Ludwig-Maximilians-Universität München
Lehrstuhl für Datenbanksysteme und Data Mining
Prof. Dr. Thomas Seidl

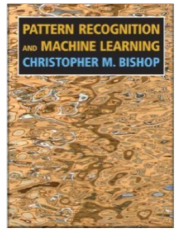
# Knowledge Discovery and Data Mining I

Winter Semester 2018/19

# Agenda

# Additional Literature for this Chapter

Christopher M. Bishop: *Pattern Recognition and Machine Learning*. Springer, Berlin 2006.



# Introduction: Example

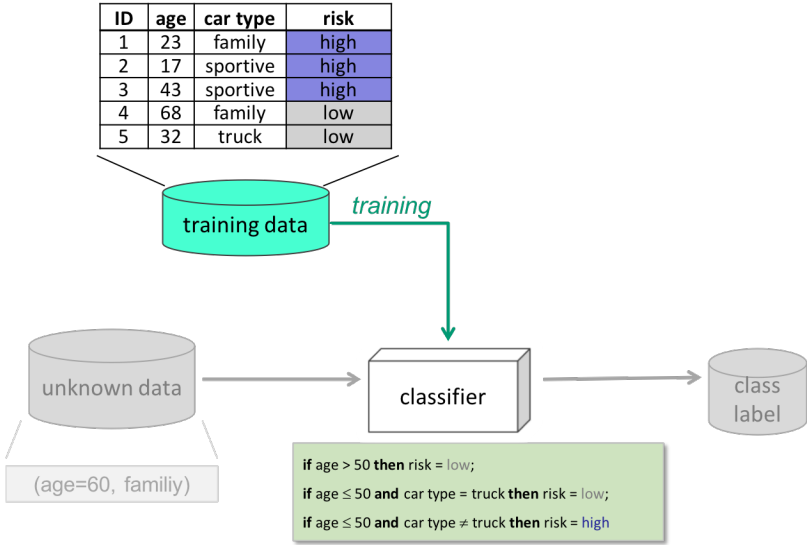
- Training data

| age | car_type | max_speed | risk |
|---|---|---|---|
| 23 | family | 180 | high |
| 17 | sportive | 240 | high |
| 43 | sportive | 246 | high |
| 68 | family | 183 | low |
| 32 | truck | 110 | low |

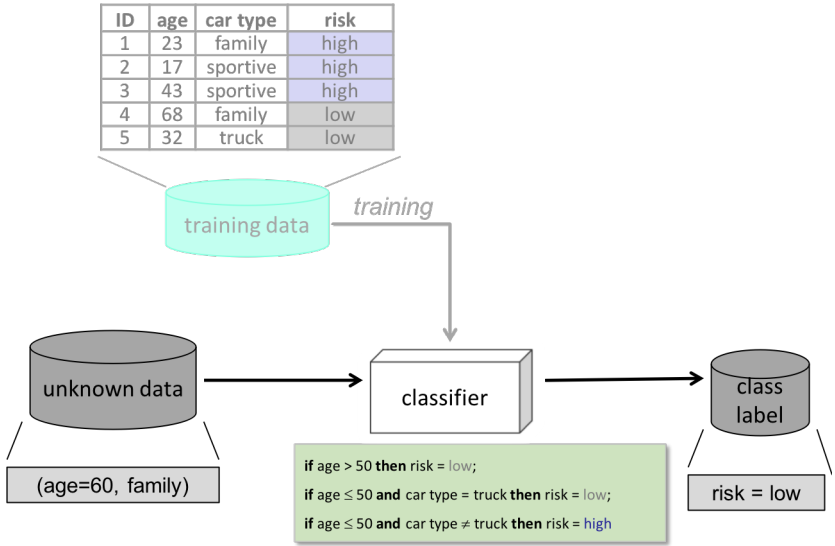
- Simple classifier

**if** age $>$ 50 **then** risk $=$ low
**if** age $\leq$ 50 **and** car type $=$ truck **then** risk $=$ low
**if** age $\leq$ 50 **and** car type $\neq$ truck **then** risk $=$ high

# Classification: Training Phase (Model Construction)



# Classification: Prediction Phase (Application)



# Classification

*The systematic assignment of new observations to known categories according to criteria learned from a training set.*

## Formal Setup

- A *classifier* $K$ for a *model* $M(\theta)$ is a function $K_{M(\theta)} : D \to Y$, where
  - $D$: data space
    - Often $d$-dim. space with attributes $a_1, \ldots, a_d$ (not necessarily a vector space)
    - Some other space, e.g. metric space
  - $Y = \{y_1, \ldots, y_k\}$: set of $k$ distinct *class labels*
  - $O \subseteq D$: set of *training objects* $o$ with known class labels $y \in Y$
- *Classification*: Application of classifier $K$ on objects from $D \setminus O$
- Model $M(\theta)$ is the "type" of the classifier, and $\theta$ are the model parameters
- *Supervised learning*: find/learn optimal parameters $\theta$ for $M(\theta)$ given $O$

# Supervised vs. Unsupervised Learning

## Unsupervised Learning (clustering)

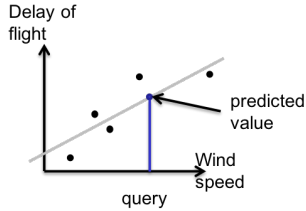
- The class labels of training data are unknown
- Given a set of measurements, observations, etc. with the aim of establishing the existence of classes or clusters in the data
  - Classes (=clusters) are to be determined

## Supervised Learning (classification)

- Supervision: The training data (observations, measurements, etc.) are accompanied by labels indicating the class of the observations
  - Classes are known in advance (a priori)
- New data is classified based on information extracted from the training set

# Numerical Prediction

- Related problem to classification: numerical prediction
  - Determine the numerical value of an object
  - Method: e.g., regression analysis
  - Example: Prediction of flight delays




- Numerical prediction is *different* from classification
  - Classification refers to predict categorical class label
  - Numerical prediction models continuous-valued functions
- Numerical prediction is *similar* to classification
  - First, construct a model
  - Second, use model to predict unknown value
  - Major method for numerical prediction is regression:
    - Linear and multiple regression
    - Non-linear regression

# Goals for this Section

1. Introduction of different classification models
2. Learning techniques for these models

| age | car_type | max_speed | risk |
|---|---|---|---|
| 23 | family | 180 | high |
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| 43 | sportive | 246 | high |
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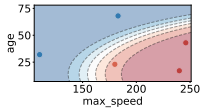
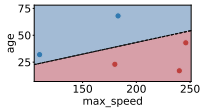
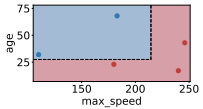


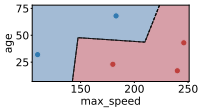

Bayes classifier




Linear classifier




Decision tree




$k$-NN classifier

# Quality Measures for Classifiers

- Classification accuracy or classification error (complementary)
- Compactness of the model
  - Decision tree size, number of decision rules, ...
- Interpretability of the model
  - Insights and understanding of the data provided by the model
- Efficiency
  - Time to generate the model (training time)
  - Time to apply the model (prediction time)
- Scalability for large databases
  - Efficiency in disk-resident databases
- Robustness
  - Robust against noise or missing values

# Evaluation of Classifiers: Notions

- Using training data to build a classifier and to estimate the model's accuracy may result in misleading and overoptimistic estimates
  - $\rightsquigarrow$ Overspecialization of the learning model to the training data
- *Train-and-Test*: Decomposition of labeled data set $O$ into two partitions
  - Training data is used to train the classifier
    - Construction of the model by using information about the class labels
  - Test data is used to evaluate the classifier
    - Temporarily hide class labels, predict them anew and compare with original class labels
- Train-and-Test is not applicable if the set of objects for which the class label is known is very small

# Evaluation of Classifiers: Cross Validation

## $m$-fold Cross Validation

- Decompose data set evenly into $m$ subsets of (nearly) equal size
- Iteratively use $(m-1)$ partitions for training data and the remaining single partition as test data
- Combine the $m$ classification accuracy values to an overall classification accuracy

## Leave-one-out: Special case of cross validation ($m = n$)

- For each of the objects $o$ in the data set $O$:
  - Use set $O \setminus \{o\}$ as training set
  - Use the singleton set $\{o\}$ as test set
  - Compute classification accuracy by dividing the number of correct predictions through the database size $|O|$
- Particularly well applicable to nearest-neighbor classifiers

# Quality Measures: Accuracy and Error

- Let $K$ be a classifier
- Let $C(o)$ denote the correct class label of an object $o$
- Measure the quality of $K$:
  - Predict the class label for each object $o$ from a data set $T \subseteq O$
  - Determine the fraction of correctly predicted class labels

## Classification Accuracy of $K$

$$G_T(K) = \frac{|\{o \in T \mid K(o) = C(o)\}|}{|T|}$$

## Classification Error of $K$

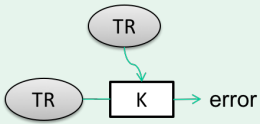
$$F_T(K) = \frac{|\{o \in T \mid K(o) \neq C(o)\}|}{|T|}$$
$$= 1 - G_T(K)$$

# Quality Measures: Accuracy and Error

- Let $K$ be a classifier
- Let $TR \subseteq O$ be the training set: Used to build the classifier
- Let $TE \subseteq O$ be the test set: Used to test the classifier

