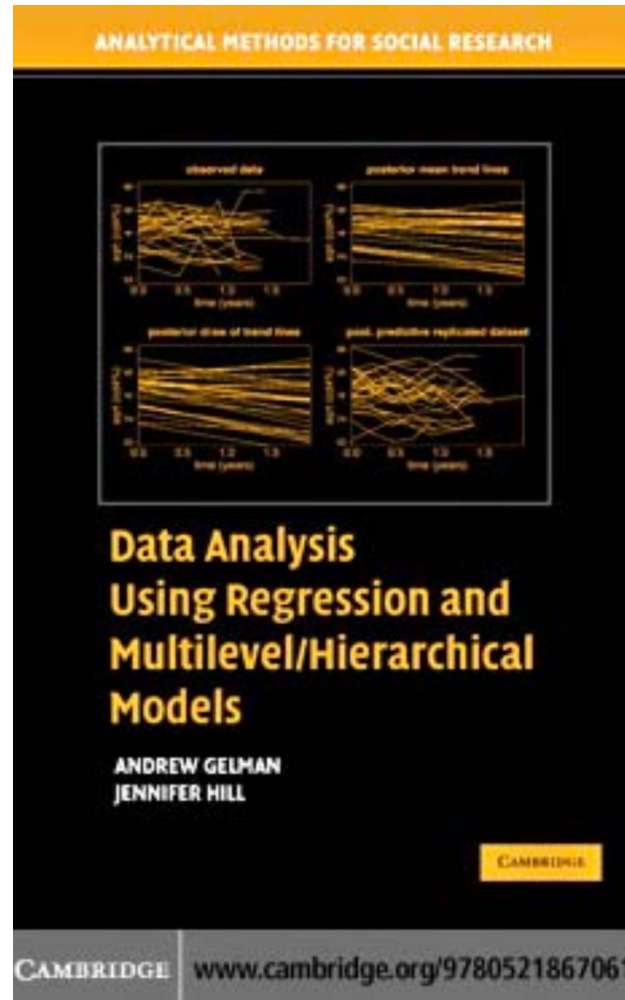


Lecture 5:

Classification

Homework (after Eastern)



Homework (after Eastern)

Passwords

Homework (after Eastern)

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Homework (after Eastern)

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Classification fundamentals

Classification: definition

Given

- a collection of class labels
- a collection of data objects labelled with a class label

Find a descriptive profile of each class, which will allow the assignment of unlabeled objects to the appropriate class

Definitions

Training set

Collection of labeled data objects used to learn the classification model

Test set

Collection of labeled data objects used to validate the classification model

Classification techniques

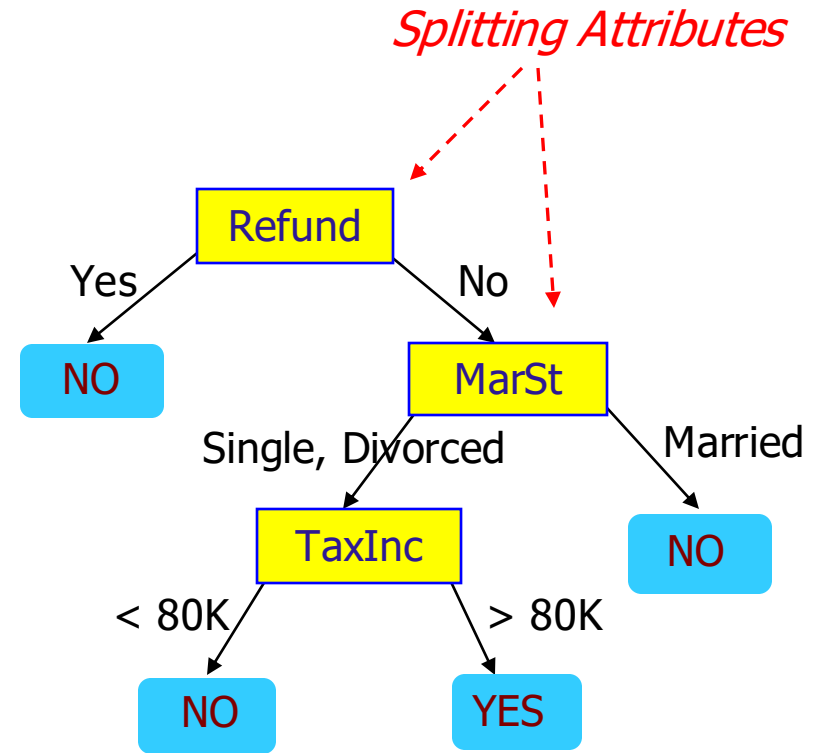
1. Decision trees
 2. Classification rules
 3. Association rules
 4. Neural Networks
 5. Naïve Bayes and Bayesian Networks
 6. k-Nearest Neighbours (k-NN)
 7. Support Vector Machines (SVM)
- ...

Decision trees

Example of decision tree

categorical
categorical
continuous
class

Tid	Refund	Marital Status	Taxable Income	Cheat
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



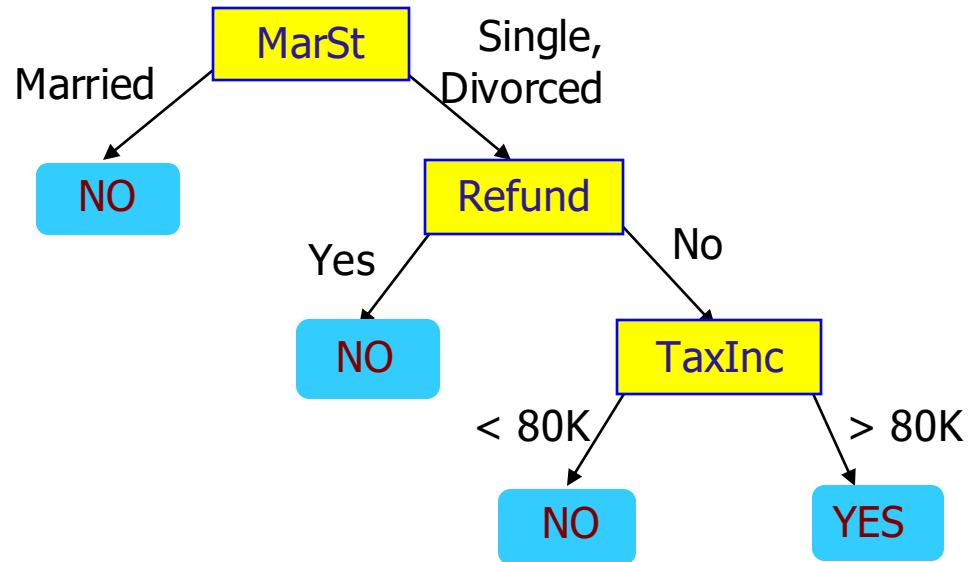
Training Data

Model: Decision Tree

Another example of decision tree

categorical
categorical
continuous
class

<i>Tid</i>	Refund	Marital Status	Taxable Income	Cheat
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
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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



There could be more than one tree that fits the same data!

Decision tree induction

Many algorithms to build a decision tree

Hunt's Algorithm (one of the earliest)

CART

ID3, C4.5, C5.0

SLIQ, SPRINT

Decision Tree Based Classification

Advantages

- Inexpensive to construct

- Extremely fast at classifying unknown records

- Easy to interpret for small-sized trees

- Accuracy is comparable to other classification techniques for many simple data sets

Disadvantages

- accuracy may be affected by missing data

Evaluation of decision trees

Accuracy

For simple datasets, comparable to other classification techniques

Interpretability

Model is interpretable for small trees

Single predictions are interpretable

Incrementality

Not incremental

■ Efficiency

- Fast model building
- Very fast classification

■ Scalability

- Scalable both in training set size and attribute number

■ Robustness

- Difficult management of missing data

Random Forest

Ensemble learning technique

multiple base models are combined
to improve accuracy and stability
to avoid overfitting

Random forest = set of decision trees

a number of decision trees are built at training time
the class is assigned by majority voting

Random Forest

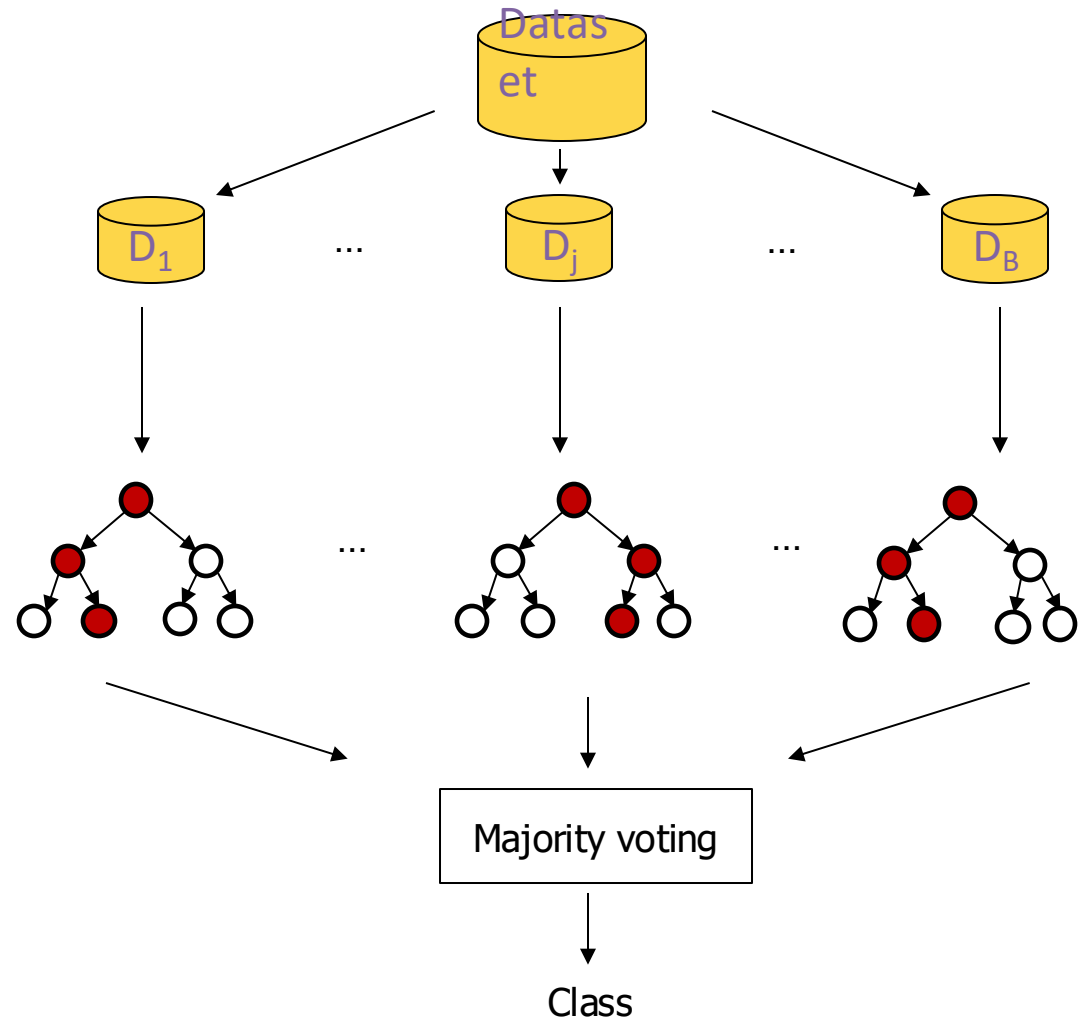
Original Training data

Random subsets

Multiple decision trees

For each subset, a tree is learned on a *random* set of features

Aggregating classifiers



Bootstrap aggregation

Given a training set D of n instances, it selects B times a *random* sample with replacement from D and trains trees on these dataset samples

For $b = 1, \dots, B$

Sample with replacement n' training examples, $n' \leq n$

A dataset subset D_b is generated

Train a classification tree on D_b

Random Forest – Algorithm Recap

- Given a training set D of n instances with p features
- For $b = 1, \dots, B$
 - Sample randomly with replacement n' training examples. A subset D_b is generated
 - Train a classification tree on D_b
 - During the tree construction, for each candidate split
 - $m \ll p$ random features are selected (typically $m \approx \sqrt{p}$)
 - the best split is computed among these m features
- Class is assigned by majority voting among the B predictions

Random Forest

Strong points

- higher accuracy than decision trees
- fast training phase
- robust to noise and outliers
- provides global feature importance, i.e. an estimate of which features are important in the classification

Weak points

- results can be difficult to interpret
 - A prediction is given by hundreds of trees
 - but at least we have an indication through feature importance

