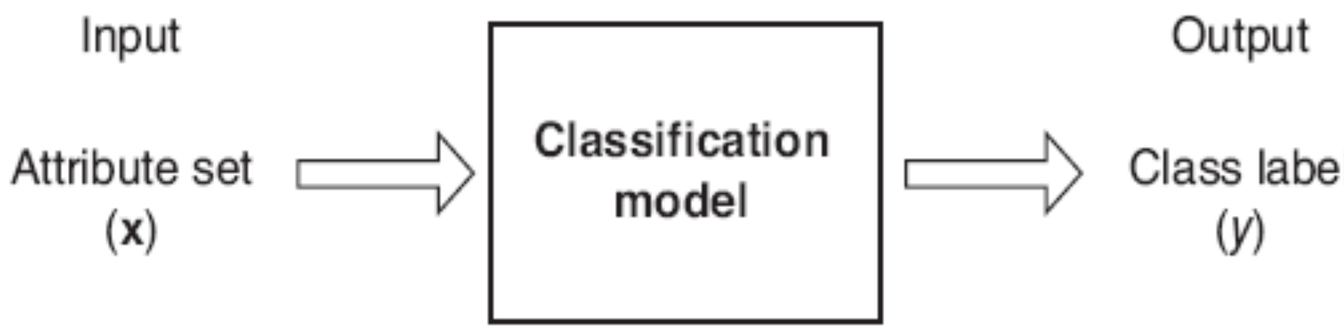


Figure 4.2. Classification as the task of mapping an input attribute set $\mathbf{x}$ into its class label y.

Figure from Introduction to Data Mining (Tan, Steinbach and Kumar)

Why classification?

- The target function f is known as a **classification model**
- Descriptive modeling: **Explanatory tool** to distinguish between objects of different classes (e.g., description of who can pay back his loan)
- Predictive modeling: Predict a class of a previously **unseen** record

Typical applications

- credit approval
- target marketing
- medical diagnosis
- treatment effectiveness analysis

General approach to classification

- **Training set** consists of records with **known class labels**

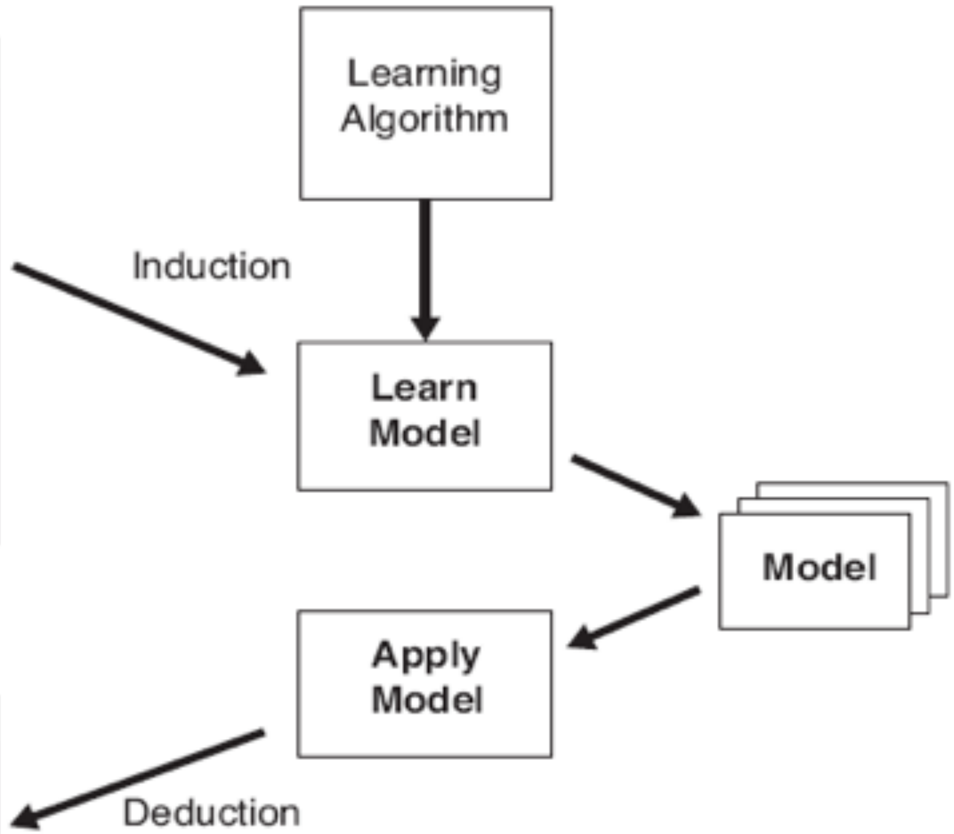
- Training set is used to **build a classification model**