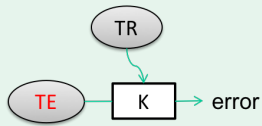
## Resubstitution Error of $K$

$$F_{TR}(K) = \frac{|\{o \in TR \mid K(o) \neq C(o)\}|}{|TR|}$$




## (True) Classification Error of $K$

$$F_{TE}(K) = \frac{|\{o \in TE \mid K(o) \neq C(o)\}|}{|TE|}$$



# Quality Measures: Confusion Matrix

- Results on the test set: Confusion matrix

| | | classified as ... | | | | |
|---|---|---|---|---|---|---|
| | | class 1 | class 2 | class 3 | class 4 | class 5 |
| correct label | class 1 | 35 | 1 | 1 | 1 | 4 |
| | class 2 | 0 | 31 | 1 | 1 | 5 |
| | class 3 | 3 | 1 | 50 | 1 | 2 |
| | class 4 | 1 | 0 | 1 | 10 | 2 |
| | class 5 | 3 | 1 | 9 | 16 | 13 |

(correctly classified in green)

- Based on the confusion matrix, we can compute several accuracy measures, including:
  - Classification Accuracy/Error
  - Precision and Recall

# Quality Measures: Precision and Recall

## Recall

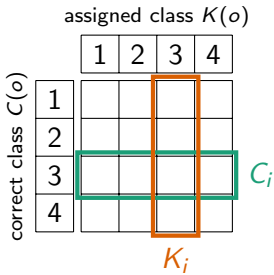
Fraction of test objects of class $i$, which have been identified correctly.

$$Recall_{TE}(K, i) = \frac{|\{o \in C_i \mid K(o) = C(o)\}|}{|C_i|}$$

## Precision

Fraction of test objects assigned to class $i$, which have been identified correctly.

$$Precision_{TE}(K, i) = \frac{|\{o \in C_i \mid K_i(o) = C(o)\}|}{|K_i|}$$



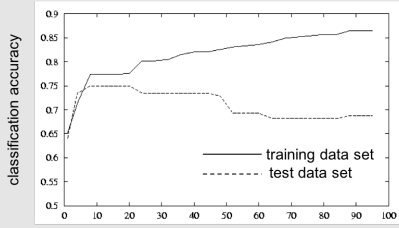

$$C_i = \{o \in TE \mid C(o) = i\}$$
$$K_i = \{o \in TE \mid K(o) = i\}$$

# Overfitting

## Characterization of Overfitting

The classifier adapts too closely to the training dataset and may therefore fail to accurately predict class labels for test objects unseen during training.

## Example: Decision Tree




**Generalization** ← ***classifier*** → **specialization**

"overfitting"

# Overfitting

## Overfitting

- Occurs when the classifier is too optimized to the (noisy) training data
- As a result, the classifier yields worse results on the test data set
- Potential reasons:
  - Bad quality of training data (noise, missing values, wrong values)
  - Different statistical characteristics of training data and test data

## Overfitting Avoidance

- Removal of *noisy/erroneous/contradicting* training data
- Choice of an appropriate *size* of the training set
  - Not too small, not too large
- Choice of appropriate sample
  - Sample should describe all aspects of the domain and not only parts of it

# Underfitting

## Underfitting

- Occurs when the classifiers model is too simple, e.g. trying to separate classes linearly that can only be separated by a quadratic surface
- Happens seldomly

$\rightsquigarrow$ *Trade-off*: Usually one has to find a good balance between over- and underfitting.

# Agenda

# Bayes Classification

- Probability based classification
  - Based on likelihood of observed data, estimate explicit probabilities for classes
  - Classify objects depending on costs for possible decisions and the probabilities for the classes
- Incremental
  - Likelihood functions built up from classified data
  - Each training example can incrementally increase/decrease the probability that a hypothesis (class) is correct
  - Prior knowledge can be combined with observed data.
- Good classification results in many applications

# Bayes' Theorem

## Probability Theory

- Conditional probability: $P(A \mid B) = \frac{P(A \wedge B)}{P(B)}$ ("prob. of A given B")
- Product Rule: $P(A \wedge B) = P(A \mid B) \cdot P(B)$

## Bayes' Theorem

- $P(A \wedge B) = P(A \mid B) \cdot P(B)$
- $P(B \wedge A) = P(B \mid A) \cdot P(A)$
- Since $P(A \wedge B) = P(B \wedge A)$, $P(A \mid B) \cdot P(B) = P(B \mid A) \cdot P(A)$, and thus

$$P(A \mid B) = \frac{P(B \mid A) \cdot P(A)}{P(B)}$$

# Bayes Classifier

- Bayes' rule: $P(c_j \mid x) = \frac{P(x|c_j) \cdot P(c_j)}{p(x)}$ for object $x$ and class $c_j \in \mathcal{C}$.
- We are interested in maximizing this, i.e.

$$\underset{c_j \in \mathcal{C}}{\operatorname{argmax}} \left(P(c_j \mid x)\right) = \underset{c_j \in \mathcal{C}}{\operatorname{argmax}} \left( \frac{P(x \mid c_j) \cdot P(c_j)}{p(x)} \right) \overset{(*)}{=} \underset{c_j \in \mathcal{C}}{\operatorname{argmax}} \left(P(x \mid c_j) \cdot P(c_j)\right)$$

  where $(*)$ assumes the value of $p(x)$ is constant and hence does not change the result.
- Final decision rule:

$$K(x) = c_{\text{max}} = \underset{c_j \in \mathcal{C}}{\operatorname{argmax}} \left(P(x \mid c_j) \cdot P(c_j)\right)$$

- But how to obtain $P(c_j)$ and $P(x \mid c_j)$.

# Bayes Classifier: Density Estimation

## A-Priori Class Probabilities

Estimate the a-priori probabilities $P(c_j)$ of classes $c_j \in \mathcal{C}$ by using the observed relative frequency of the individual class labels $c_j$ in the training set, i.e.,

$$P(c_j) = \frac{N_{c_j}}{N}$$

## Conditional Probabilities

- *Non-parametric* methods: Kernel methods Parzen's window, Gaussian kernels, etc.
- *Parametric* methods, e.g.
  - Single Gaussian distribution: Computed by maximum likelihood estimators (MLE)
  - *Mixture* models: e.g. Gaussian Mixture Model computed by EM algorithm

# Bayes Classifier: Density Estimation

**Problem**

Curse of dimensionality often lead to problems in high dimensional data $\rightsquigarrow$ Density functions become too uninformative

**Solution**

- Dimensionality reduction
- Usage of statistical independence of single attributes (extreme case: naïve Bayes)

# Naïve Bayes Classifier

## Assumptions

- Objects are given as $d$-dimensional vectors, $x = (x_1, \ldots, x_d)$
- For any given class $c_j$ the attribute values $x_i$ are conditionally independent, i.e.

$$P(x_1, \ldots, x_d \mid c_j) = \prod_{i=1}^{d} P(x_i \mid c_j) = P(x_1 \mid c_j) \cdot \ldots \cdot P(x_d \mid c_j)$$

## Decision Rule

$$K_{\text{naïve}}(x) = \operatorname*{argmax}_{c_j \in \mathcal{C}} \left( P(c_j) \cdot \prod_{i=1}^{d} P(x_i \mid c_j) \right)$$

# Naïve Bayes Classifier

## Categorical Attribute $x_i$

$P(x_i \mid c_j)$ can be estimated as the relative frequency of samples having value $v_i$ as the $i$th attribute in class $c_j$ in the training set.

## Continuous Attribute $x_i$

$P(x_i \mid c_j)$ can, for example, be estimated through a Gaussian distribution determined by $\mu_{ij}, \sigma_{ij}$.

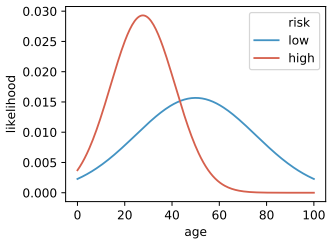
$\rightsquigarrow$ Computationally easy in both cases.

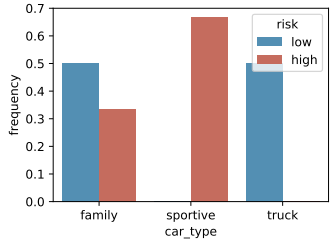
# Naïve Bayes Classifier: Example

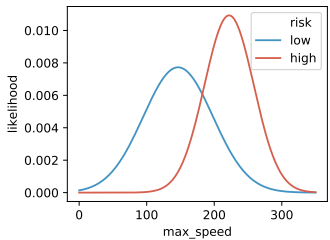
| age | car_type | max_speed | risk |
|---|---|---|---|
| 23 | family | 180 | high |
| 17 | sportive | 240 | high |
| 43 | sportive | 246 | high |
| 68 | family | 183 | low |
| 32 | truck | 110 | low |

## Model Setup

- $Age \sim N(\mu, \sigma^2)$ (normal distribution)
- $car\_type \sim$ relative frequencies
- $max\_speed \sim N(\mu, \sigma^2)$ (normal distribution)



# Naïve Bayes Classifier: Example (cont'd)

## Query

$q = (age = 60; car\_type = family; max\_speed = 190)$

## Example

We have:

- $P(high) = \frac{3}{5}$
- $\mu_{age,high} = \frac{83}{3}, \sigma^2_{age,high} = \frac{1112}{3} \implies P(age = 60 \mid high) \approx 0.00506$
- $P(car\_type = family \mid high) = \frac{1}{3}$
- $\mu_{max\_speed,high} = 222, \sigma^2_{max\_speed,high} = 2664 \implies P(max\_speed = 190 \mid high) \approx 0.00638$

and hence

$$\begin{aligned} P(high)P(q \mid high) &= P(high)P(age = 60 \mid high)P(car\_type = family \mid high)P(max\_speed = 190 \mid high) \\ &\approx 6.45166 \cdot 10^{-6} \end{aligned}$$

Analogously, we obtain $P(low)P(q \mid low) = 15.72290 \cdot 10^{-6} \implies K_{\ddot{\text{naive}}}(q) = low$.