Evaluation of random forests

Accuracy

Higher than decision trees

Interpretability

Model and prediction are not interpretable

A prediction may be given by hundreds of trees

Provide global feature importance

an estimate of which features are important in the classification

Incrementality

Not incremental

■ Efficiency

- Fast model building
- Very fast classification

■ Scalability

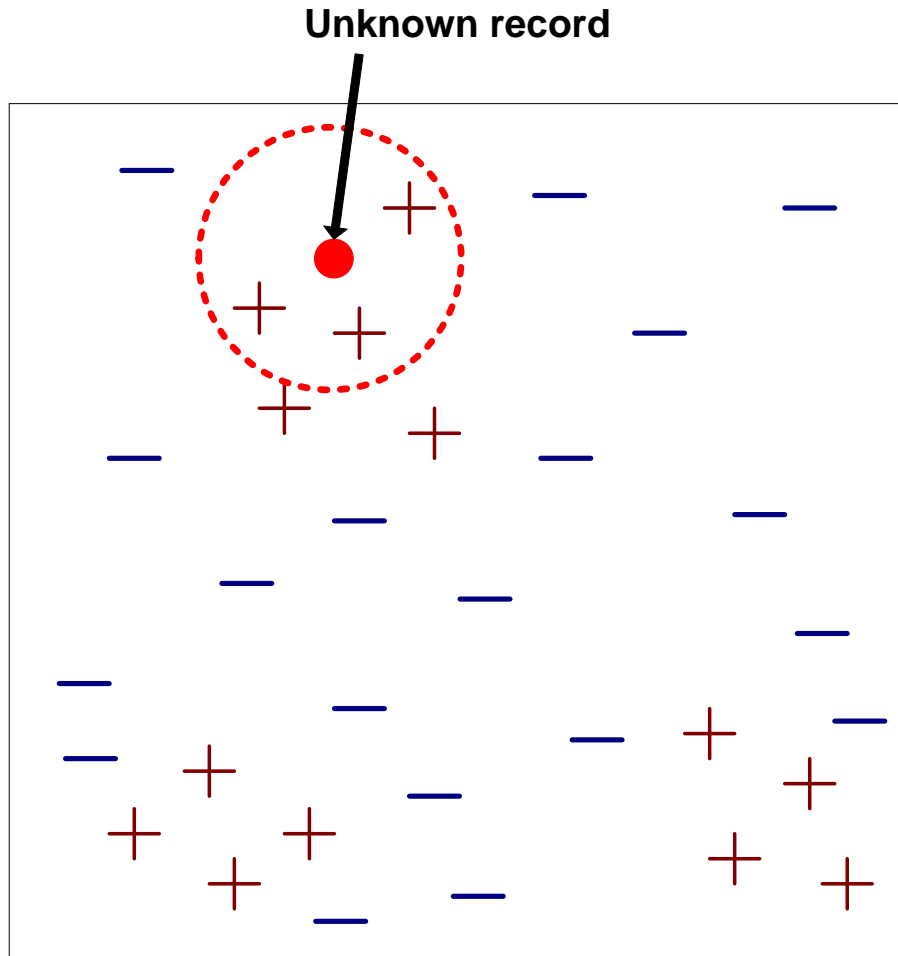
- Scalable both in training set size and attribute number

■ Robustness

- Robust to noise and outliers

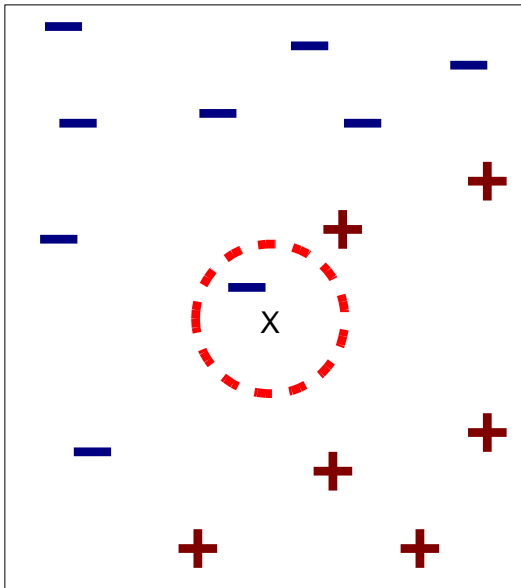
K-Nearest Neighbor

Nearest-Neighbor Classifiers

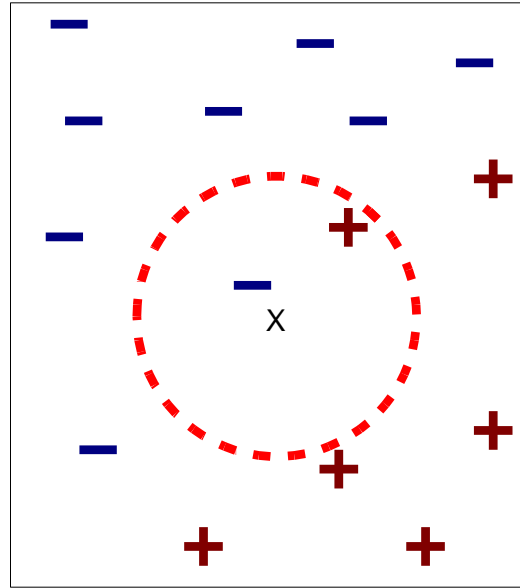


- Requires
 - The set of stored records
 - Distance Metric to compute distance between records
 - The value of k , the number of nearest neighbors to retrieve
- To classify an unknown record
 - Compute distance to other training records
 - Identify k nearest neighbors
 - Use class labels of nearest neighbors to determine the class label of unknown record (e.g., by taking majority vote)

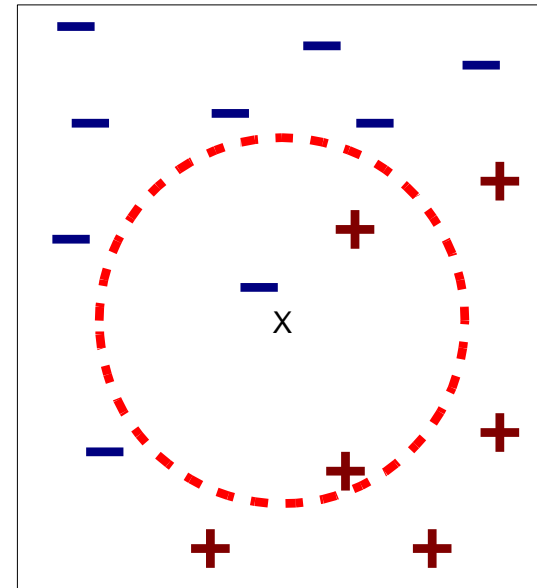
Definition of Nearest Neighbor



(a) 1-nearest neighbor



(b) 2-nearest neighbor

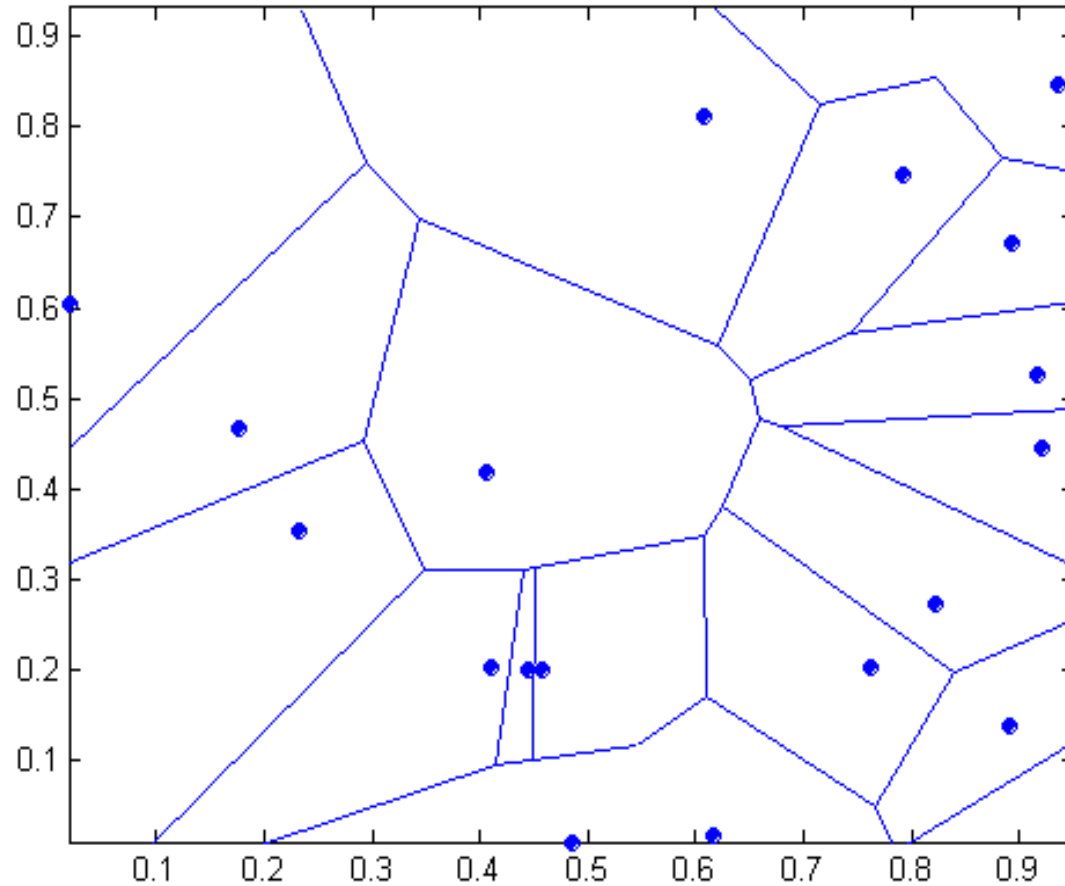


(c) 3-nearest neighbor

K-nearest neighbors of a record x are data points that have the k smallest distance to x

1 nearest-neighbor

Voronoi Diagram



From: Tan, Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

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

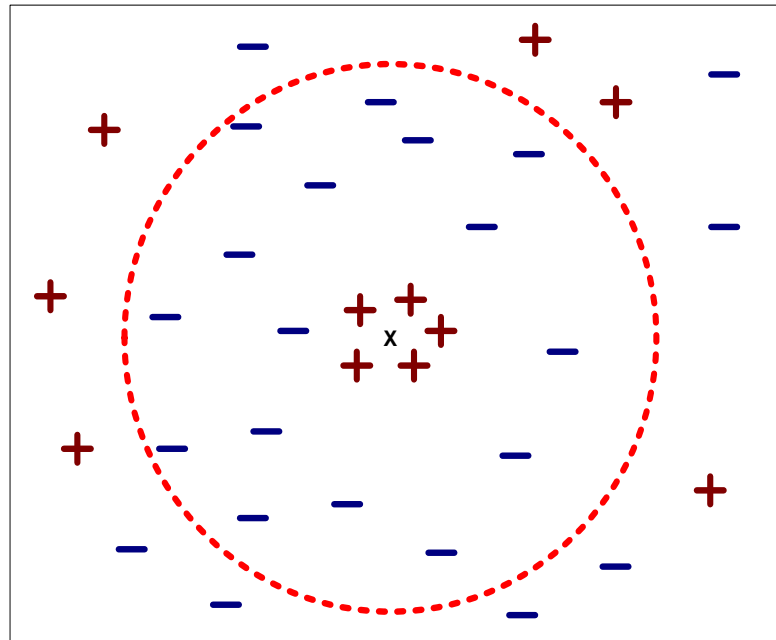
weight factor, $w = 1/d^2$

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

Attribute domain should be normalized to prevent distance measures from being dominated by one of the attributes

Example: height [1.5m to 2.0m] vs. income [\$10K to \$1M]

Problem with distance measures

High dimensional data

curse of dimensionality

Evaluation of KNN

Accuracy

Comparable to other classification techniques for simple datasets

Interpretability

Model is not interpretable
Single predictions can be "described" by neighbors

Incrementality

Incremental
Training set *must* be available

■ Efficiency

- (Almost) no model building
- Slower classification, requires computing distances

■ Scalability

- Weakly scalable in training set size
- Curse of dimensionality for increasing attribute number

■ Robustness

- Depends on distance computation

Bayesian Classification (FINISH POINT)

Elena Baralis
Politecnico di Torino

Bayes theorem

Let C and X be random variables

$$P(C, X) = P(C | X) P(X)$$

$$P(C, X) = P(X | C) P(C)$$

Hence

$$P(C | X) P(X) = P(X | C) P(C)$$

and also

$$P(C | X) = P(X | C) P(C) / P(X)$$

Bayesian classification: Example

Outlook	Temperature	Humidity	Windy	Class
sunny	hot	high	false	N
sunny	hot	high	true	N
overcast	hot	high	false	P
rain	mild	high	false	P
rain	cool	normal	false	P
rain	cool	normal	true	N
overcast	cool	normal	true	P
sunny	mild	high	false	N
sunny	cool	normal	false	P
rain	mild	normal	false	P
sunny	mild	normal	true	P
overcast	mild	high	true	P
overcast	hot	normal	false	P
rain	mild	high	true	N

Bayesian classification: Example

outlook	
$P(\text{sunny} p) = 2/9$	$P(\text{sunny} n) = 3/5$
$P(\text{overcast} p) = 4/9$	$P(\text{overcast} n) = 0$
$P(\text{rain} p) = 3/9$	$P(\text{rain} n) = 2/5$
temperature	
$P(\text{hot} p) = 2/9$	$P(\text{hot} n) = 2/5$
$P(\text{mild} p) = 4/9$	$P(\text{mild} n) = 2/5$
$P(\text{cool} p) = 3/9$	$P(\text{cool} n) = 1/5$
humidity	
$P(\text{high} p) = 3/9$	$P(\text{high} n) = 4/5$
$P(\text{normal} p) = 6/9$	$P(\text{normal} n) = 1/5$
windy	
$P(\text{true} p) = 3/9$	$P(\text{true} n) = 3/5$
$P(\text{false} p) = 6/9$	$P(\text{false} n) = 2/5$

$P(p) = 9/14$
$P(n) = 5/14$

Bayesian classification: Example

Data to be labeled

$$X = \langle \text{rain, hot, high, false} \rangle$$

For class p

$$\begin{aligned} P(X|p) \cdot P(p) &= \\ &= P(\text{rain}|p) \cdot P(\text{hot}|p) \cdot P(\text{high}|p) \cdot P(\text{false}|p) \cdot P(p) = \\ &= \frac{3}{9} \cdot \frac{2}{9} \cdot \frac{3}{9} \cdot \frac{6}{9} \cdot \frac{9}{14} = 0.010582 \end{aligned}$$

For class n

$$\begin{aligned} P(X|n) \cdot P(n) &= \\ &= P(\text{rain}|n) \cdot P(\text{hot}|n) \cdot P(\text{high}|n) \cdot P(\text{false}|n) \cdot P(n) = \\ &= \frac{2}{5} \cdot \frac{2}{5} \cdot \frac{4}{5} \cdot \frac{2}{5} \cdot \frac{5}{14} = \mathbf{0.018286} \end{aligned}$$