- The classification model is applied to the **test set** that consists of records with **unknown labels**

General approach to classification

Training Set

Tid	Attrib1	Attrib2	Attrib3	Class
1	Yes	Large	125K	No
2	No	Medium	100K	No
3	No	Small	70K	No
4	Yes	Medium	120K	No
5	No	Large	95K	Yes
6	No	Medium	60K	No
7	Yes	Large	220K	No
8	No	Small	85K	Yes
9	No	Medium	75K	No
10	No	Small	90K	Yes



Test Set

Tid	Attrib1	Attrib2	Attrib3	Class
11	No	Small	55K	?
12	Yes	Medium	80K	?
13	Yes	Large	110K	?
14	No	Small	95K	?
15	No	Large	67K	?

Figure 4.3. General approach for building a classification model.

Figure from Introduction to Data Mining (Tan, Steinbach and Kumar)

Evaluating your classifier

- Metrics for Performance Evaluation
  - How to evaluate the performance of a classifier?
- Methods for Performance Evaluation
  - How to obtain reliable estimates?
- Methods for Classifier Comparison
  - How to compare the relative performance of different classifiers?

Evaluation of classification models

- Counts of test records that are correctly (or incorrectly) predicted by the classification model
- **Confusion matrix**

Predicted Class

Actual Class

	Class = 1	Class =
Class = 1	f_{11}	f_{10}
Class = 0	f_{01}	f_{00}

$$\text{Accuracy} = \frac{\#\text{ correct predictions}}{\text{total }\#\text{ of predictions}} = \frac{f_{11} + f_{00}}{f_{11} + f_{10} + f_{01} + f_{00}}$$

$$\text{Error rate} = \frac{\#\text{ wrong predictions}}{\text{total }\#\text{ of predictions}} = \frac{f_{10} + f_{01}}{f_{11} + f_{10} + f_{01} + f_{00}}$$

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

Metrics for Performance Evaluation

- Focus on the predictive capability of a model
  - Rather than how fast it takes to classify or build models, scalability, etc.
- Confusion Matrix:

	PREDICTED CLASS		
		Class=Yes	Class=No
ACTUAL CLASS	Class=Yes	a: TP	b: FN
	Class=No	c: FP	d: TN

a: TP (true positive)

b: FN (false negative)

c: FP (false positive)

d: TN (true negative)

Metrics for Performance Evaluation…

		PREDICTED CLASS	
		Class=Yes	Class=No
ACTUAL CLASS	Class=Yes	a (TP)	b (FN)
	Class=No	c (FP)	d (TN)

- Most widely-used metric:

$$\text{Accuracy} = \frac{a+d}{a+b+c+d} = \frac{TP+TN}{TP+TN+FP+FN}$$

Limitation of Accuracy

- Consider a 2-class problem
  - Number of Class 0 examples = 9990
  - Number of Class 1 examples = 10

- If model predicts everything to be class 0, accuracy is 9990/10000 = 99.9 %
  - Accuracy is misleading because model does not detect any class 1 example

Cost Matrix

	PREDICTED CLASS	
ACTUAL CLASS		

	C(i|j)	**Class=Yes**	**Class=No**
ACTUAL CLASS	**Class=Yes**	C(Yes|Yes)	C(No|Yes)
	Class=No	C(Yes|No)	C(No|No)