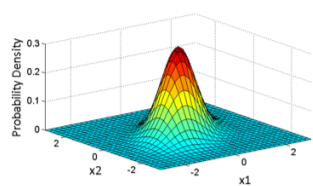
# Bayesian Classifier

- Assuming dimensions of $x = (x_1, \ldots, x_d)$ are *not* independent
- Assume multivariate normal distribution (i.e. Gaussian)

$$P(x \mid C_j) = \frac{1}{\sqrt{(2\pi)^d \det(\Sigma_j)}} \exp\left(-\frac{1}{2}(x - \mu_j)\Sigma_j^{-1}(x - \mu_j)^T\right)$$

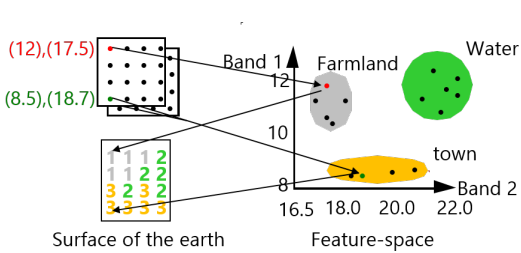
with

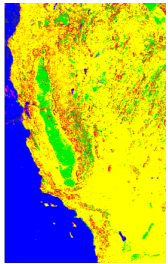
- $\mu_j$: mean vector of class $C_j$
- $\Sigma_j$ is the $d \times d$ covariance matrix
- $\det(\Sigma_j)$ is the determinant of $\Sigma_j$, and $\Sigma_j^{-1}$ its inverse



# Example: Interpretation of Raster Images

- Scenario: Automated interpretation of raster images
  - Take an image from a certain region (in $d$ different frequency bands, e.g., infrared, etc.)
  - Represent each pixel by $d$ values: $(x_1, \ldots, x_d)$
- Basic assumption: different surface properties of the earth ("landuse") follow a characteristic reflection and emission pattern



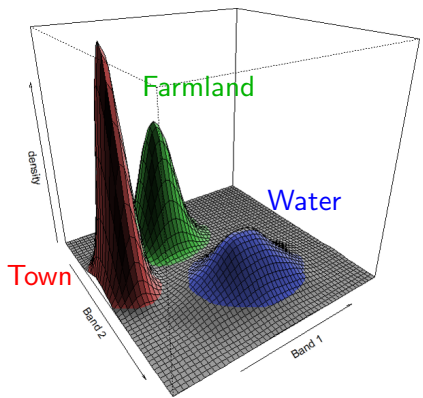



# Example: Interpretation of Raster Images

Application of the Bayes classifier:

- Estimation of the $P(x \mid c)$ without assumption of conditional independence
- Assumption of $d$-dimensional normal (= Gaussian) distributions for the value vectors of a class

Probability of class membership



# Example: Interpretation of Raster Images

## Method

Estimate the following measures from training data

- $\mu_j$: $d$-dimensional mean vector of all feature vectors of class $C_j$
- $\Sigma_j$: $d \times d$ covariance matrix of class $C_j$

## Problems

- if likelihood of respective class is very low
- if several classes share the same likelihood

$\rightsquigarrow$ Mitigate e.g. by applying some minimum likelihood threshold; do not classify regions below.

# Bayesian Classifiers: Discussion

## Pro

- High classification accuracy for many applications if density function defined properly
- Incremental computation: many models can be adopted to new training objects by updating densities
  - For Gaussian: store count, sum, squared sum to derive mean, variance
  - For histogram: store count to derive relative frequencies
- Incorporation of expert knowledge about the application in the prior $P(C_i)$

## Contra

- Limited applicability: often, required conditional probabilities are not available
- Lack of efficient computation: in case of a high number of attributes (particularly for Bayesian belief networks)

# The Independence Hypothesis

## The Independence Hypothesis . . .

- . . . makes efficient computation possible
- . . . yields optimal classifiers when satisfied
- . . . but is seldom satisfied in practice, as attributes (variables) are often correlated.

## Attempts to overcome this limitation

- *Bayesian networks*, that combine Bayesian reasoning with causal relationships between attributes
- *Decision trees*, that reason on one attribute at the time, considering most important attributes first

# Agenda

# Linear Discriminant Function Classifier

## Idea

Separate points of two classes by a hyperplane

- I.e., classification model is a hyperplane
- Points of one class in one half space, points of second class in the other half space

| age | car_type | max_speed | risk |
|---|---|---|---|
| 23 | family | 180 | high |
| 17 | sportive | 240 | high |
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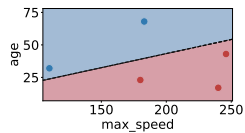
| 68 | family | 183 | low |
| 32 | truck | 110 | low |

## Questions

- How to formalize the classifier?
- How to find optimal parameters of the model?



# Basic Notions

Recall some general algebraic notions for a vector space $V$:

- $\langle x, y \rangle$denotes an inner product of two vectors $x, y \in V$
  - E.g., the scalar product $\langle x, y \rangle = x^T y = \sum_{i=1}^{d} x_i y_i$
- $H(w, w_0)$ denotes a hyperplane with normal vector $w$ and constant term $w_0$:

$$x \in H \Leftrightarrow \langle x, w \rangle + w_0 = 0$$

- The normal vector w may be normalized to $w'$:

$$w' = \frac{1}{\sqrt{\langle w, w \rangle}} w \implies \langle w', w' \rangle = 1$$

- Distance of a point $x$ to the hyperplane $H(w', w_0)$:

$$dist(x, H(w', w_0)) = |\langle w', x \rangle + w_0|$$

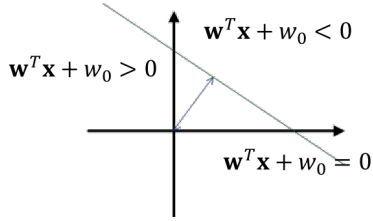
# Formalization

- Consider a two-class example (generalizations later on):
  - $D$: $d$-dimensional vector space with attributes $a_1, \ldots, a_d$
  - $Y = \{-1, 1\}$ set of 2 distinct class labels $y_j$
  - $O \subseteq D$: Set of objects $o = (o_1, \ldots, o_d)$ with known class labels $y \in Y$ and cardinality $|O| = N$
- A hyperplane $H(w, w_0)$ with normal vector $w$ and constant term $w_0$

$$x \in H \Leftrightarrow w^T x + w_0 = 0$$

**Classification Rule**

$$K_{H(w,w_0)}(x) = \text{sign}(w^T x + w_0)$$



# Optimal Parameter Estimation

## How to estimate optimal parameters $w, w_0$?

1. Define an objective/loss function $L(\cdot)$ that assigns a value (e.g. the error on the training set) to each parameter-configuration
2. Optimal parameters minimize/maximize the objective function

## How does an objective function look like?

- Different choices possible
- Most intuitive: Each misclassified object contributes a constant (loss) value $\rightsquigarrow$ 0-1 loss

# Optimal Parameter Estimation

## 0-1 Loss Objective for Linear Classifier

- $L(w, w_0) = \sum_{i=1}^{N} I(y_i \neq K_{H(w,w_0)}(x_i))$
- $\min_{w,w_0} L(w, w_0)$

where $I(condition) = 1$ if condition holds, 0 otherwise

- Minimize the overall number of training errors, but ...
  - NP-hard to optimize in general (non-smooth, non-convex)
  - Small changes of $w, w_0$ can lead to large changes of the loss

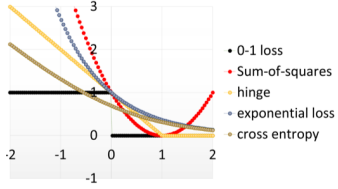
# Loss Functions

## Alternative Convex Loss Functions

| | | |
|---|---|---|
| Sum-of-squares loss | $(w^T x_i + w_0 - y_i)^2$ | |
| Hinge loss | $\max\{0, (1 - y_i(w^T x_i + w_0)\}$ | (SVM) |
| Exponential loss | $\exp(-y_i(w^T x_i + w_0))$ | (AdaBoost) |
| Cross-entropy error | $-y_i \log g(x_i) + (1 - y_i) \log(1 - g(x_i))$ | (Logistic Regression) |
| | where $g(x_i) = \frac{1}{1+\exp(-(w^T x_i + w_0))}$ | |

... and many more

- Optimizing different loss function leads to several classification algorithms
- Next, we derive the optimal parameters for the sum-of-squares loss



# Optimal Parameters for SSE loss

## Objective Function

$$SSE(w, w_0) = \frac{1}{2} \sum_{i=1}^{N} (w^T x_i + w_0 - y_i)^2$$

- Minimize the error function for getting optimal parameters
- Use standard optimization technique:
  1. Calculate first derivative
  2. Set derivative to zero and compute the global minimum (SSE is a convex function)

# Optimal Parameters for SSE Loss

- Transform the problem for simpler computations:
  - $w^T x + w_0 = \sum_{i=1}^{d} w_i x_i + w_0 = \sum_{i=0}^{d} w_i x_i$ with $x_0 = 1$
  - For $w$ let $\tilde{w} = (w_0, \ldots, w_d)^T$
- Combine the values to matrices

$$\tilde{X} = \begin{pmatrix} 1 & x_{1,1} & \ldots & x_{1,d} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{N,1} & \ldots & x_{N,d} \end{pmatrix}, \qquad Y = \begin{pmatrix} y_1 \\ \vdots \\ y_N \end{pmatrix}$$