Evaluation of Naïve Bayes Classifiers

Accuracy

Similar or lower than decision trees

Naïve hypothesis simplifies model

Interpretability

Model and prediction are not interpretable

The weights of contributions in a single prediction may be used to explain

Incrementality

Fully incremental

Does *not* require availability of training data

■ Efficiency

- Fast model building
- Very fast classification

■ Scalability

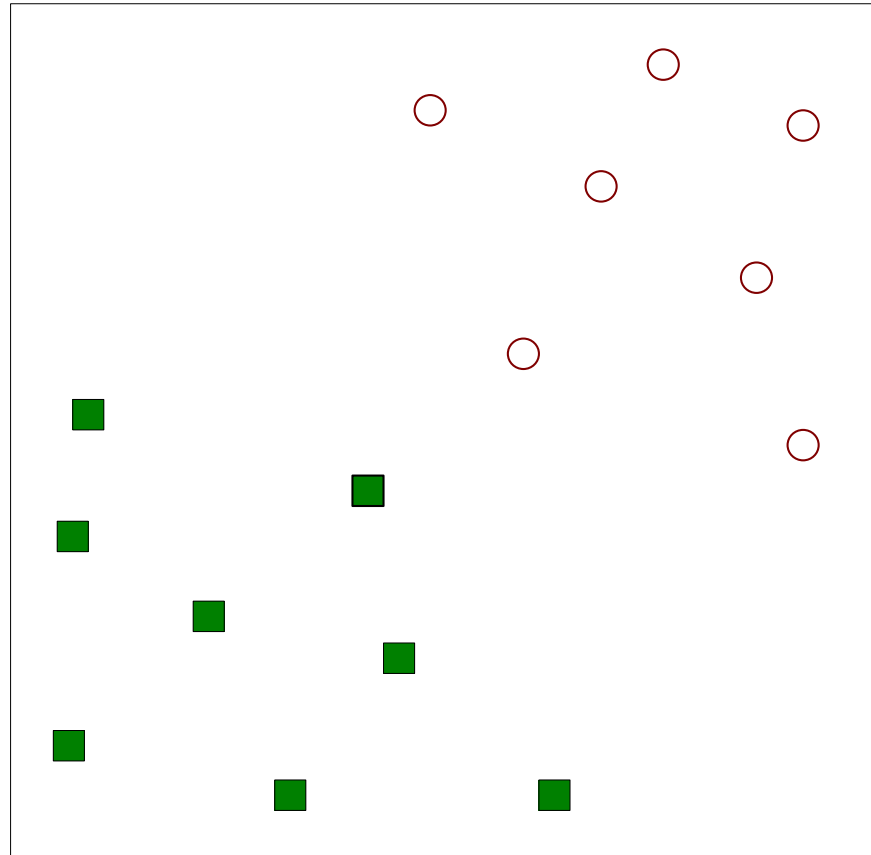
- Scalable both in training set size and attribute number

■ Robustness

- Affected by attribute correlation

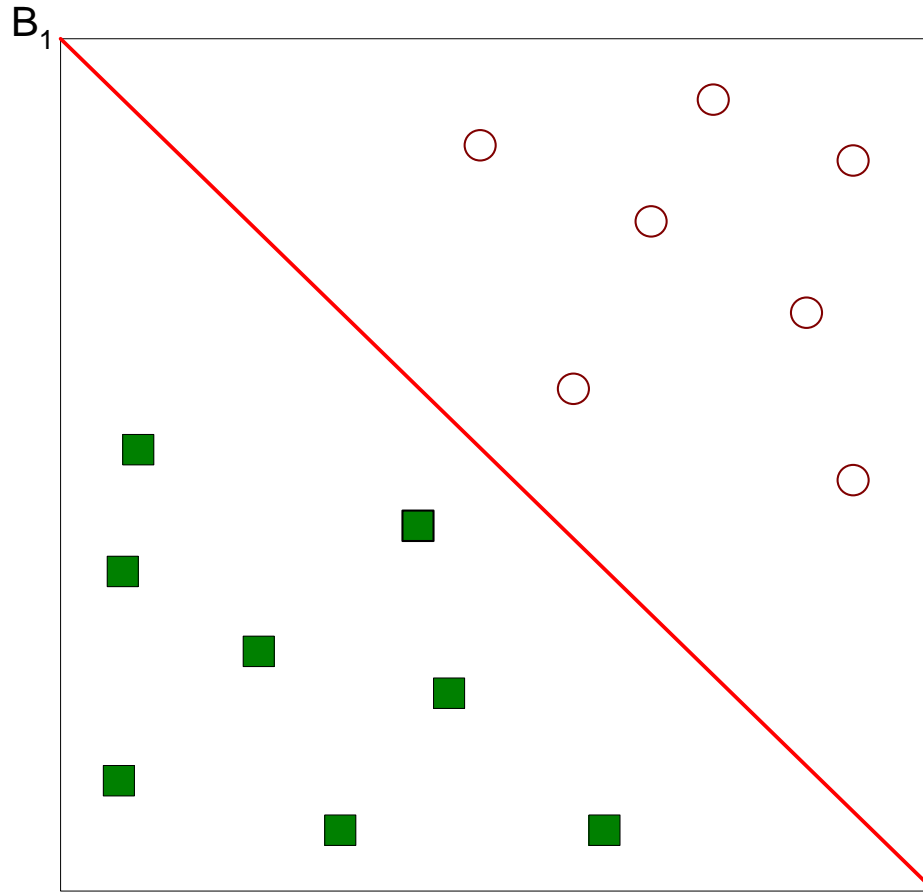
Support Vector Machines

Support Vector Machines



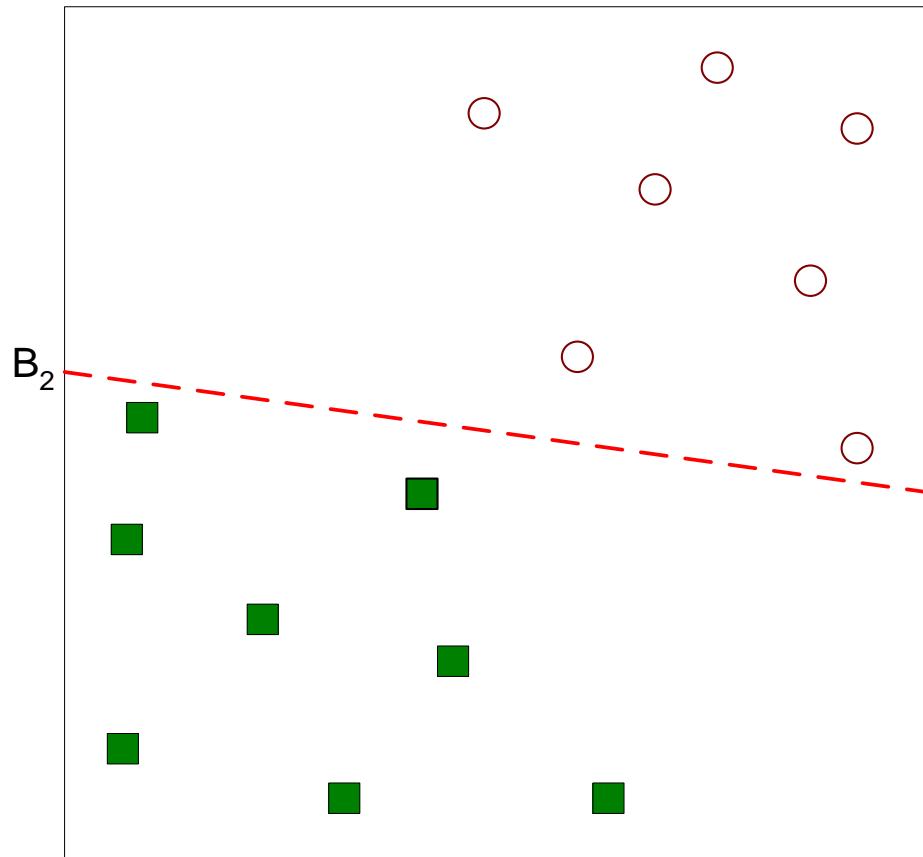
Find a linear hyperplane (decision boundary) that will separate the data