C(i|j): Cost of misclassifying class **j** example as class **i**

Computing Cost of Classification

Cost Matrix	PREDICTED CLASS		
	C(i|j)	+	-
ACTUAL CLASS	+	-1	100
	-	1	0

Model M_1	PREDICTED CLASS		
		+	-
ACTUAL CLASS	+	150	40
	-	60	250

Accuracy = 80%

Cost = 3910

Model M_2	PREDICTED CLASS		
		+	-
ACTUAL CLASS	+	250	45
	-	5	200

Accuracy = 90%

Cost = 4255

Cost vs Accuracy

Count	PREDICTED CLASS		
ACTUAL CLASS		Class=Yes	Class=No
	Class=Yes	a	b
	Class=No	c	d

Cost	PREDICTED CLASS		
ACTUAL CLASS		Class=Yes	Class=No
	Class=Yes	p	q
	Class=No	q	p

Accuracy is proportional to cost if

1. C(Yes|No)=C(No|Yes) = q
2. C(Yes|Yes)=C(No|No) = p

$N = a + b + c + d$

$\text{Accuracy} = (a + d)/N$

$$\begin{aligned}\text{Cost} &= p\,(a + d) + q\,(b + c)\\ &= p\,(a + d) + q\,(N - a - d)\\ &= q\,N - (q - p)(a + d)\\ &= N\,[q - (q-p) \times \text{Accuracy}]\end{aligned}$$

Cost-Sensitive Measures

$$\text{Precision (p)} = \frac{a}{a+c} = \frac{TP}{TP+FP}$$

$$\text{Recall (r)} = \frac{a}{a+b} = \frac{TP}{TP+FN}$$

$$\text{F - measure (F)} = \frac{2rp}{r+p} = \frac{2a}{2a+b+c} = \frac{2TP}{2TP+FP+FN}$$

- Precision is biased towards **C(Yes|Yes) & C(Yes|No)**
- Recall is biased towards **C(Yes|Yes) & C(No|Yes)**
- F-measure is biased towards all except **C(No|No)**

$$\text{Weighted Accuracy} = \frac{w_1 a + w_4 d}{w_1 a + w_2 b + w_3 c + w_4 d}$$