- Then the sum-of-squares error is equal to

$$SSE(\tilde{w}) = \frac{1}{2}(\tilde{X}\tilde{w} - Y)^T(\tilde{X}\tilde{w} - Y)$$

# Optimal Parameters for SSE Loss

- Take the derivative:

$$\frac{\partial}{\partial \tilde{w}} SSW(\tilde{w}) = \tilde{X}^T(\tilde{X}\tilde{w} - Y)$$

- Solve $\frac{\partial}{\partial \tilde{w}} SSE(\tilde{w}) = 0$:

$$\begin{aligned} \tilde{X}^T(\tilde{X}\tilde{w} - Y) &= 0 \\ \Leftrightarrow \tilde{X}^T\tilde{X}\tilde{w} &= \tilde{X}^T Y \\ \Leftrightarrow \tilde{w} &= \underbrace{(\tilde{X}^T\tilde{X})^{-1}\tilde{X}^T}_{\substack{\text{Left-inverse of } \tilde{X} \\ \text{(”Moore-Penrose Inverse”)}}} Y \end{aligned}$$

# Optimal Parameters for SSE Loss

- Set $\hat{w} = (\tilde{X}^T \tilde{X})^{-1} \tilde{X}^T Y$
- Classify new point $x$ with $x_0 = 1$ using

## Classification Rule

$$K_{H(\hat{w})}(x) = \text{sign}(\hat{w}x)$$

# Example SSE

- Data (consider only age and max. speed):

$$\tilde{X} = \begin{pmatrix} 1 & 23 & 180 \\ 1 & 17 & 240 \\ 1 & 43 & 246 \\ 1 & 68 & 183 \\ 1 & 32 & 110 \end{pmatrix}, \qquad Y = \begin{pmatrix} 1 \\ 1 \\ 1 \\ -1 \\ -1 \end{pmatrix}$$

| age | car_type | max_speed | risk |
|---|---|---|---|
| 23 | family | 180 | high |
| 17 | sportive | 240 | high |
| 43 | sportive | 246 | high |
| 68 | family | 183 | low |
| 32 | truck | 110 | low |

- Encode classes as $\{\text{high} = 1, \text{low} = -1\}$

$$(\tilde{X}^T\tilde{X})^{-1}\tilde{X}^T = \begin{pmatrix} 0.7491 & -0.0836 & -0.8603 & -0.4736 & 1.6684 \\ -0.0087 & -0.0114 & 0.0049 & 0.0194 & -0.0043 \\ -0.0012 & 0.0036 & 0.0046 & -0.0002 & -0.0068 \end{pmatrix}$$

$$\implies \hat{w} = (\tilde{X}^T\tilde{X})^{-1}\tilde{X}^T Y = \begin{pmatrix} w_0 \\ w_{age} \\ w_{maxspeed} \end{pmatrix} = \begin{pmatrix} -1.3896 \\ -0.0302 \\ 0.0141 \end{pmatrix}$$

# Example SSE

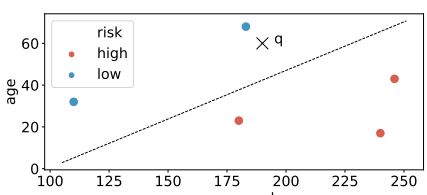
- Model parameters:

$$\hat{w} = (\tilde{X}^T \tilde{X})^{-1} \tilde{X}^T Y = \begin{pmatrix} w_0 \\ w_{age} \\ w_{maxspeed} \end{pmatrix} = \begin{pmatrix} -1.3896 \\ -0.0302 \\ 0.0141 \end{pmatrix}$$

$$\implies K_{H(\hat{w})}(x) = \text{sign}\left( \begin{pmatrix} -0.0302 \\ 0.0141 \end{pmatrix}^T x - 1.3896 \right)$$

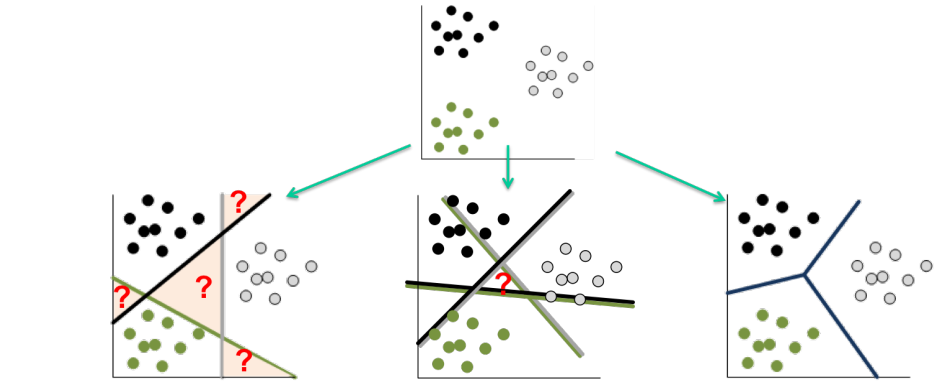
- Query: $q = (age = 60; max\_speed = 190)$

$$\text{sign}(\hat{w}^T \tilde{q}) = \text{sign}(-0.5323) = -1$$
$$\implies class = low$$



# Extension to Multiple Classes

Assume we have more than two ($k > 2$) classes. What to do?




One-vs-the-rest
("one-vs-all")
→k classifiers

One-vs-one (Majority vote of classifiers)
→ $\frac{k(k-1)}{2}$ classifiers

Multiclass linear classifier

→ k classifiers

# Extension to Multiple Classes

## Idea of Multiclass Linear Classifier

- Take $k$ linear functions of the form $H_{w_j,w_{j,0}}(x) = w_j^T x + w_{j,0}$
- Decide for class $y_j$:

$$y_j = \underset{j=1,\ldots,k}{\operatorname{argmax}} H_{w_j,w_{j,0}}(x)$$

- Advantage: No ambiguous regions except for points on decision hyperplanes
- The optimal parameter estimation is also extendable to $k$ classes $y_1, \ldots, y_k$

# Discussion (SSE)

## Advantages

- Simple approach
- Closed form solution for parameters
- Easily extendable to non-linear spaces (later on)

## Disadvantages

- Sensitive to outliers $\rightsquigarrow$ not a stable classifier
  - How to define and efficiently determine the maximum stable hyperplane?
- Only good results for linearly separable data
- Expensive computation of selected hyperplanes

$\rightsquigarrow$ Approach to solve problems: Support Vector Machines (SVMs) [Vapnik 1979, 1995]

# Agenda

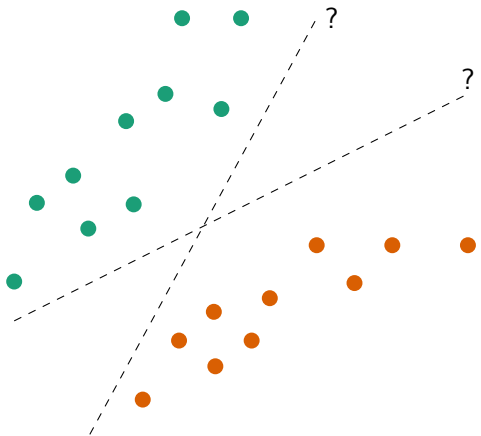
# Maximum Margin Hyperplane

**Question**

How to define the notion of the "best" hyperplane differently?

**Criteria**

- Stability at insertion
- Distance to the objects of both classes

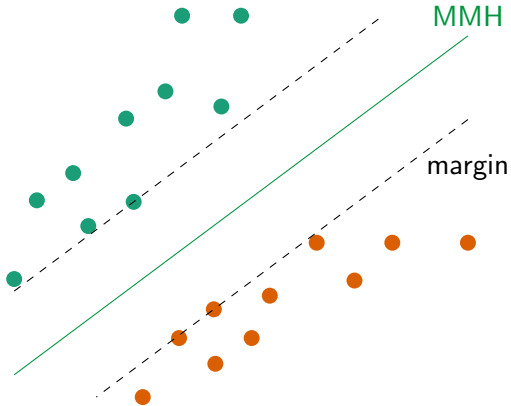


# Support Vector Machines: Principle

## Basic Idea

Linear separation with the *Maximum Margin Hyperplane (MMH)*:

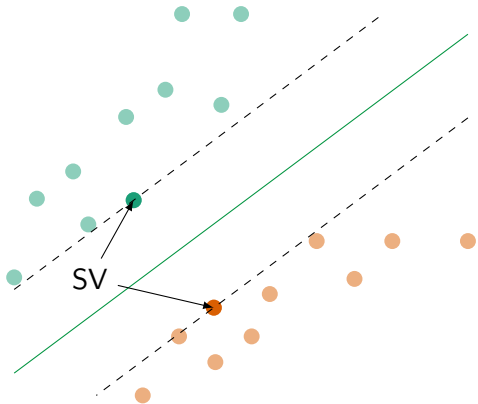
- Distance to points from any of the two sets is maximal, i.e., at least $\xi$
- Minimal probability that the separating hyperplane has to be moved due to an insertion
  $\rightsquigarrow$ Best generalization behavior; MMH is "maximally stable"



# Support Vector Machines: Principle

## Support Vectors

MMH only depends on points $p_i$ whose distance to the hyperplane is exactly $\xi$. These $p_i$ are called *support vectors* (SV).