Support Vector Machines



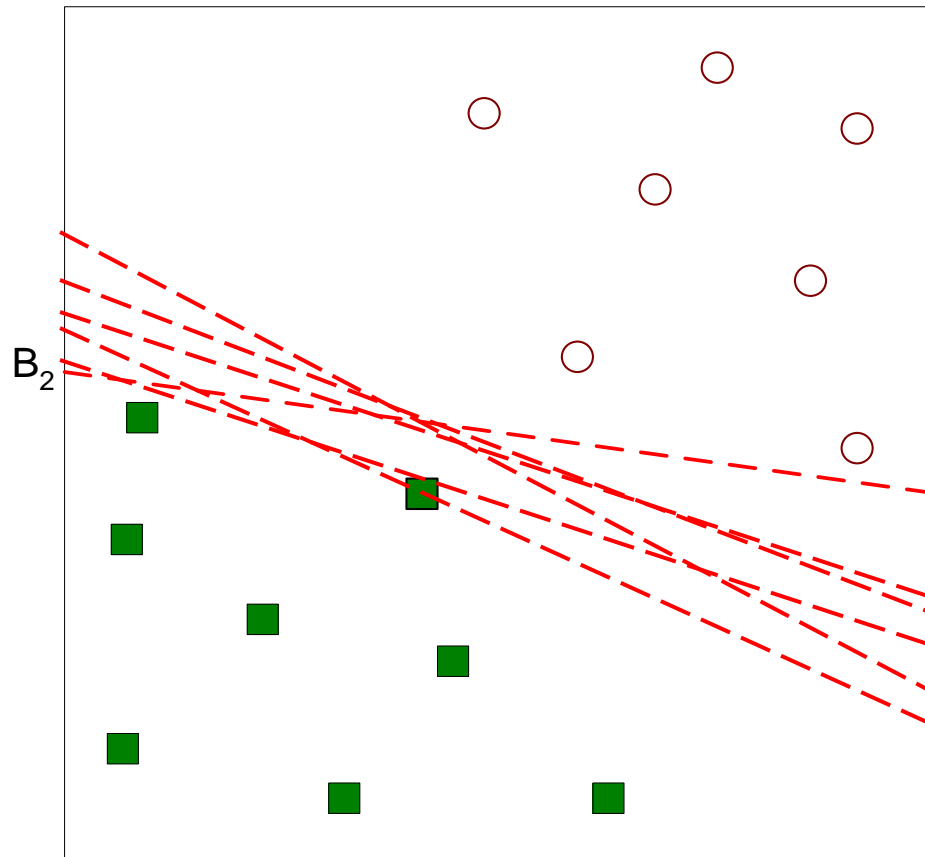
One Possible Solution

Support Vector Machines



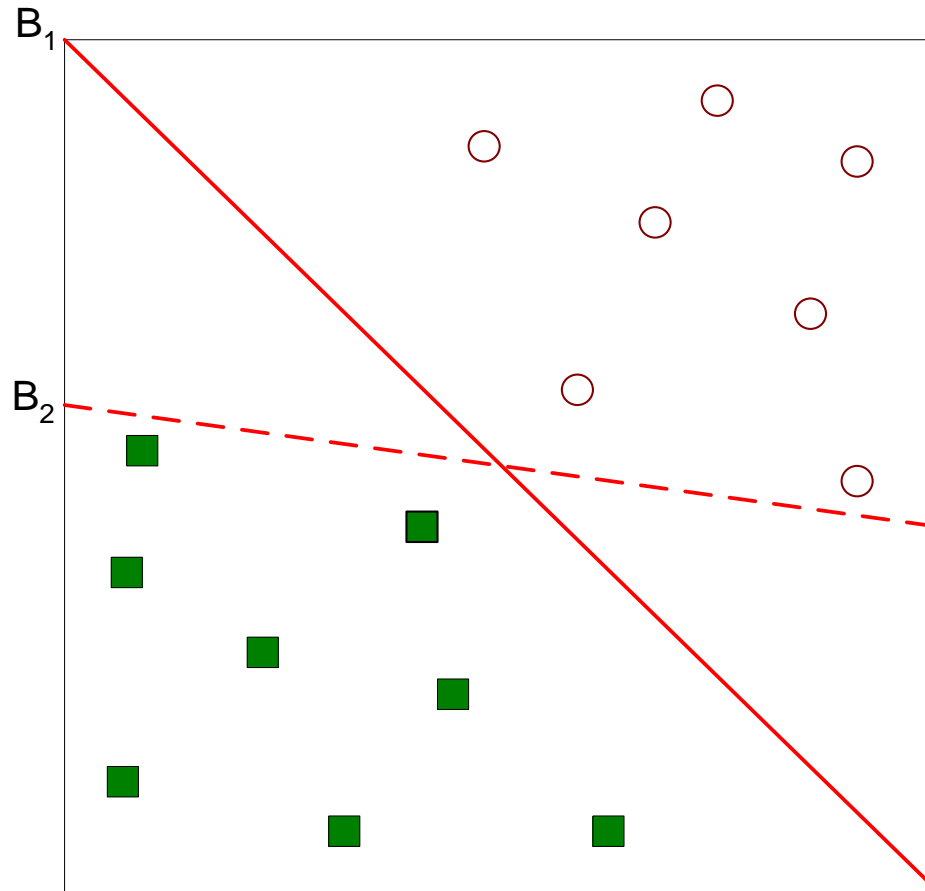
Another possible solution

Support Vector Machines



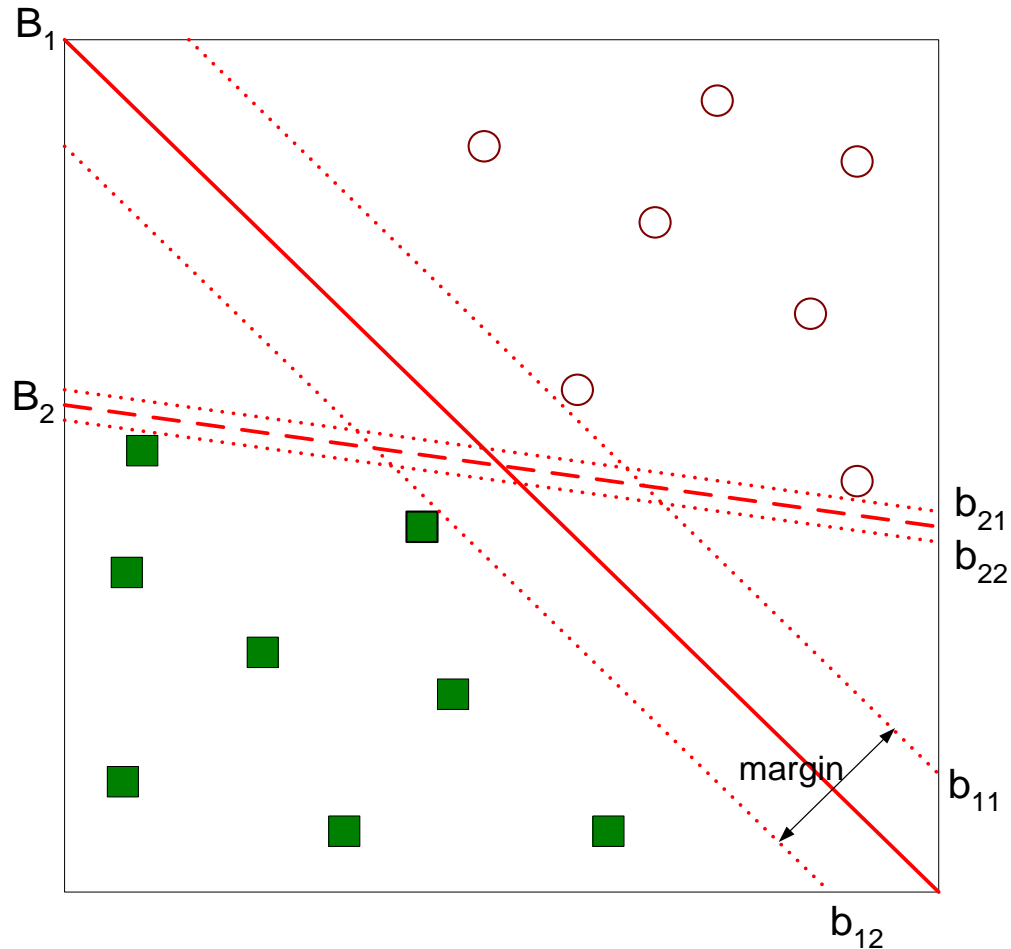
Other possible solutions

Support Vector Machines



Which one is better? B_1 or B_2 ?
How do you define better?

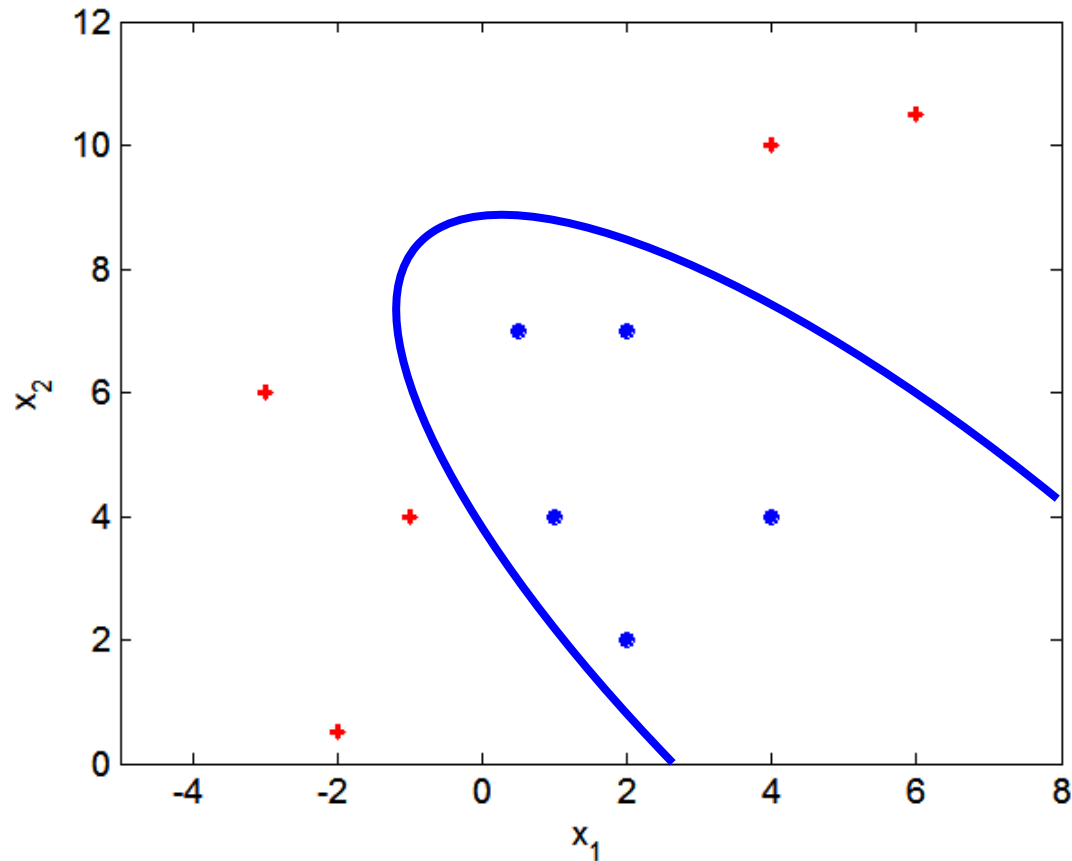
Support Vector Machines



Find hyperplane **maximizes** the margin \Rightarrow B1 is better than B2

Nonlinear Support Vector Machines

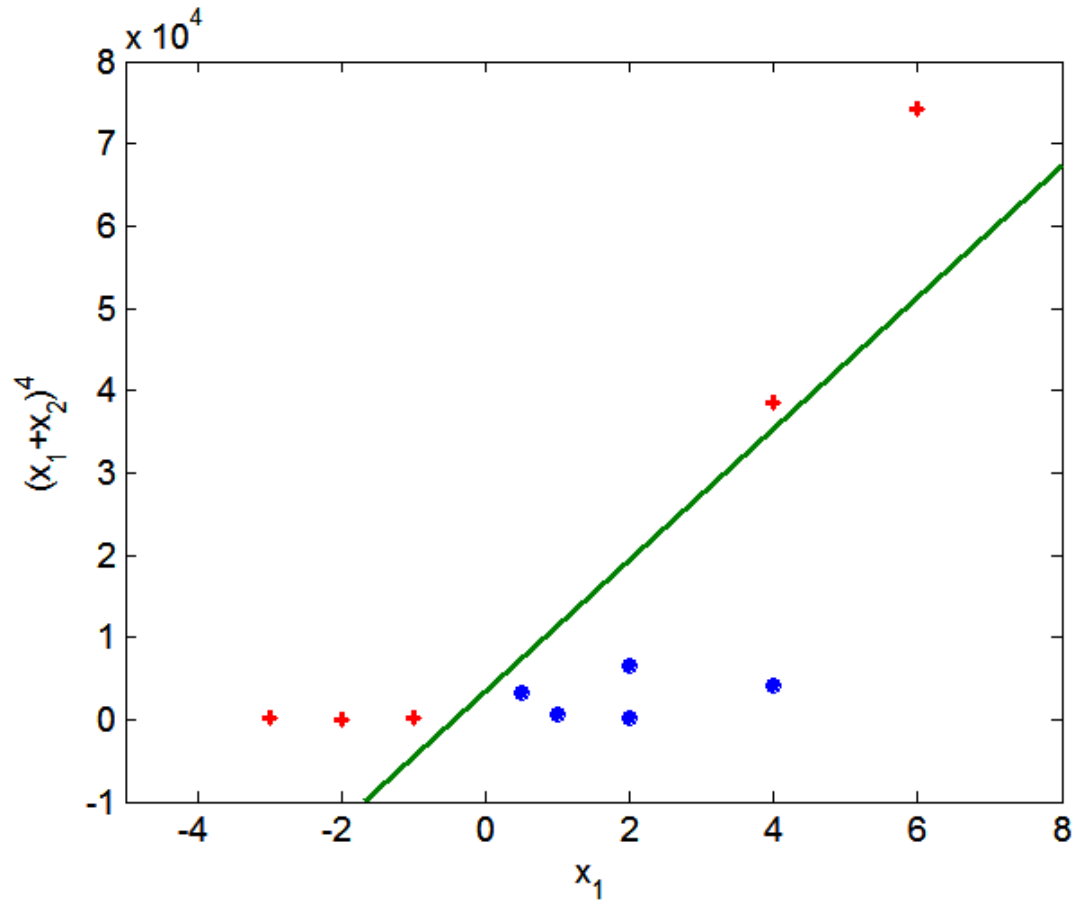
What if decision boundary is not linear?



From: Tan, Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

Nonlinear Support Vector Machines

Transform data into higher dimensional space



From: Tan, Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

Evaluation of Support Vector Machines

Accuracy

Among best performers

Interpretability

Model and prediction are not interpretable

Black box model

Incrementality

Not incremental

■ Efficiency

- Model building requires significant parameter tuning
- Very fast classification

■ Scalability

- Medium scalable both in training set size and attribute number

■ Robustness

- Robust to noise and outliers

Artificial Neural Networks

Elena Baralis

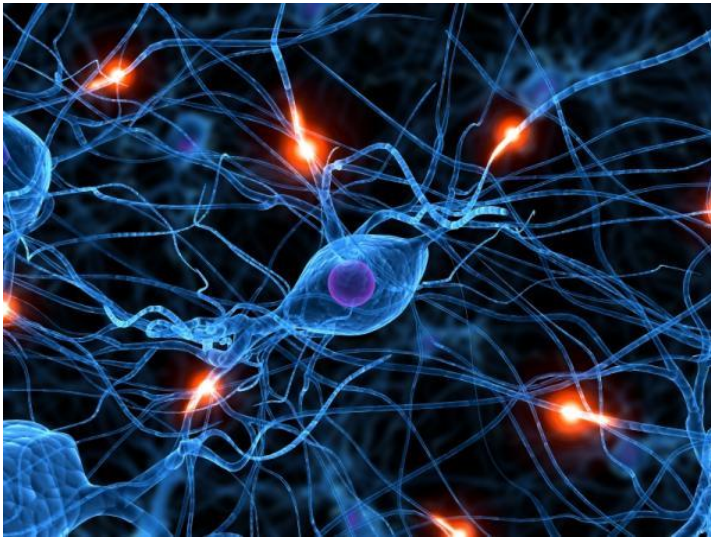
Politecnico di Torino

Artificial Neural Networks

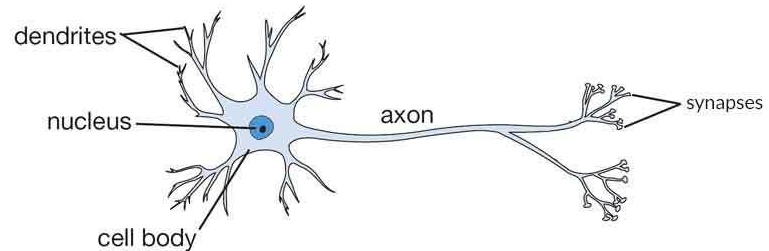
Inspired to the structure of the human brain

Neurons as elaboration units

Synapses as connection network



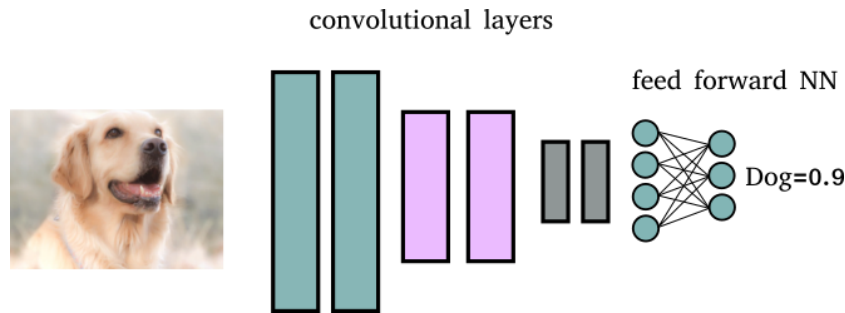
Biological Neuron



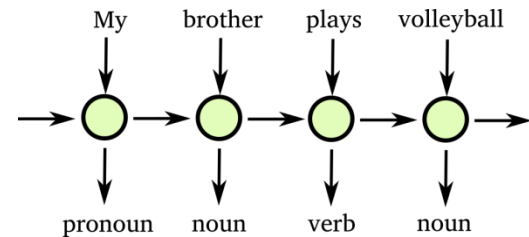
Artificial Neural Networks

Different tasks, different architectures

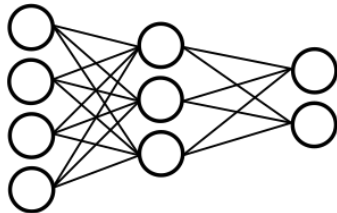
image understanding: convolutional NN (CNN)



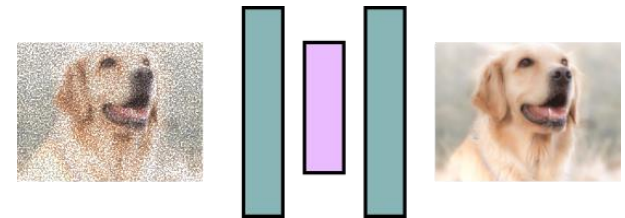
time series analysis: recurrent NN (RNN)