Model Evaluation

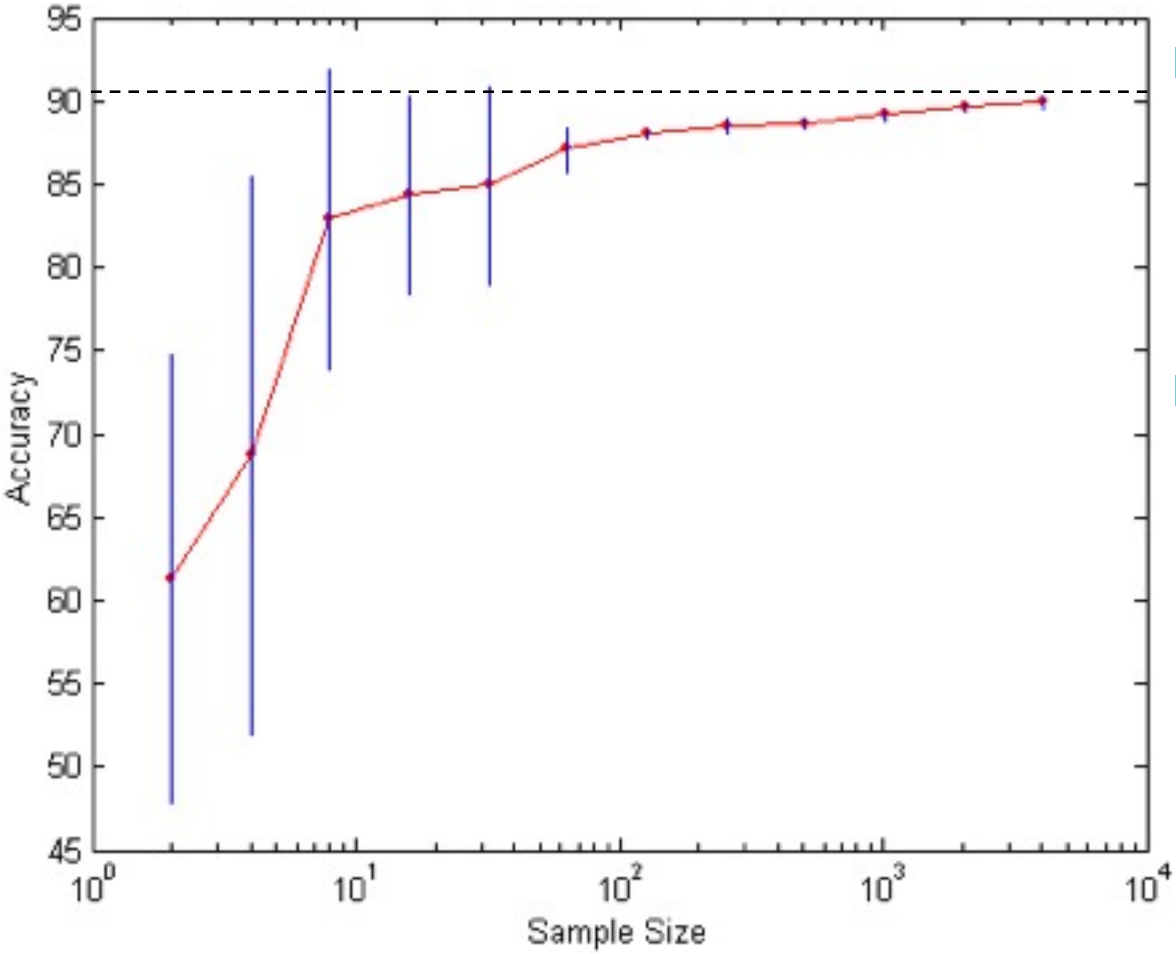
- Metrics for Performance Evaluation
  - How to evaluate the performance of a model?
- Methods for Performance Evaluation
  - How to obtain reliable estimates?
- Methods for Model Comparison
  - How to compare the relative performance of different models?

Methods for Performance Evaluation

- How to obtain a reliable estimate of performance?

- Performance of a model may depend on other factors besides the learning algorithm:
  - Class distribution
  - Cost of misclassification
  - Size of training and test sets

Learning Curve



- Learning curve shows how accuracy changes with varying sample size
- Requires a sampling schedule for creating learning curve

Effect of small sample size:
- Bias in the estimate
- Variance of estimate

Methods of Estimation

- **Holdout**
  - Reserve **2/3** for training and **1/3** for testing
- **Random subsampling**
  - Repeated holdout
- **Cross validation**
  - Partition data into **k** disjoint subsets
  - **k**-fold: train on **k-1** partitions, test on the remaining one
  - **Leave-one-out**: **k=n**
- **Bootstrap**
  - Sampling with replacement