# Formalisation

- Let $\mathbf{x_i} \in \mathbb{R}^d$ denote the data points, and $y_i = +1$, if first class, else $y_i = -1$.
- A hyperplane in Hesse normal form is represented by a normal vector $\mathbf{w} \in \mathbb{R}^d$ of unit length (i.e., $\|\mathbf{w}\|_2 = 1$), and a (signed) distance from the origin $b \in \mathbb{R}$.
- In the following slides, we will define the requirements which the MMH shall fulfil.

# Requirements of the MMH

The parameters $(\mathbf{w}, b)$ of the MMH shall fulfil the following two requirements:

## No Error

The classification is accurate for all points, i.e.

$$y_i \cdot (\langle \mathbf{w}, \mathbf{x_i} \rangle + b) > 0 \iff \begin{cases} y_i = -1 & \langle \mathbf{w}, \mathbf{x_i} \rangle + b < 0 \\ y_i = +1 & \langle \mathbf{w}, \mathbf{x_i} \rangle + b > 0 \end{cases}$$

## Requirement: Maximal Margin

Let $\xi = \min_{\mathbf{x_i} \in TR} |\langle \mathbf{w}, \mathbf{x_i} \rangle + b|$ denote the minimum distance of any training object $\mathbf{x_i}$ to the hyperplane $H(\mathbf{w}, b)$. The margin $\xi$ should be as large as possible.

# Computation of the MMH

- *Task*: Maximise $\xi$ subject to $y_i \cdot (\langle \mathbf{w}, \mathbf{x_i} \rangle + b) > \xi$ for all $i \in \{1, \ldots, n\}$.
- Scaling the constraints by $\xi^{-1}$ yields $y_i \cdot (\langle \xi^{-1}\mathbf{w}, \mathbf{x_i} \rangle + \xi^{-1} b) > 1$ for all $i \in \{1, \ldots, n\}$.
- Define $\mathbf{w}' = \xi^{-1}\mathbf{w}$, and $b' = \xi^{-1} b$.
- Maximizing $\xi$ corresponds to minimizing $\langle \mathbf{w}', \mathbf{w}' \rangle = \frac{\langle \mathbf{w}, \mathbf{w} \rangle}{\xi^2}$.

## Primary Optimization Problem

$$\begin{aligned} \min \quad & \|\mathbf{w}'\|_2^2 \\ s.t. \quad & y_i \cdot (\langle \mathbf{w}', \mathbf{x_i} \rangle + b') > 1 \qquad i \in \{1, \ldots, n\} \end{aligned}$$

# Computation of the MMH

## Primary Optimization Problem

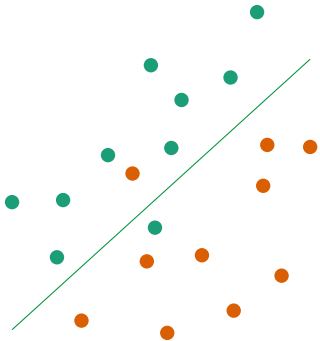
$$\begin{aligned} \min \quad & \|\mathbf{w}'\|_2^2 \\ s.t. \quad & y_i \cdot (\langle \mathbf{w}', \mathbf{x_i} \rangle + b') > 1 \qquad i \in \{1, \ldots, n\} \end{aligned}$$

- Convex optimization problem: Quadratic programming problem with linear constraints
  $\Longrightarrow$ Solution can be obtained by Lagrangian Theory.

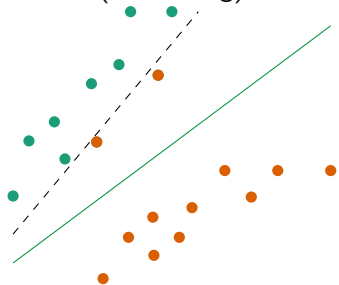
# Soft Margin Optimization

- Problem of MMH optimization: How to treat non-(linearly separable) data?
- Two typical problems:

data points not linearly separable



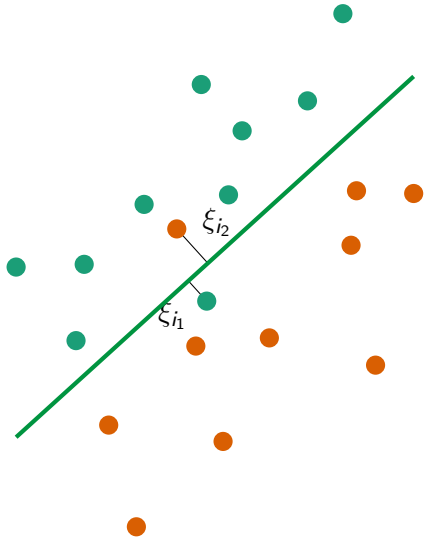
complete separation not optimal (overfitting)



- Trade-off between training error and size of margin

# Soft Margin Optimization

- Additionally regard the number of training errors when optimizing:
  - $\xi_i$ is the distance from $\mathbf{x_i}$ to the margin (often called *slack variable*):
    - $\xi_i = 0 \implies \mathbf{x_i}$ on correct side
    - $\xi_i > 0 \implies \mathbf{x_i}$ on wrong side
- Introduce parameter $C$ to weight the misclassification against the size of the margin.



# Soft Margin Optimization

## Primary Optimization Problem With Soft Margin

$$
\begin{aligned}
\min \quad & \frac{1}{2}\|\mathbf{w}'\|_2^2 + C\sum_{i=1}^{n}\xi_i & \\
s.t. \quad & y_i \cdot \left(\langle \mathbf{w}', \mathbf{x_i} \rangle + b'\right) > 1 - \xi_i & i \in \{1, \ldots, n\} \\
& \xi_i \geq 0 & i \in \{1, \ldots, n\}
\end{aligned}
$$

# Soft Margin Optimization

## Wolfe-Dual with Lagrange Multipliers

$$\max \quad \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \langle \mathbf{x_i}, \mathbf{x_j} \rangle$$

$$s.t. \quad \sum_{i=1}^{n} \alpha_i y_i = 0$$

$$0 \leq \alpha_i \leq C \qquad i \in \{1, \ldots, n\}$$

- $\alpha_i = 0$: $\mathbf{x_i}$ is not a support vector
- $\alpha_i = C$: $\mathbf{x_i}$ is support vector with $\xi_i > 0$
- $0 < \alpha_i < C$: $\mathbf{x_i}$ is support vector with $\xi_i = 0$

# Soft Margin SVM

## Decision Rule

$$H(x) = sign\left(\sum_{\mathbf{x_i} \in SV} \alpha_i y_i \langle \mathbf{x_i}, \mathbf{x} \rangle + b\right)$$

where $SV$ denotes the set of support vectors.

# SVM: Discussion

## Pro

- generate classifiers with a high classification accuracy
- relatively weak tendency to overfitting (generalization theory)
- efficient classification of new objects due to often small number of support vectors
- compact models

## Contra

- training times may be long (appropriate feature space may be very high-dimensional)
- expensive implementation

# Agenda

# Non-Linearly Separable Data Sets

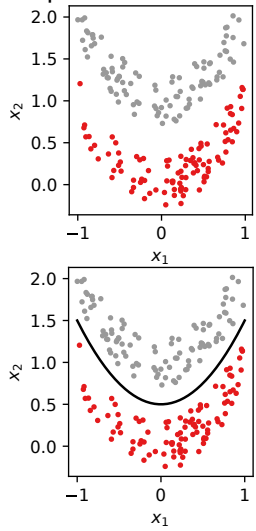
**Problem**

For real data sets, a linear separation with a high classification accuracy often is not possible.

**Idea**

Transform the data non-linearly into a new space, and try to separate the data in the new space linearly (extension of the hypotheses space)

Example for quadratically separable data set



# Extension of the Hypotheses Space

## Principle

$$\text{input space} \xrightarrow{\phi} \text{extented feature space}$$

$\rightsquigarrow$ Try to linearly separate in the extended feature space.

## Example

$$\phi(x, y) = \left(1, x, y, x^2, xy, y^2\right)$$

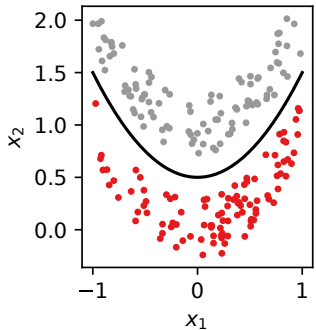
Here: A hyperplane in the extended feature space is a polynomial of degree 2 in the input space

# Extension of the Hypotheses Space: Example (1)

Input Space (2 attributes):

$$x = (x_1, x_2)$$

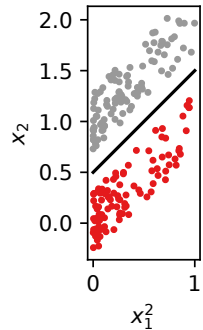
$$x_2 = x_1^2 + 0.5$$




Extended Space (6 attributes):

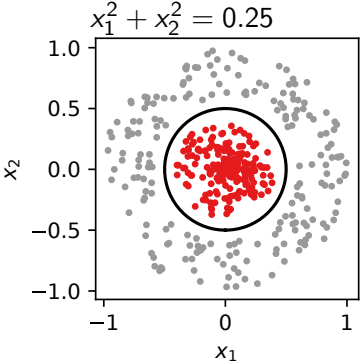
$$\phi(x) = \left(1, x, y, x^2, xy, y^2\right)$$

$$x_2 = (x_1^2) + 0.5$$

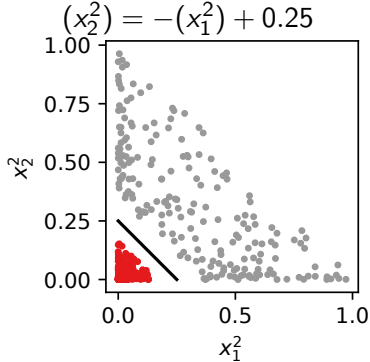


# Extension of the Hypotheses Space: Example (2)

Input Space (2 attributes):
$x = (x_1, x_2)$




Extended Space (3 attributes):
$\phi(x) = (x_1^2, x_2^2, x_1 x_2)$



# Extension of Linear Discriminant Function Classifier

- Linear classifier can be easily extended to non-linear spaces
- Recap: linear classifier $K_{H(w,w_0)}(x) = sign(w^T x + w_0)$
- Extend to non-linear case:
  - Transform all data points $x$ to new feature space $\phi(x)$
  - Data Matrix $X$ becomes a matrix $\Phi$
  - The optimal hyperplane vector becomes ...