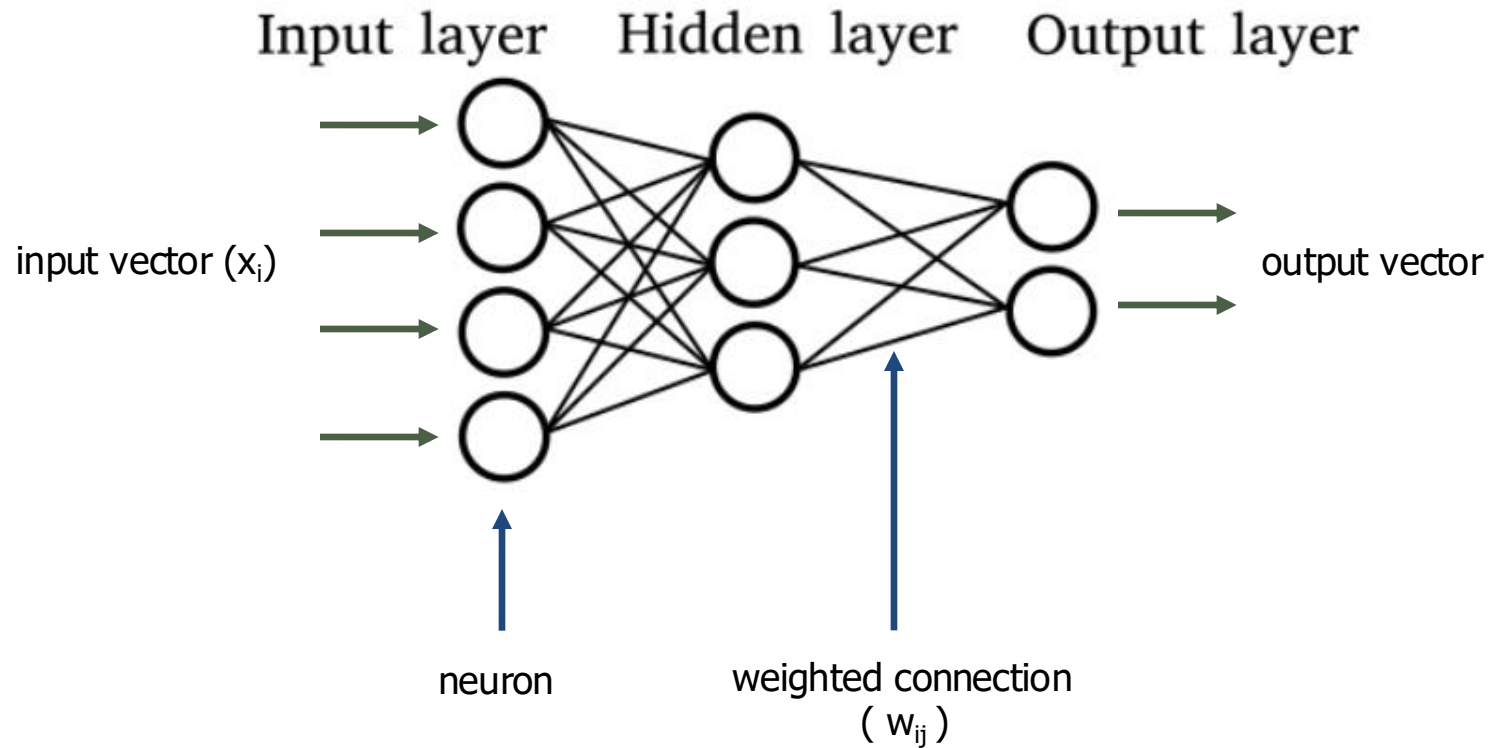
numerical vectors classification: feed forward NN (FFNN)



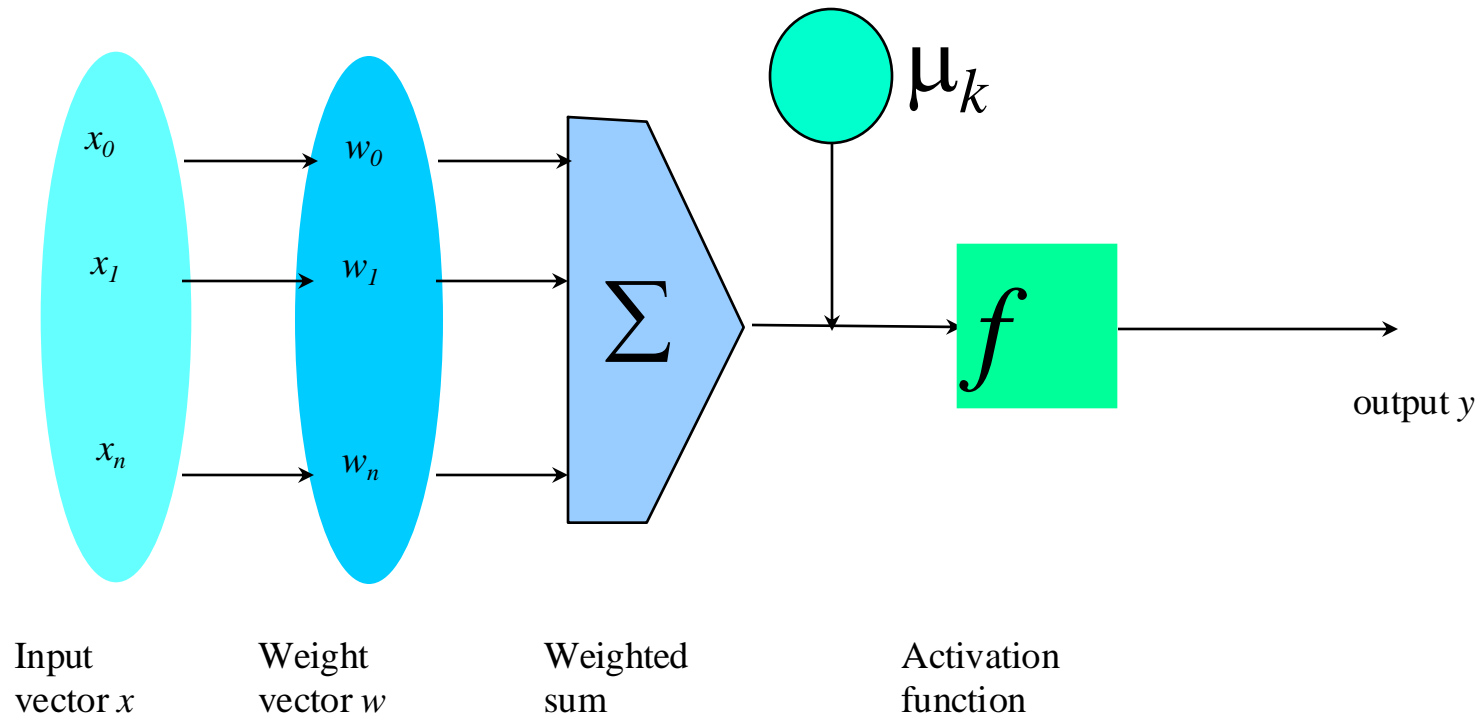
denoising: auto-encoders



Feed Forward Neural Network

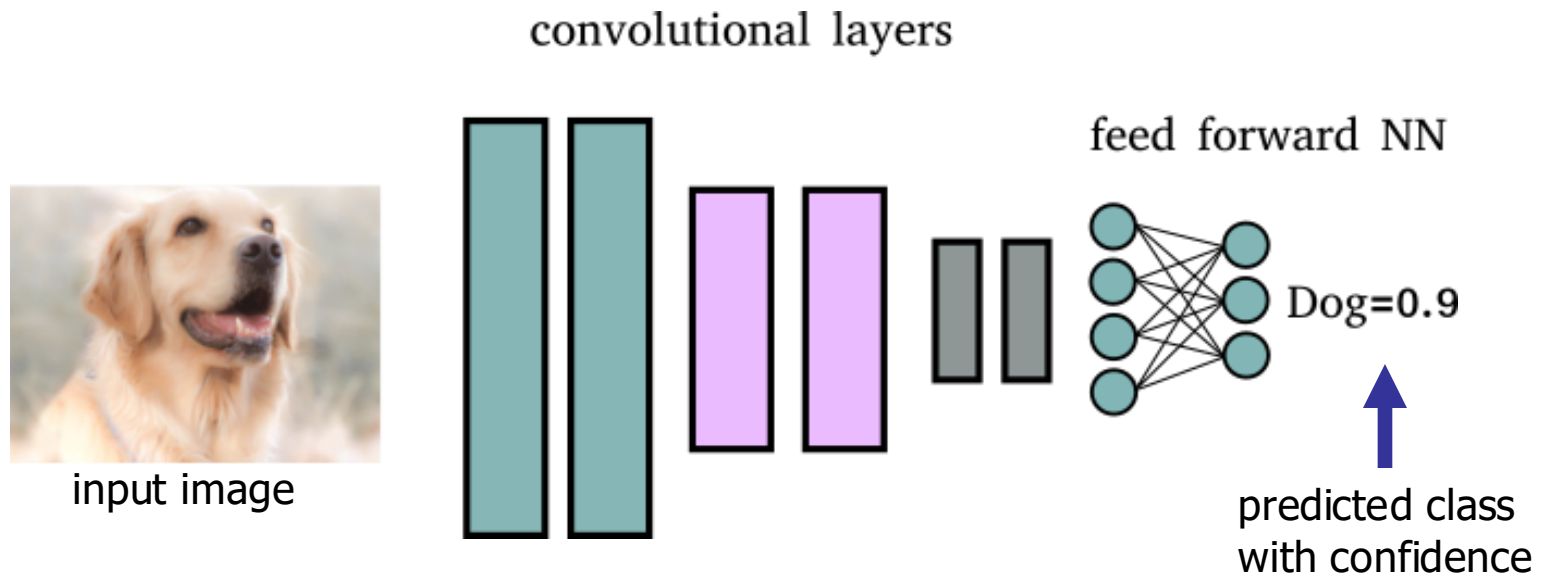


Structure of a neuron



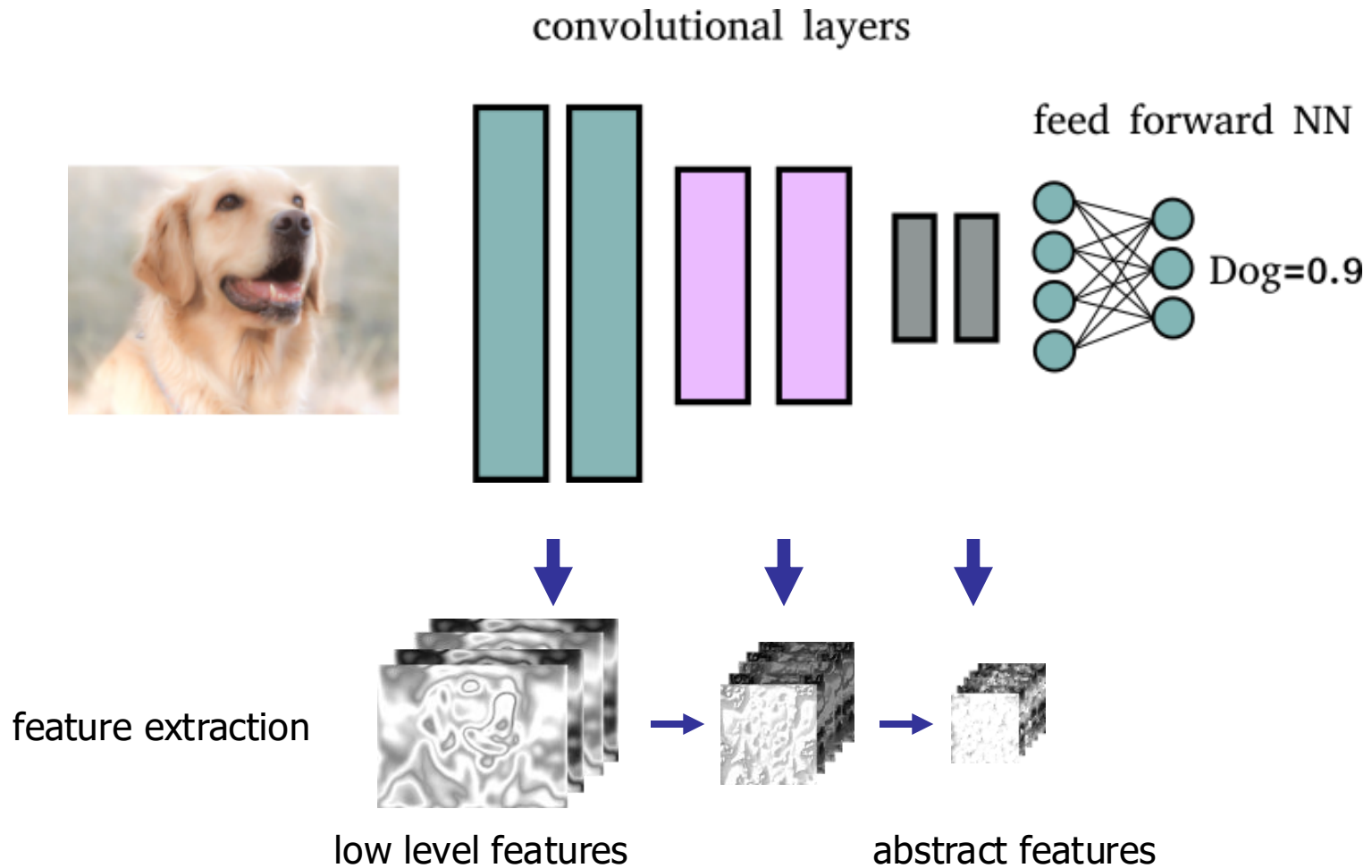
Convolutional Neural Networks

- Allow automatically extracting **features** from images and performing **classification**