Definition

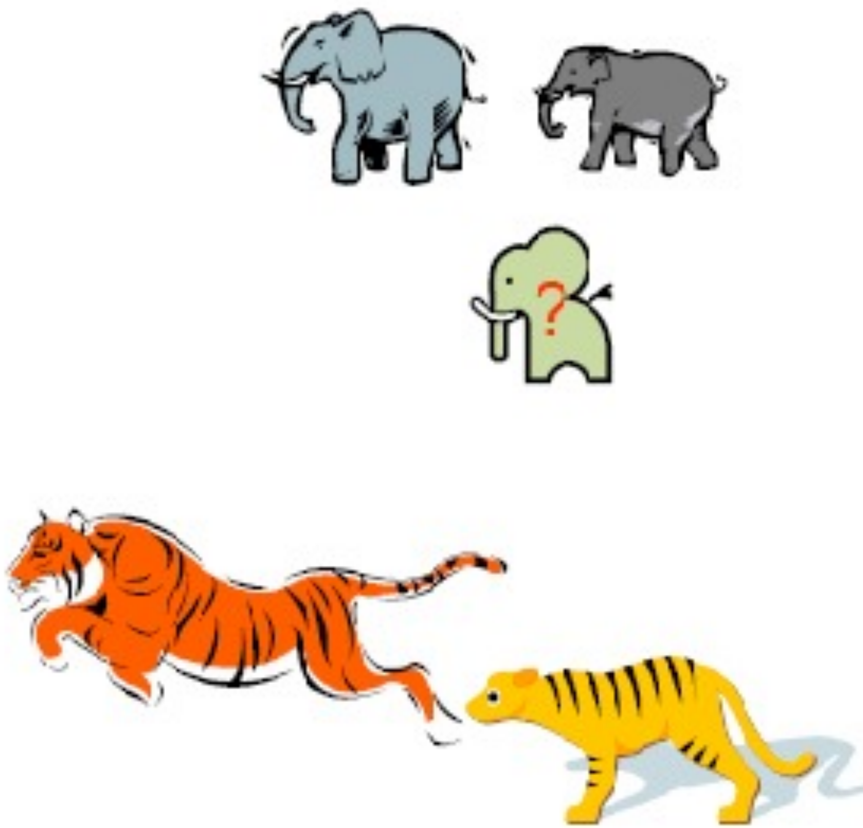
- Given: a set **X** of **n** points in $\mathbf{R}^d$
- Nearest neighbor: for any query point $\mathbf{q} \in \mathbf{R}^d$ return the point $\mathbf{x} \in \mathbf{X}$ minimizing $\mathbf{D(x,q)}$