$$\tilde{w}_{opt,\phi} = (\Phi^T \Phi)^{-1} \Phi^T Y$$

  - ... and that's all!
- New classification rule: $K_{H(w_\phi, w_{0,\phi})}(x) = sign(w_\phi^T \phi(x) + w_{0,\phi})$
- SVM can be extended in a similar way

# Non-linear Classification: Discussion

## Pro

- By explicit feature transformation a much richer hypotheses space
- Simple extension of existing techniques
- Efficient evaluation, if transformed feature space not too high-dimensional

## Contra

- Explicit mapping to other feature spaces can become problematic
- Meaningful transformation is usually not known a-priori
- Complex data distributions may require very high-dimensional features spaces $\rightsquigarrow$ High memory consumption, High computational costs

# Implicit Mappings: Kernel Methods

## Explicit Mapping

Explicit mapping of the data into the new feature space:

- After transformation, any vector-based distance is applied
- Resulting feature space may be very high dimensional $\rightsquigarrow$ Potential problems: Inefficient calculation, storage overhead

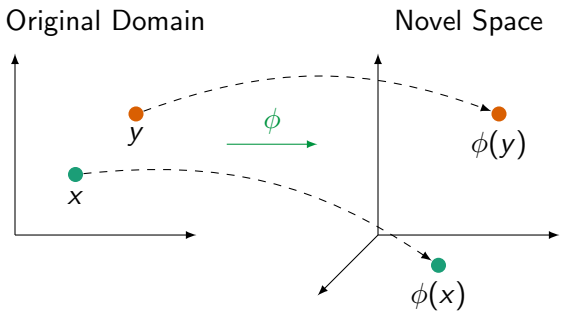
Often, we do not need the transformed data points themselves, but just the distances between them!

# Implicit Mappings: Kernel Methods

## "Kernel Trick"

Just *implicitly* map the data to a feature space: Determine a function $K_\phi$, which computes the distance in the kernel space without explicitly computing $\phi(\cdot)$

$$K_\phi(x, y) = \langle \phi(x), \phi(y) \rangle$$

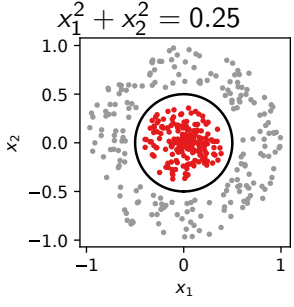


# Kernel: Example

- Assume the original domain is $\mathcal{X} = \mathbb{R}^2$
- We transform a point $x = (x_1, x_2)$ to $\phi(x) = \left(x_1^2, x_2^2, x_1 x_2\right)$, i.e. the novel feature space is $\mathcal{H} = \mathbb{R}^3$, and $\kappa : \mathcal{X} \to \mathcal{H}$.

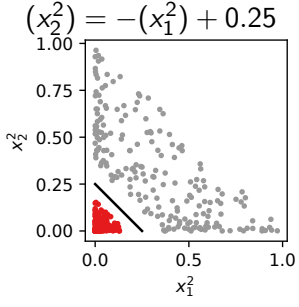
Input Space (2 attributes):

$$x = (x_1, x_2)$$




Extended Space (3 attributes):

$$\phi(x) = \left(x_1^2, x_2^2, x_1 x_2\right)$$



# Kernel: Example

- Original point $x = (x_1, x_2)$; transformed point $\phi(x) = \left(x_1^2, x_2^2, \sqrt{2} \cdot x_1 x_2\right)$
- We want to calculate the dot product in the novel feature space $\mathcal{H}$:

$$\begin{aligned}
\langle \phi(x), \phi(y) \rangle &= \left\langle \left(x_1^2, x_2^2, \sqrt{2} \cdot x_1 x_2\right), \left(y_1^2, y_2^2, \sqrt{2} \cdot y_1 y_2\right) \right\rangle \\
&= x_1^2 y_1^2 + x_2^2 y_2^2 + 2 x_1 x_2 y_1 y_2 \\
&= (x_1 y_1 + x_2 y_2)^2 \\
&= \langle x, y \rangle^2
\end{aligned}$$

- We do not have to explicitly map the points to the feature space $\mathcal{H}$!
- Simply calculate squared dot product in the original domain $\mathcal{X}$!
- $\kappa : \mathcal{X} \times \mathcal{X} \to \mathbb{R}, (x, y) \mapsto \langle x, y \rangle^2$ is called a (valid) kernel

# Why is the dot product useful?

- Kernels correspond to dot products in some feature space
- With the dot product we are able to compute:
  - The norm/length of a vector $\|x\| = \sqrt{\langle x, x \rangle}$
  - The distance between two vectors:

$$\|x - y\|^2 = \langle x - y, x - y \rangle = \langle x, x \rangle + \langle y, y \rangle - 2 \langle x, y \rangle$$

  - The angle between two vectors:

$$\angle(x, y) = \arccos \frac{\langle x, y \rangle}{\|x\| \cdot \|y\|}$$

# Formal Definitions

## Definition: Kernel Function

A *kernel function* $\kappa : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is a symmetric function, i.e., $\kappa(x, y) = \kappa(y, x)$, mapping pairs of objects $x, y \in \mathcal{X}$ to real numbers.

## Definition: Mercer Kernel

For all finite $\{x_1, \ldots, x_n\} = X \subseteq \mathcal{X}$, let $\kappa(X) := (\kappa(x_i, x_j))_{i,j} \in \mathbb{R}^{n \times n}$. A kernel function $\kappa$ is called *Mercer kernel*, valid kernel, admissible kernel, or positive semi-definite, if for all such finite $X$, the matrix $\kappa(X)$ is positive semi-definite, i.e. for all $c \in \mathbb{R}^n$, it holds

$$c^T \kappa(X) c \geq 0$$

# Formal Definitions (cont'd)

## Definition: Dot Product

A dot product in a vector space $\mathcal{H}$ is a function $\langle \cdot, \cdot \rangle : \mathcal{H} \times \mathcal{H} \to \mathbb{R}$ satisfying:

- $\langle x, x \rangle = 0$ for $x = 0$
- $\langle x, x \rangle > 0$ for $x \neq 0$
- $\langle x, y \rangle = \langle y, x \rangle$ (Symmetry)
- $\langle \alpha x + \beta y, z \rangle = \alpha \langle x, z \rangle + \beta \langle y, z \rangle$ (Bi-linearity)

## Definition: Hilbert Space

A vector space $\mathcal{H}$ endowed with a dot product $\langle \cdot, \cdot \rangle : \mathcal{H} \times \mathcal{H} \to \mathbb{R}$ for which the induced norm gives a complete metric space, is termed *Hilbert Space*.

# Interpretation of Kernel Functions

**Theorem**

Let $\kappa : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ be a valid kernel on $\mathcal{X}$. There exists a possibly infinite-dimensional Hilbert space $\mathcal{H}$ and a mapping $\phi : \mathcal{X} \to \mathcal{H}$ such that $\kappa(x, y) = \langle \phi(x), \phi(y) \rangle_{\mathcal{H}}$ for all $x, y \in \mathcal{X}$ where $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ denotes the dot product in a Hilbert space $\mathcal{H}$.

$\rightsquigarrow$ every kernel $\kappa$ can be seen as a dot product in some feature space $\mathcal{H}$.

**Advantages**

- Feature space $\mathcal{H}$ can be infinite-dimensional
- Not really necessary to know which feature space $\mathcal{H}$ we have
- Computation of kernel is done in original domain $\mathcal{X}$

# Kernel SVM

## Wolfe-Dual Optimization Problem with Lagrange Multipliers

$$\max \quad \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \kappa(x_i, x_j)$$

$$s.t. \quad \sum_{i=1}^{n} \alpha_i y_i = 0$$

$$0 \leq \alpha_i \leq C \qquad i \in \{1, \ldots, n\}$$

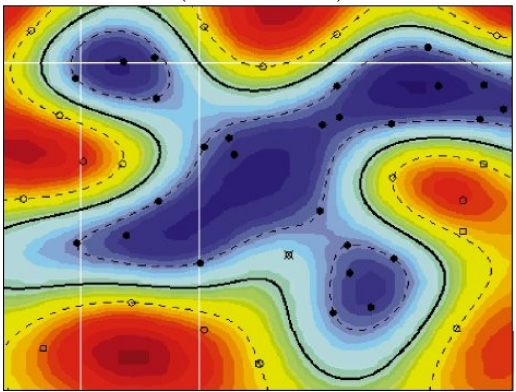
## Decision Rule

$$H(x) = sign\left( \sum_{x_i \in SV} \alpha_i y_i \kappa(x_i, x) + b \right)$$

# Example for Mercer Kernels

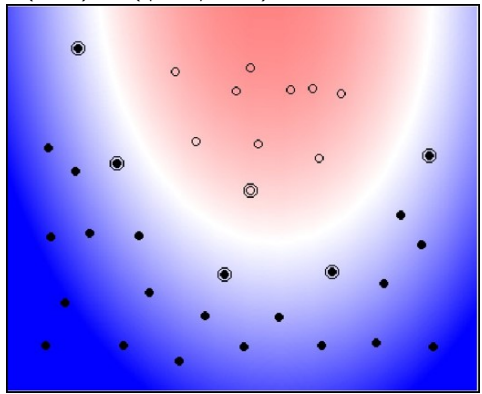
Radial Basis Kernel

$\kappa(x, y) = \exp\left(-\gamma \|x - y\|^2\right)$



Polynomial Kernel (degree 2)