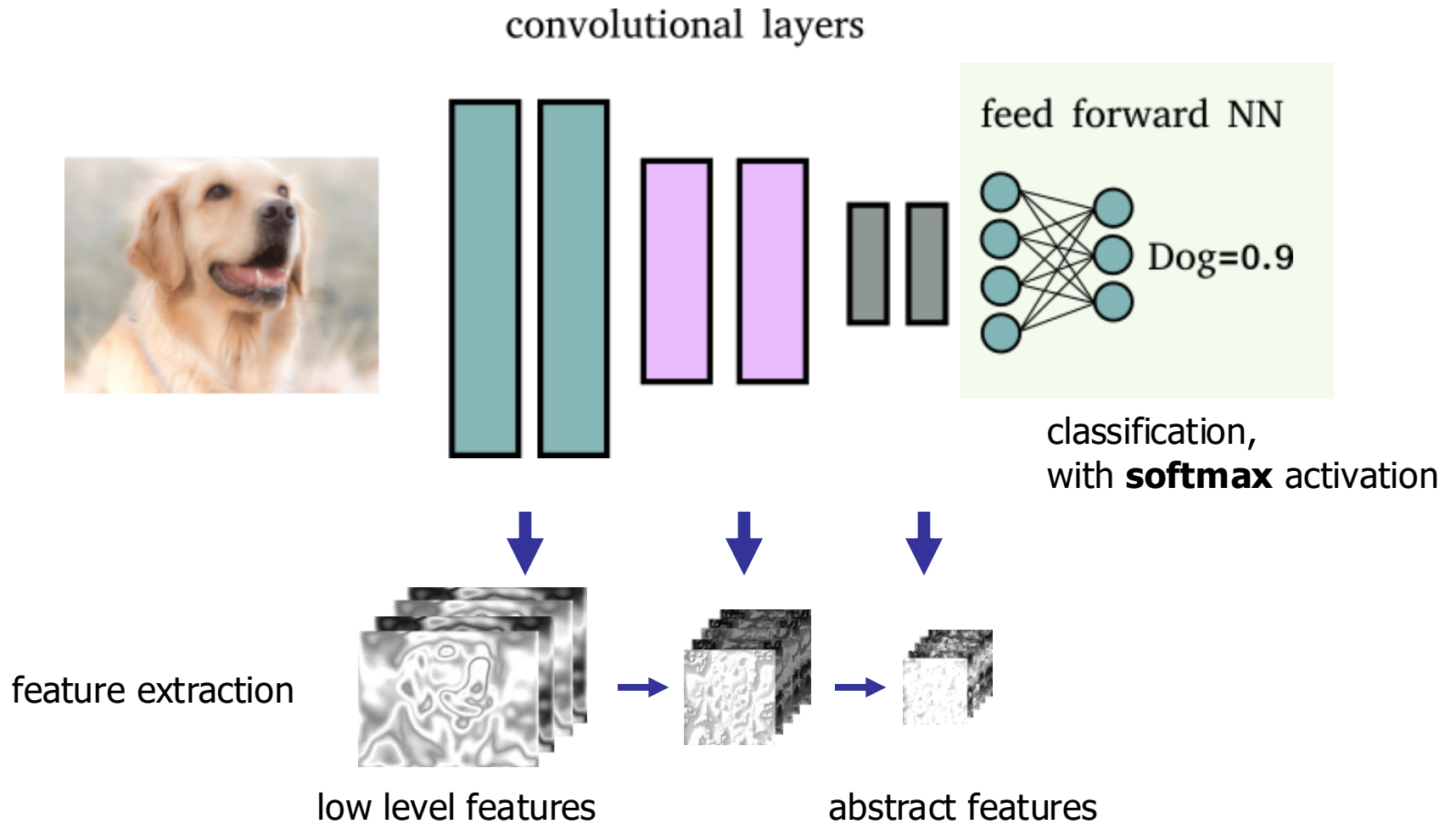


Convolutional Neural Network (CNN) Architecture

Convolutional Neural Networks



Convolutional Neural Networks



Convolutional Neural Networks

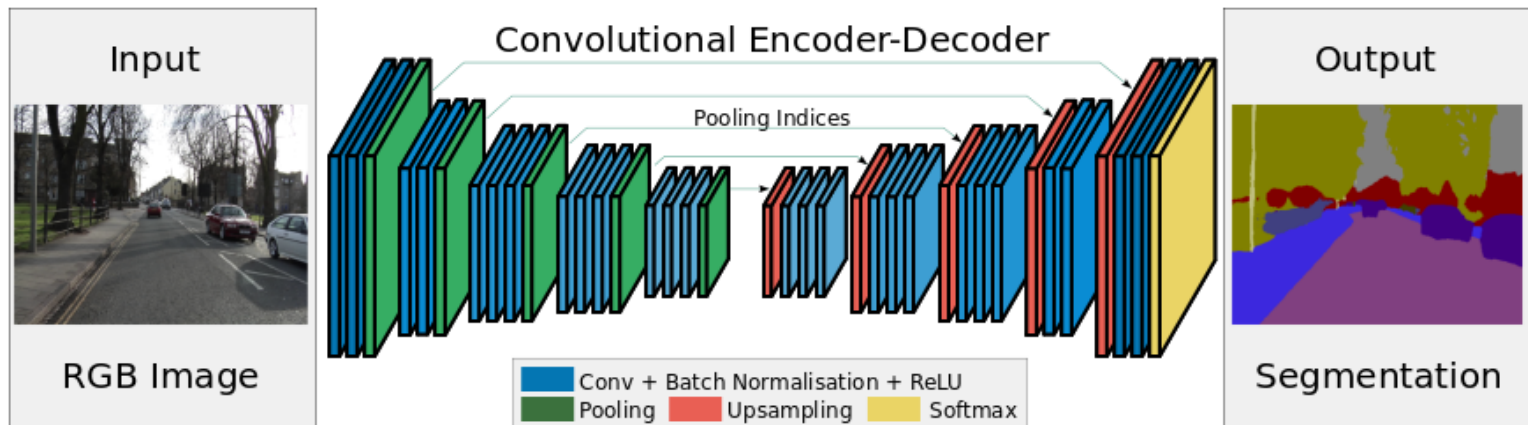
Semantic segmentation CNNs

allow assigning a class to each pixel of the input image

composed of 2 parts

encoder network: convolutional layers to extract abstract features

decoder network: deconvolutional layers to obtain the output image from the extracted features

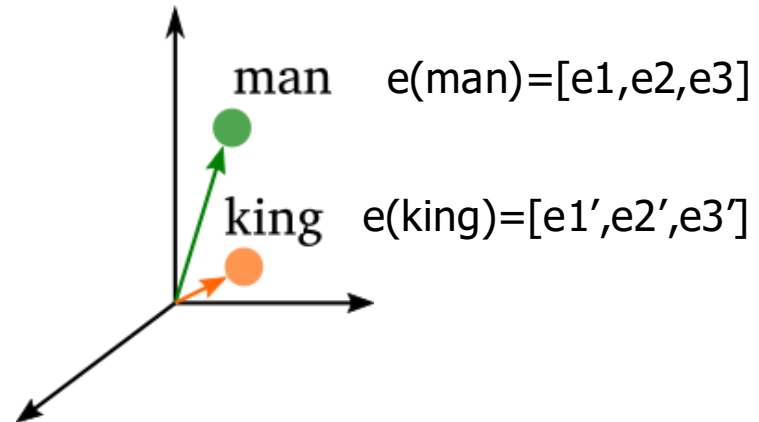
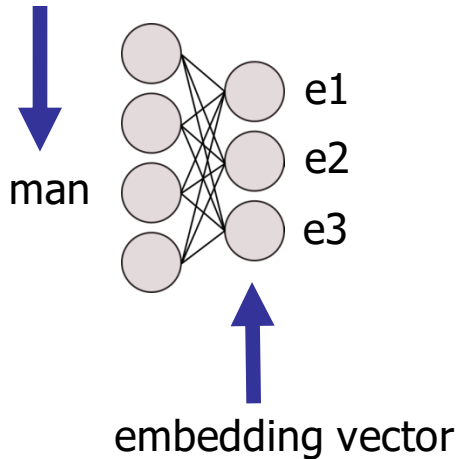


SegNet neural network

Word Embeddings (Word2Vec)

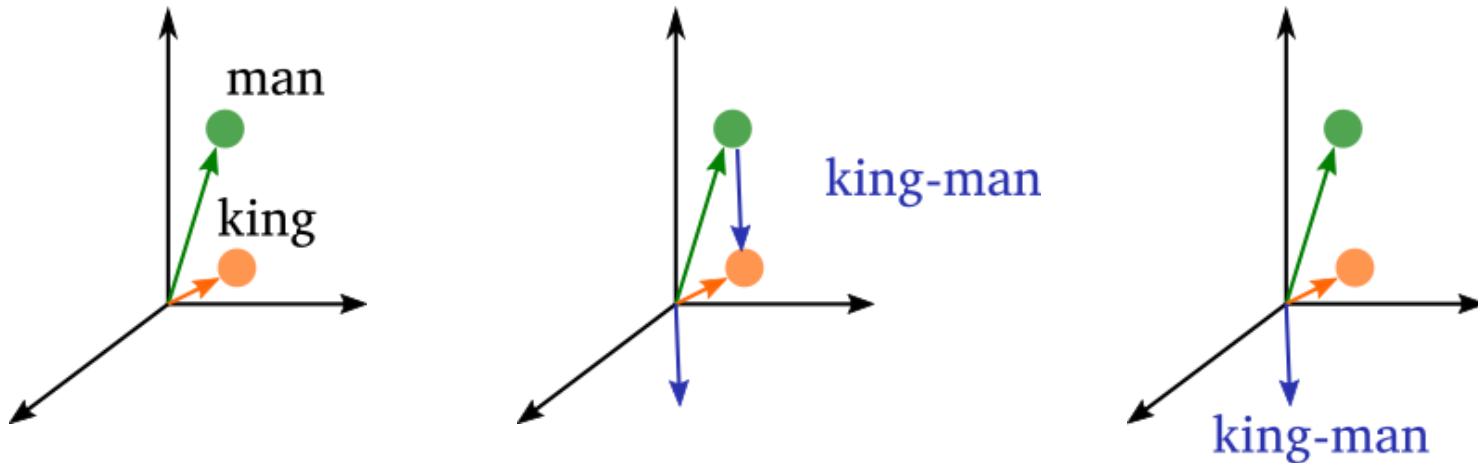
- Word *embeddings* associate words to n-dimensional vectors
 - trained on big text collections to model the word distributions in different sentences and contexts
 - able to capture the *semantic* information of each word
 - words with similar *meaning* share vectors with similar characteristics

input word



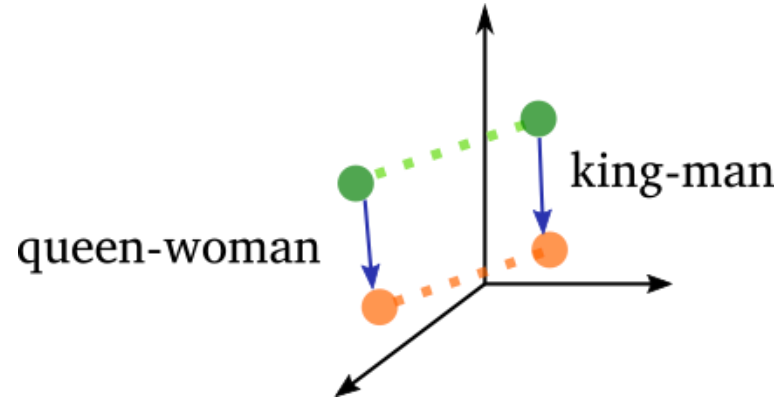
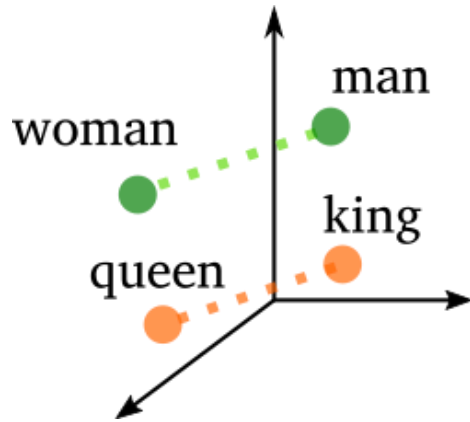
Word Embeddings (Word2Vec)

- Since each word is represented with a vector, operations among words (e.g. difference, addition) are allowed



Word Embeddings (Word2Vec)

- Semantic relationships among words are captured by vector positions



king - man = queen - woman
king - man + woman = queen

Model evaluation

Elena Baralis

Politecnico di Torino

Model evaluation

Methods for performance evaluation

Partitioning techniques for training and test sets

Metrics for performance evaluation

Accuracy, other measures

Techniques for model comparison

ROC curve

Methods for performance evaluation

Objective

reliable estimate of performance

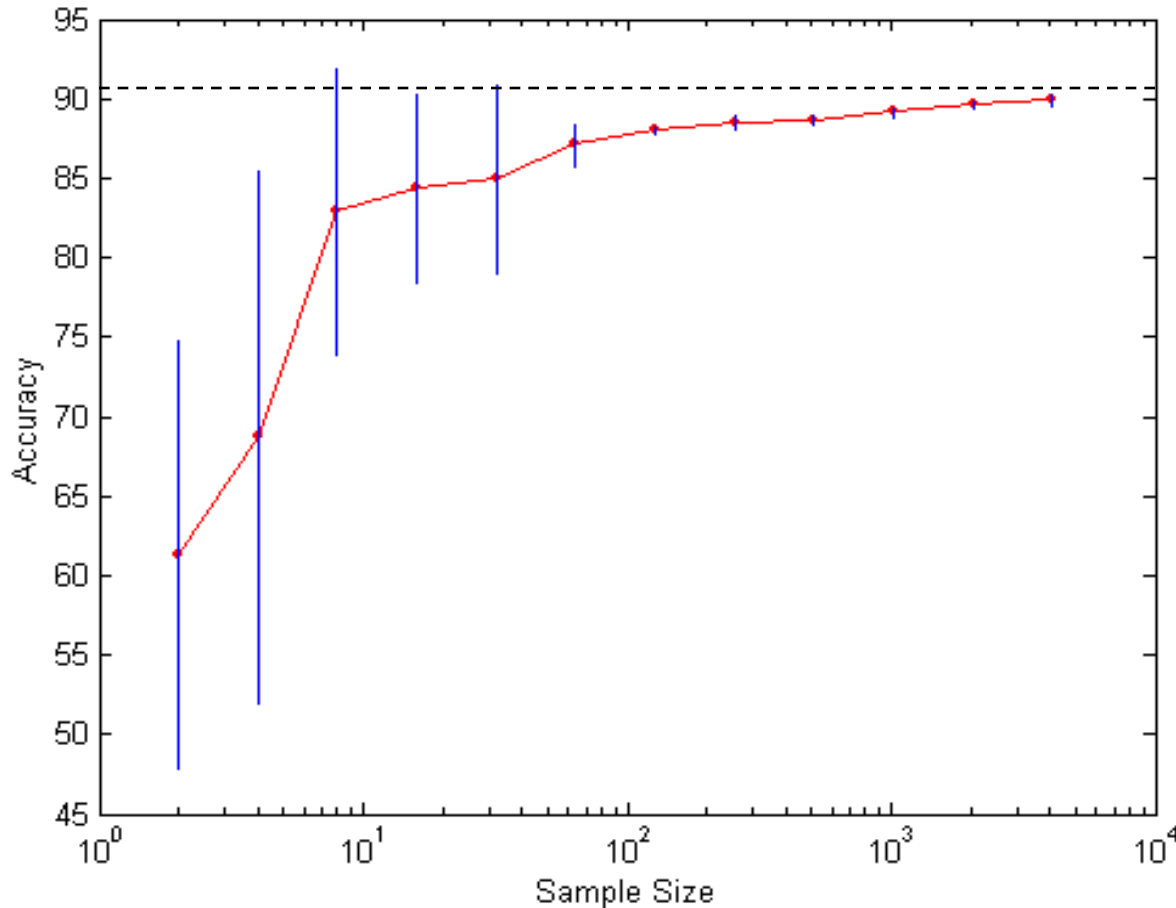
Performance of a model may depend on other factors besides the learning algorithm