- **Intuition:** Find the point in **X** that is the **closest** to **q**

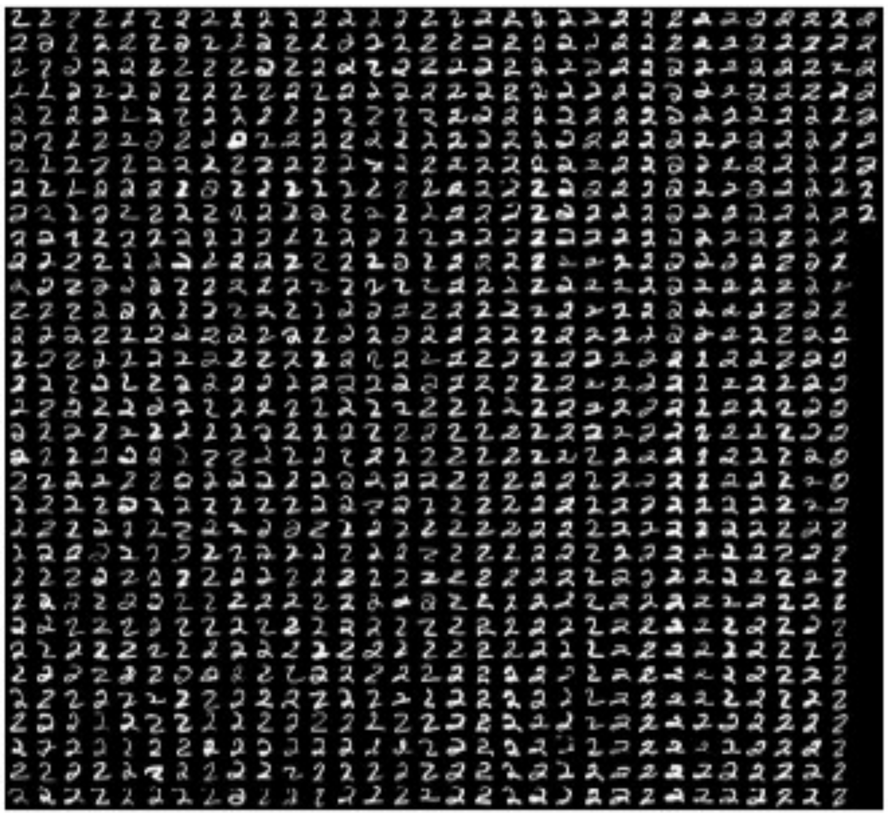
Motivation

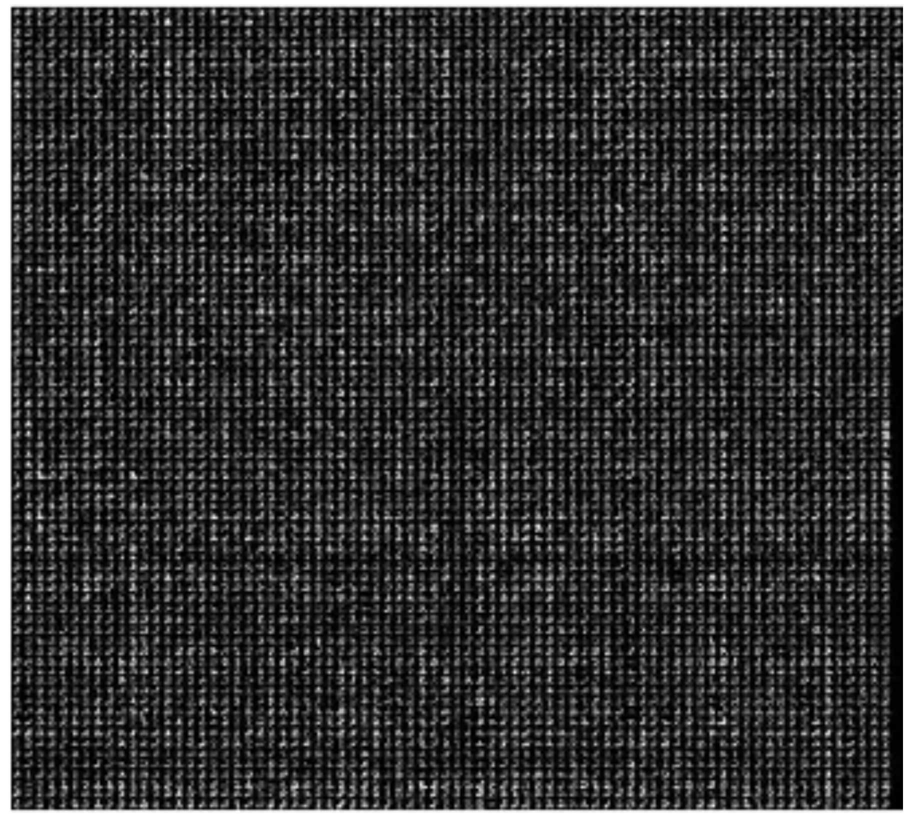
- **Learning:** Nearest neighbor rule
- **Databases:** Retrieval
- **Data mining:** Clustering
- Donald Knuth in vol.3 of **The Art of Computer Programming** called it the post-office problem, referring to the application of assigning a resident to the **nearest-post office**

Nearest-neighbor rule



MNIST dataset “2”





Methods for computing NN

- **Linear scan: O(nd)** time

- This is pretty much all what is known for exact algorithms with theoretical guarantees

- In practice:
  - **kd-trees** work "well" in "low-medium" dimensions

How to Construct an ROC curve

Instance	P(+|A)	True Class
1	0.95	+
2	0.93	+
3	0.87	-
4	0.85	-
5	0.85	-
6	0.85	+
7	0.76	-
8	0.53	+
9	0.43	-
10	0.25	+

- Use classifier that produces posterior probability for each test instance P(+|A)
- Sort the instances according to P(+|A) in decreasing order
- Apply threshold at each unique value of P(+|A)
- Count the number of TP, FP, TN, FN at each threshold
- TP rate, TPR = TP/(TP+FN)
- FP rate, FPR = FP/(FP + TN)