$\kappa(x, y) = (\langle x, y \rangle + 1)^d$



# Discussion

## Pro

- Kernel methods provide a simple method for dealing with non-linearity
- Implicit mapping allows for mapping to arbitrary-dimensional spaces:c
  Computational effort depends on the number of training examples, but not on the feature space dimensionality

## Contra

- Resulting models rarely provide an intuition
- Choice of kernel can be difficult

# Agenda

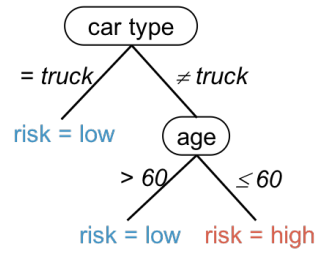
# Decision Tree Classifiers

- Approximating discrete-valued target function
- Learned function is represented as a tree:
  - A flow-chart-like tree structure
  - Internal node denotes a test on an attribute
  - Branch represents an outcome of the test
  - Leaf nodes represent class labels or class distribution
- Tree can be transformed into decision rules:
  **if** age $> 60$ **then** risk $=$ low
  **if** age $\leq 60$ **and** car type $=$ truck **then** risk $=$ low
  **if** age $\leq 60$ **and** car type $\neq$ truck **then** risk $=$ high

## Advantages

- Decision trees represent explicit knowledge
- Decision trees are intuitive to most users

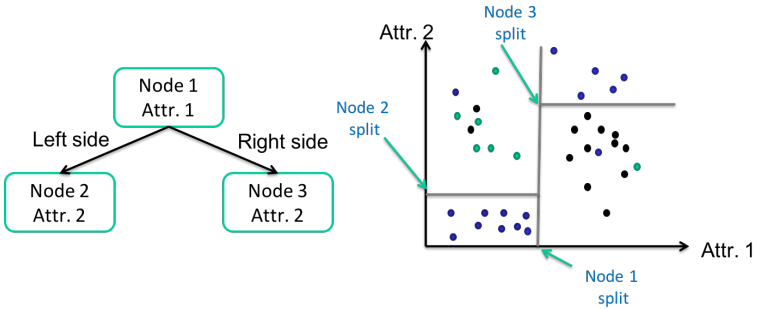
| age | car_type | max_speed | risk |
|---|---|---|---|
| 23 | family | 180 | high |
| 17 | sportive | 240 | high |
| 43 | sportive | 246 | high |
| 68 | family | 183 | low |
| 32 | truck | 110 | low |



# Decision Tree Classifier: Splits

## Goal

- Each tree node defines an axis-parallel $(d-1)$-dimensional hyperplane, that splits the data space.
- *Find such splits which lead to as homogenous groups as possible.*



# Decision Tree Classifiers: Basics

- Decision tree generation (training phase) consists of two phases
  1. Tree construction
     - At start, all the training examples are at the root
     - Partition examples recursively based on selected attributes
  2. Tree pruning
     - Identify and remove branches that reflect noise or outliers
- Use of decision tree: Classifying an unknown sample
  - Traverse the tree and test the attribute values of the sample against the decision tree
  - Assign the class label of the respective leaf to the query object

# Algorithm for Decision Tree Construction

- Basic algorithm (a greedy algorithm)
  - Tree is created in a *top-down recursive divide-and-conquer* manner
  - Attributes may be categorical or continuous-valued
  - At the start, all the training examples are assigned to the root node
  - Recursively partition examples at each node and push them down to the new nodes
  - Select test attributes and determine split points or split sets for the respective values based on a heuristic or statistical measure (*split strategy*, e.g., information gain)
- Conditions for stopping partitioning
  - All samples for a given node belong to the same class
  - There are no remaining attributes for further partitioning – majority voting is employed for classifying the leaf
  - There are no samples left

# Algorithm for Decision Tree Construction

- Most algorithms are versions of this basic algorithm (greedy, top-down)
  - E.g.: ID3, or its successor C4.5

## ID3 Algorithm

**procedure** ID3(*Examples*, *TargetAttr*, *Attributes*) ▷ specialized to learn boolean-valued functions
  Create *Root* node for the tree
  **if** all *Examples* are positive **then return** *Root* with *label* $= +$
  **else if** all *Examples* are negative **then return** *Root* with *label* $= -$
  **else if** *Attributes* $= \emptyset$ **then return** *Root* with *label* $=$ most common value of *TargetAttr* in *Examples*
  **else**
    $A =$ "best" decision attribute for next node ▷ how to determine the "best" attribute?
    Assign $A$ as decision attribute for *Root*
    **for** each possible value $v_i$ of $A$ **do** ▷ how to split the possible values?
      Generate branch corresponding to test $A = v_i$
      $Examples_{v_i} =$ examples that have value $v_i$ for $A$
      **if** $Examples_{v_i} = \emptyset$ **then**
        Add leaf node with *label* $=$ most common value of *TargetAttr* in *Examples*
      **else**
        Add subtree ID3($Examples_{v_i}$, *TargetAttr*, *Attributes* $\setminus \{A\}$)

# Example: Decision for "playing_tennis"

- Query: How about playing tennis today?
- Training data:

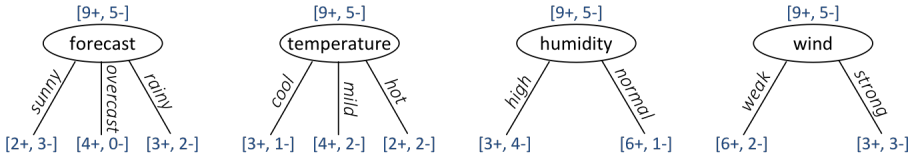
| day | forecast | temperature | humidity | wind | tennis decision |
|---|---|---|---|---|---|
| 1 | sunny | hot | high | weak | no |
| 2 | sunny | hot | high | strong | no |
| 3 | overcast | hot | high | weak | yes |
| 4 | rainy | mild | high | weak | yes |
| 5 | rainy | cool | normal | weak | yes |
| 6 | rainy | cool | normal | strong | no |
| 7 | overcast | cool | normal | strong | yes |
| 8 | sunny | mild | high | weak | no |
| 9 | sunny | cool | normal | weak | yes |
| 10 | rainy | mild | normal | weak | yes |
| 11 | sunny | mild | normal | strong | yes |
| 12 | overcast | mild | high | strong | yes |
| 13 | overcast | hot | normal | weak | yes |
| 14 | rainy | mild | high | strong | no |

- Build decision tree ...

# Split Strategies: Quality of Splits

## Given

- A set $T$ of training objects
- A (disjoint, complete) partitioning $T_1, \ldots T_m$ of $T$
- The relative frequencies $p_i$ of class $c_i$ in $T$ and in the partitions $T_1, \ldots T_m$




## Wanted

- A measure for the heterogeneity of a set $S$ of training objects with respect to the class membership
- A split of $T$ into partitions $\{T_1, \ldots, T_m\}$ such that the heterogeneity is minimized

$\rightsquigarrow$ Proposals: *Information gain*, *Gini index*, *Misclassification error*

# Attribute Selection Measures: Information Gain

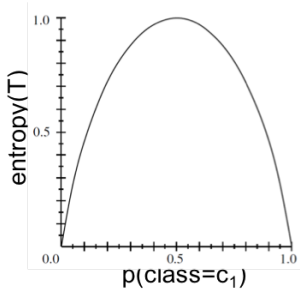
- Used in ID3/C4.5

## Entropy

- Minimum number of bits to encode a message that contains the class label of a random training object
- The entropy of a set $T$ of training objects is defined as

$$entropy(T) = -\sum_{i=1}^{k} p_i \log_2 p_i$$

  for $k$ classes with frequencies $p_i$
- $entropy(T) = 0$ if $p_i = 1$ for any class $c_i$
- $entropy(T) = 1$ if $p_i = \frac{1}{k}$ for all classes $c_i$




$k = 2$

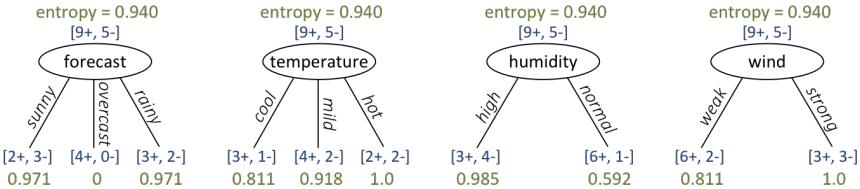
# Attribute Selection Measures: Information Gain

## Information Gain

Let $A$ be the attribute that induced the partitioning $\{T_1, \ldots, T_m\}$ of $T$. The information gain of attribute $A$ w.r.t. $T$ is defined as

$$information\_gain(T, A) = entropy(T) - \sum_{i=1}^{m} \frac{|T_i|}{|T|} entropy(T_i)$$