Class distribution

Cost of misclassification

Size of training and test sets

Learning curve



- Learning curve shows how accuracy changes with varying training sample size

- Requires a sampling schedule for creating learning curve:

- Arithmetic sampling (Langley, et al)
- Geometric sampling (Provost et al)

Effect of small sample size:

- Bias in the estimate
- Variance of estimate

Partitioning data

Several partitioning techniques

- holdout

- cross validation

Stratified sampling to generate partitions

- without replacement

Bootstrap

- Sampling with replacement

Methods of estimation

Partitioning labeled data for training, validation and test

Several partitioning techniques

- holdout

- cross validation

Stratified sampling to generate partitions

- without replacement

Bootstrap

- Sampling with replacement

Holdout

Fixed partitioning

Typically, may reserve 80% for training, 20% for test

Other proportions may be appropriate, depending on the dataset size

Appropriate for large datasets

may be repeated several times

repeated holdout

Cross validation

Cross validation

partition data into k disjoint subsets (i.e., folds)

k -fold: train on $k-1$ partitions, test on the remaining one

repeat for all folds

reliable accuracy estimation, not appropriate for very large datasets

Leave-one-out

cross validation for $k=n$

only appropriate for very small datasets

Model performance estimation

Model training step

Building a new model

Model validation step

Hyperparameter tuning

Algorithm selection

Model test step

Estimation of model performance

Model performance estimation

Typical dataset size

Training set 60% of labeled data

Validation set 20% of labeled data

Test set 20% of labeled data

Splitting labeled data

Use hold-out to split in
training+validation
test

Use cross validation to split in
training
validation

Metrics for model evaluation

Evaluate the predictive accuracy of a model

Confusion matrix

binary classifier

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

a: TP (true positive)
b: FN (false negative)
c: FP (false positive)
d: TN (true negative)

Accuracy

Most widely-used metric for model evaluation

$$\text{Accuracy} = \frac{\text{Number of correctly classified objects}}{\text{Number of classified objects}}$$

Not always a reliable metric

Accuracy

For a binary classifier

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

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

Limitations of accuracy

Consider a binary problem

Cardinality of Class 0 = 9900

Cardinality of Class 1 = 100

Model

$() \rightarrow \textit{class 0}$

Model predicts everything to be class 0

accuracy is $9900/10000 = 99.0\%$

Accuracy is misleading because the model does not detect any class 1 object

Limitations of accuracy

Classes may have different importance

Misclassification of objects of a given class is more important
e.g., ill patients erroneously assigned to the healthy patients class

Accuracy is not appropriate for
unbalanced class label distribution
different class relevance

Class specific measures

- Evaluate separately for each class C

$$\text{Recall (r)} = \frac{\text{Number of objects correctly assigned to C}}{\text{Number of objects belonging to C}}$$

$$\text{Precision (p)} = \frac{\text{Number of objects correctly assigned to C}}{\text{Number of objects assigned to C}}$$

- Maximize

$$\text{F - measure (F)} = \frac{2rp}{r + p}$$

Class specific measures

- For a binary classification problem
 - on the confusion matrix, for the positive class

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

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

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

ROC (Receiver Operating Characteristic)

Developed in 1950s for signal detection theory to analyze noisy signals

characterizes the trade-off between positive hits and false alarms

ROC curve plots

TPR, True Positive Rate (on the y-axis)

$$\text{TPR} = \text{TP}/(\text{TP}+\text{FN})$$

against

FPR, False Positive Rate (on the x-axis)

$$\text{FPR} = \text{FP}/(\text{FP} + \text{TN})$$

ROC curve

(FPR, TPR)

(0,0): declare everything
to be negative class

(1,1): declare everything
to be positive class

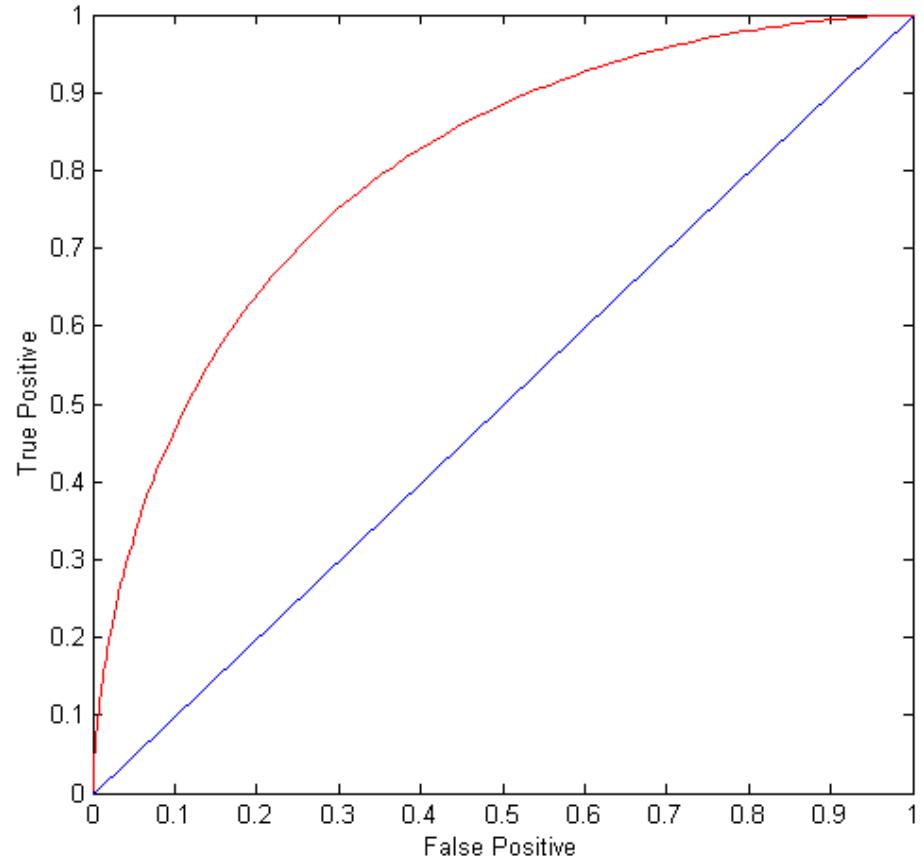
(0,1): ideal

Diagonal line

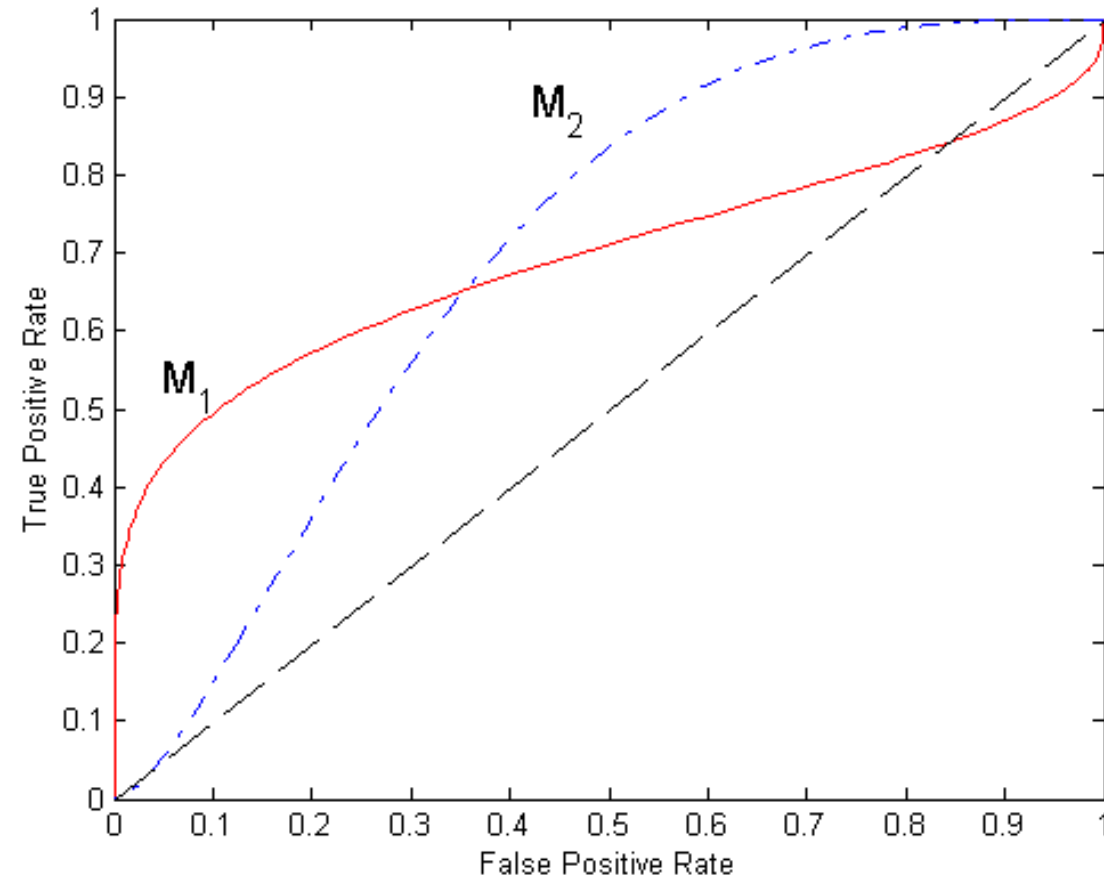
Random guessing

Below diagonal line

prediction is opposite of the tr
class



Using ROC for Model Comparison



- No model consistently outperforms the other
 - M_1 is better for small FPR
 - M_2 is better for large FPR
- Area under ROC curve
 - Ideal
Area = 1.0
 - Random guess
Area = 0.5

Next slides taken from MIT
Course of “Data Science”

There are Three Kinds of Lies

LIES

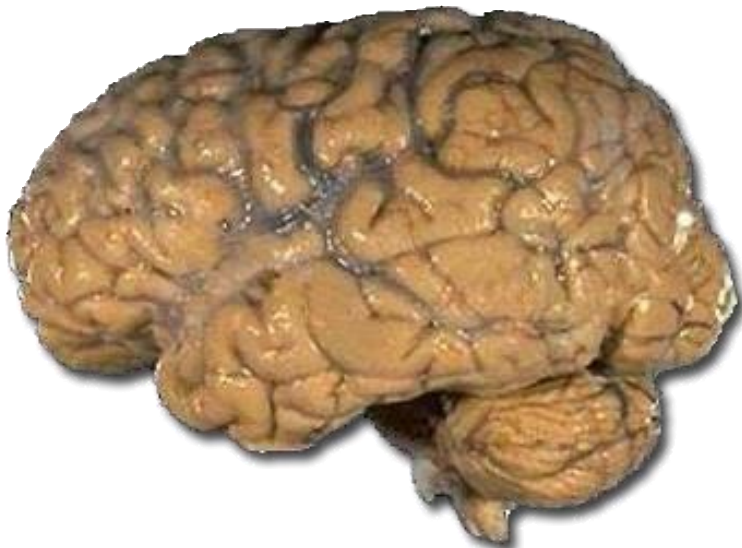
DAMNED LIES

and

STATISTICS

Humans and Statistics

Human Mind



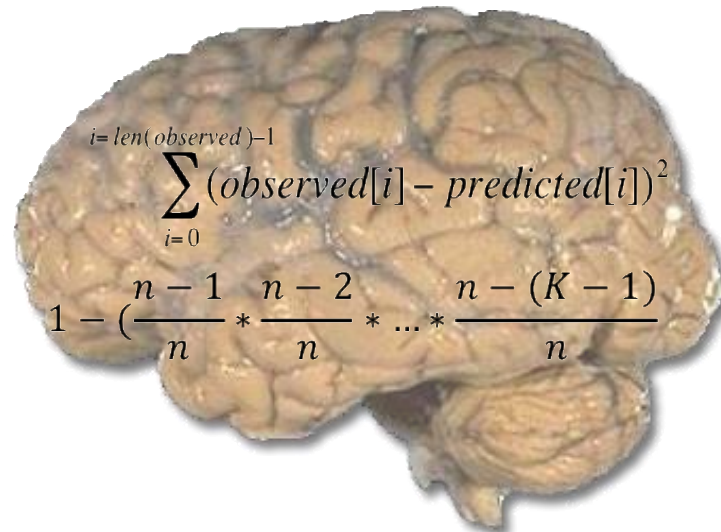
Statistics

$$1 - \left(\frac{n-1}{n} * \frac{n-2}{n} * \dots * \frac{n-(K-1)}{n} \right) \sum_{i=0}^{i=\text{len}(\text{observed})-1} (\text{observed}[i] - \text{predicted}[i])^2$$

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Humans and Statistics

“If you can't prove what you want to prove, demonstrate something else and pretend they are the same thing. In the daze that follows the collision of statistics with the human mind, hardly anyone will notice the difference.” – *Darrell Huff*



Anscombe's Quartet

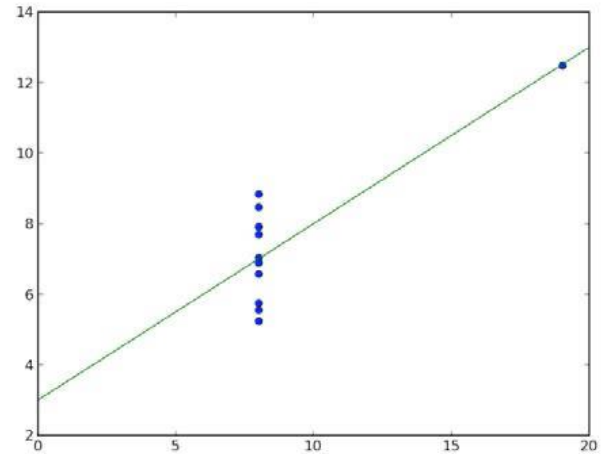
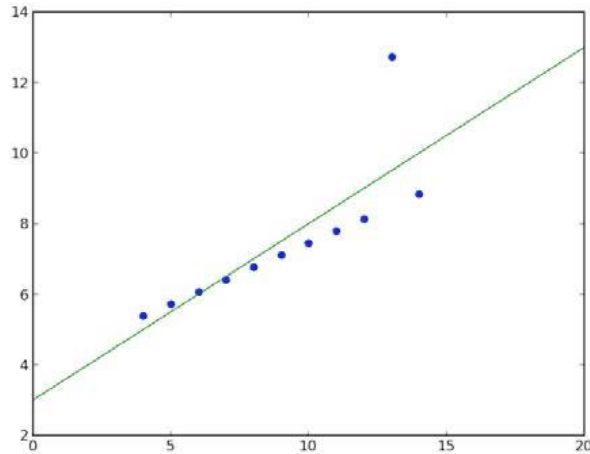
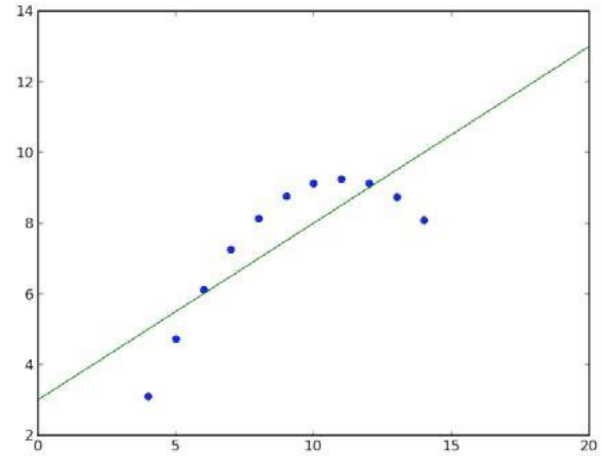
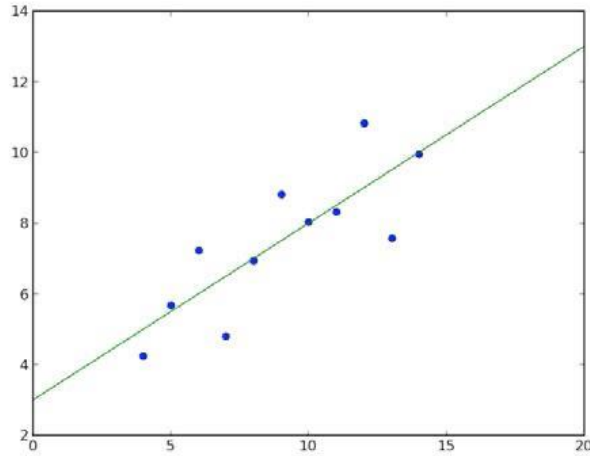
- Four groups each containing 11 x, y pairs

x	y	x	y	x	y	x	y
10.0	8.04	10.0	9.14	10.0	7.46	8.0	6.58
8.0	6.95	8.0	8.14	8.0	6.77	8.0	5.76
13.0	7.58	13.0	8.74	13.0	12.74	8.0	7.71
9.0	8.81	9.0	8.77	9.0	7.11	8.0	8.84
11.0	8.33	11.0	9.26	11.0	7.81	8.0	8.47
14.0	9.96	14.0	8.10	14.0	8.84	8.0	7.04
6.0	7.24	6.0	6.13	6.0	6.08	8.0	5.25
4.0	4.26	4.0	3.10	4.0	5.39	19.0	12.50
12.0	10.84	12.0	9.13	12.0	8.15	8.0	5.56
7.0	4.82	7.0	7.26	7.0	6.42	8.0	7.91
5.0	5.68	5.0	4.74	5.0	5.73	8.0	6.89

Summary Statistics

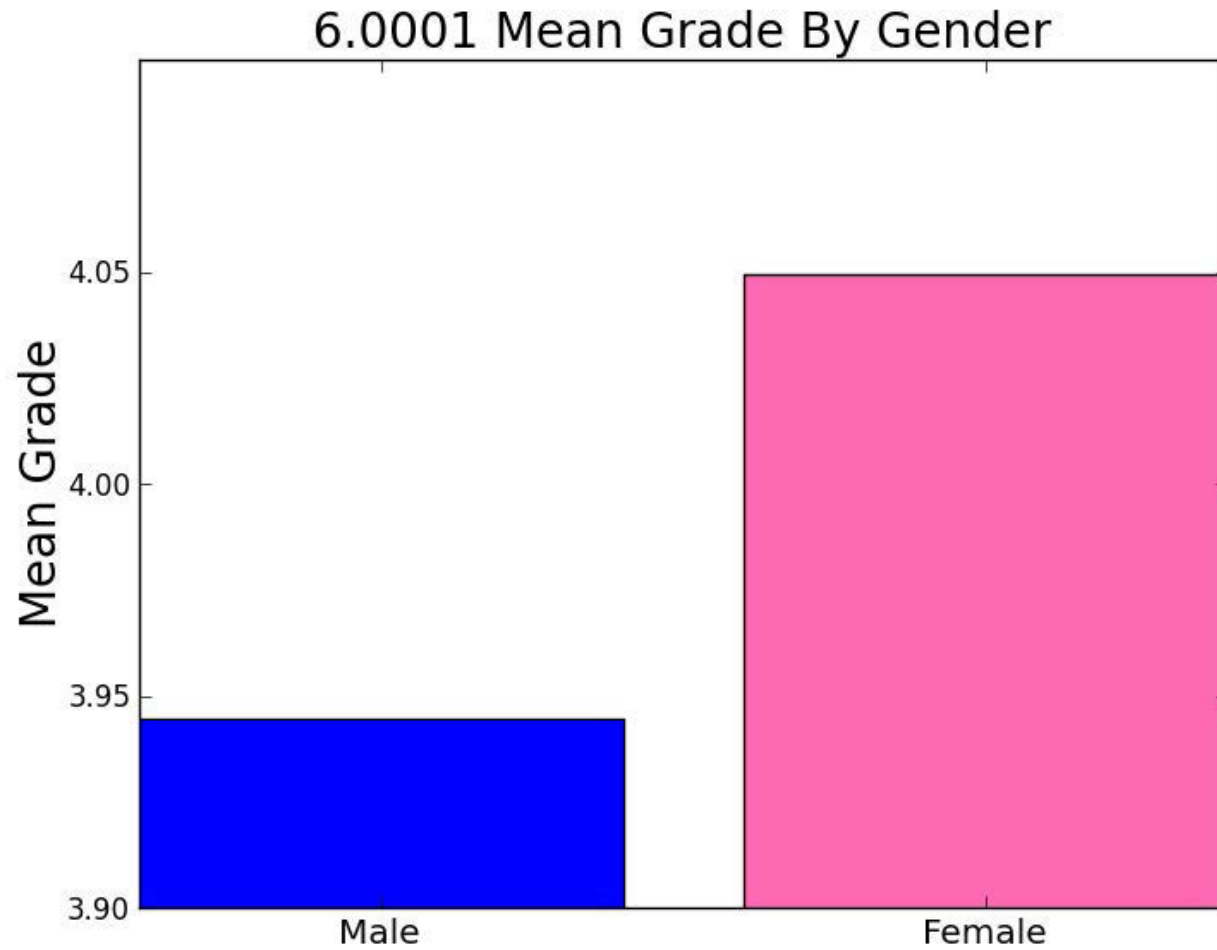
- Summary statistics for groups identical
 - Mean $x = 9.0$
 - Mean $y = 7.5$
 - Variance of $x = 10.0$
 - Variance of $y = 3.75$
 - Linear regression model: $y = 0.5x + 3$
- Are four data sets really similar?

Let's Plot the Data

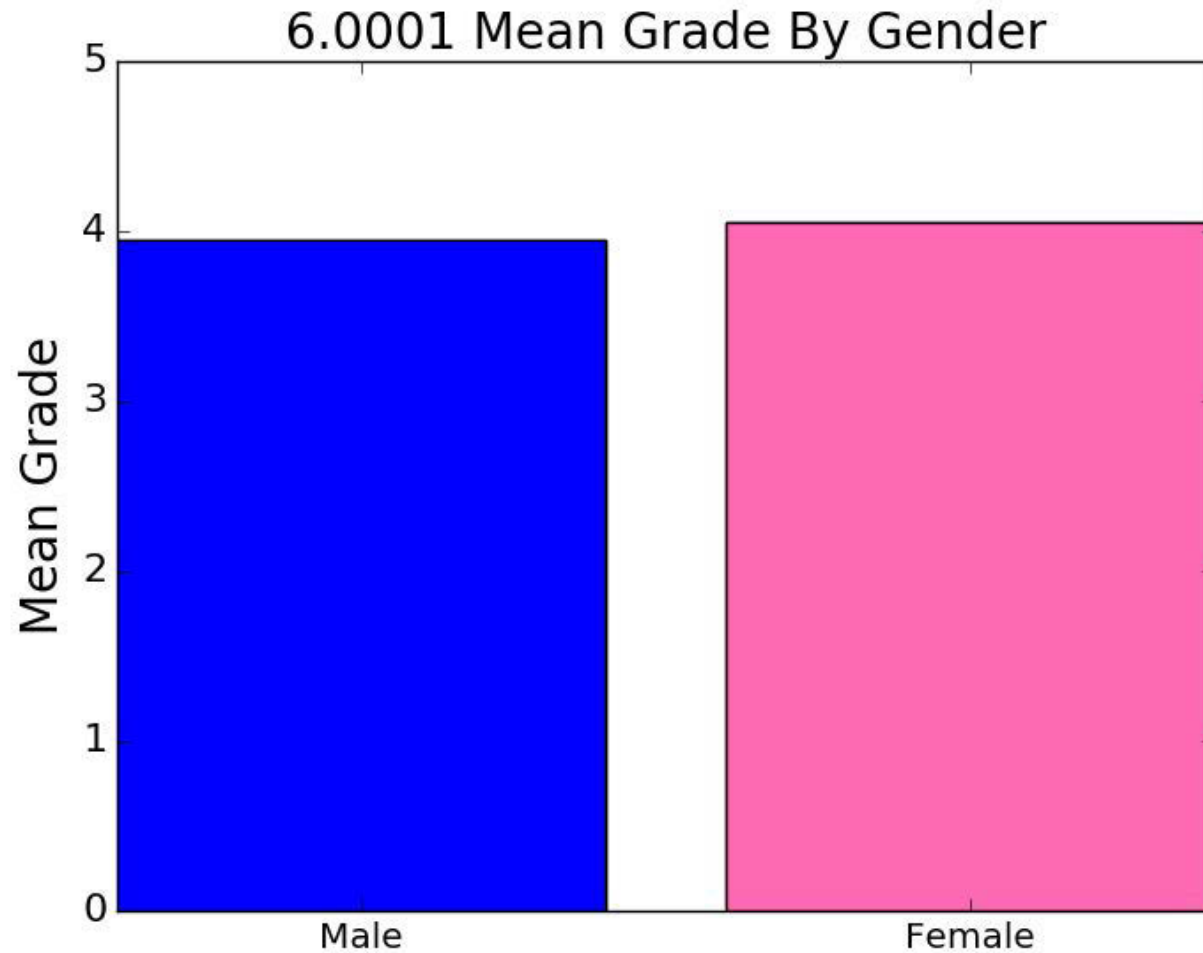


Moral: Statistics about the data is not the same as the data
Moral: Use visualization tools to look at the data itself

Lying with Pictures



Telling the Truth with Pictures



Moral: Look carefully at the axes labels and scales

Lying with Pictures



Moral: Ask whether the things being compared are actually comparable

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Garbage In, Garbage Out

“On two occasions I have been asked [by members of Parliament], ‘Pray, Mr. Babbage, if you put into the machine wrong figures, will the right answers come out?’ I am not able rightly to apprehend the kind of confusion of ideas that could provoke such a question.” – Charles Babbage (1791-1871)

Calhoun's Response to Errors in Data

“there were so many errors they balanced one another, and led to the same conclusion as if they were all correct.”

Was it the case that the measurement errors are unbiased and independent of each of other, and therefore almost identically distributed on either side of the mean?

No, later analysis showed that the errors were not random but systematic.

“it was the census that was insane and not the colored people.” — James Freeman Clarke

Moral: Analysis of bad data can lead to dangerous conclusions.

Sampling

- All statistical techniques are based upon the assumption that by sampling a subset of a population we can infer things about the population as a whole
- As we have seen, *if random sampling is used*, one can make meaningful mathematical statements about the expected relation of the sample to the entire population
- Easy to get random samples in simulations
- Not so easy in the field, where some examples are more convenient to acquire than others

Non-representative Sampling

- “Convenience sampling” not usually random, e.g.,
 - Survivor bias, e.g., course evaluations at end of course or grading final exam in 6.0002 on a strict curve
 - Non-response bias, e.g., opinion polls conducted by mail or online
- When samples not random and independent, we can still do things like computer means and standard deviations, but **we should not draw conclusions from them** using things like the empirical rule and central limit theorem.
- **Moral: Understand how data was collected, and whether assumptions used in the analysis are satisfied. If not, be wary.**