# Attribute Selection: Example (Information Gain)

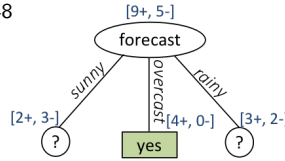



$$information\_gain(T, forecast) = 0.94 - \frac{5}{14}0.971 - \frac{4}{14}0 - \frac{5}{14}0.971 = 0.246$$

$$information\_gain(T, temperature) = 0.94 - \frac{4}{14}0.811 - \frac{6}{14}0.981 - \frac{4}{14}1 = 0.029$$

$$information\_gain(T, humidity) = 0.94 - \frac{7}{14}0.985 - \frac{7}{14}0.592 = 0.151$$

$$information\_gain(T, wind) = 0.94 - \frac{8}{14}0.811 - \frac{6}{14}1 = 0.048$$

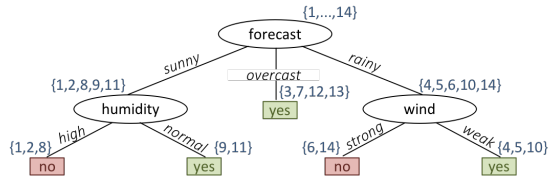



Result: "forecast" yields the highest information gain

# Example: Decision Tree for "playing_tennis"

| day | forecast | temperature | humidity | wind | tennis decision |
|---|---|---|---|---|---|
| 1 | sunny | hot | high | weak | no |
| 2 | sunny | hot | high | strong | no |
| 3 | overcast | hot | high | weak | yes |
| 4 | rainy | mild | high | weak | yes |
| 5 | rainy | cool | normal | weak | yes |
| 6 | rainy | cool | normal | strong | no |
| 7 | overcast | cool | normal | strong | yes |
| 8 | sunny | mild | high | weak | no |
| 9 | sunny | cool | normal | weak | yes |
| 10 | rainy | mild | normal | weak | yes |
| 11 | sunny | mild | normal | strong | yes |
| 12 | overcast | mild | high | strong | yes |
| 13 | overcast | hot | normal | weak | yes |
| 14 | rainy | mild | high | strong | no |

Final decision tree:



# Attribute Selection Measures: Gini Index

- Used in IBM's IntelligentMiner

## Gini Index

The Gini index for a set $T$ of training objects is defined as

$$gini(T) = 1 - \sum_{i=1}^{k} p_i^2$$

- Small value of Gini index $\equiv$ low heterogeneity
- Large value of Gini index $\equiv$ high heterogeneity

## Gini Index (of an attribute $A$)

Let $A$ be the attribute that induced the partitioning $\{T_1, \ldots, T_m\}$ of $T$. The Gini index of attribute $A$ w.r.t. $T$ is defined as

$$gini_A(T) = \sum_{i=1}^{m} \frac{|T_i|}{|T|} gini(T_i)$$

# Attribute Selection Measures: Misclassification Error

## Misclassification Error

The Misclassification Error for a set $T$ of training objects is defined as

$$Error(T) = 1 - \max_{c_i} p_i$$

- Small value of Error $\equiv$ low heterogeneity
- Large value of Error $\equiv$ high heterogeneity

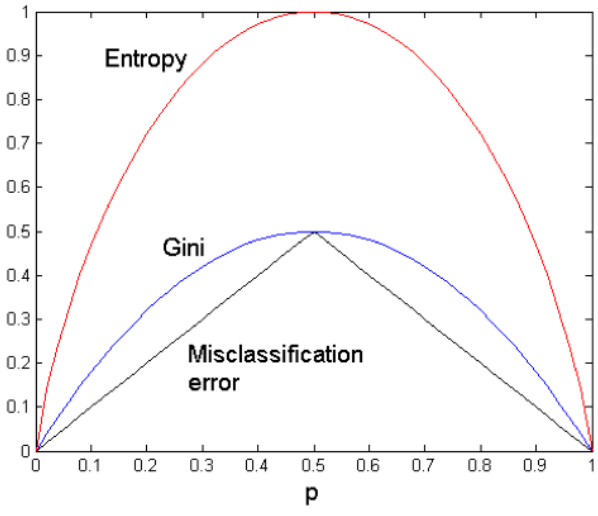
## Misclassification Error (of an attribute $A$)

Let $A$ be the attribute that induced the partitioning $\{T_1, \ldots, T_m\}$ of $T$. The Misclassification Error of attribute $A$ w.r.t. $T$ is defined as

$$Error_A(T) = \sum_{i=1}^{m} \frac{|T_i|}{|T|} Error(T_i)$$

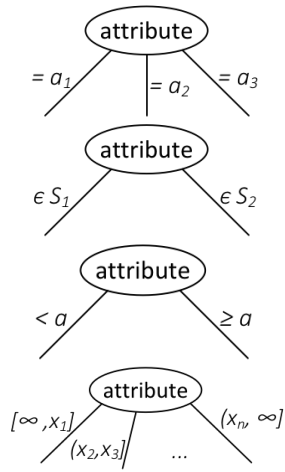
# Attribute Selection Measures: Comparison

For two-class problems:



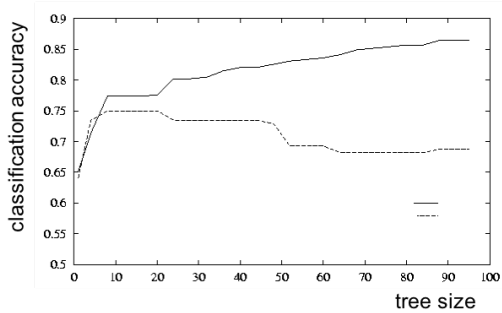
# Split Strategies: Types of Splits

- Categorical attributes
  - Split criteria based on equality "$attribute = a$"
  - Based on subset relationships "$attribute \in set$"
    $\rightsquigarrow$ many possible choices (subsets)
    - Choose the best split according to, e.g., gini index
- Numerical attributes
  - Split criteria of the form "$attribute < a$"
    $\rightsquigarrow$ many possible choices for the split point
    - One approach: Order test samples w.r.t. their attribute value; consider every mean value between two adjacent samples as possible split point; choose best one according to, e.g., gini index
  - Partition the attribute value into a discrete set of intervals (Binning)



# Avoid Overfitting in Classification

- The generated tree may overfit the training data
  - Too many branches, some may reflect anomalies due to noise or outliers
  - Result has poor accuracy for unseen samples




- Two approaches to avoid overfitting for decision trees:
  1. Post-pruning = pruning of overspecialized branches
  2. Pre-pruning = halt tree construction early

# Avoid Overfitting in Classification

## Post-pruning

Pruning of overspecialized branches:

- Remove branches from a "fully grown" tree and get a sequence of progressively pruned trees
- Use a set of data different from the training data to decide which is the "best pruned tree"

# Avoid Overfitting in Classification

## Pre-pruning

Halt tree construction early, do not split a node if this would result in the goodness measure falling below a threshold.

- Choice of an appropriate value for *minimum support*
  - Minimum support: minimum number of data objects a leaf node contains
  - In general, *minimum support* $\gg 1$
- Choice of an appropriate value for *minimum confidence*
  - Minimum confidence: minimum fraction of the majority class in a leaf node
  - Typically, *minimum confidence* $\ll 100\%$
  - Leaf nodes can absorb errors or noise in data records
- Discussion
  - With Pre-pruning it is difficult to choose appropriate thresholds
  - Pre-pruning has less information for the pruning decision than post-pruning $\rightsquigarrow$ can be expected to produce decision trees with lower classification quality
  - Tradeoff: tree construction time vs. classification quality

# Pruning of Decision Trees: Approach Post-pruning

## Reduced-Error Pruning [1]

- Decompose classified data into training set and test set
- Create a decision tree $E$ for the training set
- Prune $E$ using the test set $T$
  - Determine the interior node $v$ of $E$ whose pruning reduces the number of misclassified data points on $T$ the most (i.e., replace the subtree $S$ with root $v$ by a leaf. Determine the value of the leaf by majority voting)
  - Prune
  - Finish if no such interior node exists
- Only applicable if a sufficient number of classified data is available

[1] J.R. Quinlan. Rule induction with statistical data – a comparison with multiple regression. In Journal of the Operational Research Society, 38, pages 347-352, 1987

# Pruning of Decision Trees: Approach Post-pruning

## Minimal Cost Complexity Pruning [1]

- Does not require a separate test set
  - Applicable to small training sets as well
- Pruning of the decision tree by using the training set
  - Classification error is no appropriate quality measure
- New quality measure for decision trees:
  - Trade-off of classification error and tree size
  - Weighted sum of classification error and tree size
- General observation
  - The smaller decision trees yield the better generalization

[1] L. Breiman, J. Friedman, R. Olshen, and C. Stone. Classification and Regression Trees. Wadsworth International Group, 1984

# Minimal Cost Complexity Pruning: Notions

- Size $|E|$ of a decision tree $E$: number of leaf nodes
- Cost-complexity quality measure of $E$ with respect to training set $T$, classification error $F_T$ and complexity parameter $\alpha \geq 0$:

$$CC_T(E, \alpha) = F_T(E) + \alpha|E|$$

- For the *smallest minimal subtree* $E(\alpha)$ of $E$ w.r.t. $\alpha$, it is true that:
  1. There is no subtree of $E$ with a smaller cost complexity
  2. If $E(\alpha)$ and $B$ both fulfill (1), then is $E(\alpha)$ a subtree of $B$
- $\alpha = 0$: $E(\alpha) = E$
  - Only error matters
- $\alpha \to \infty$: $E(\alpha) =$ root node of $E$
  - Only tree size matters
- $0 < \alpha < \infty$: $E(\alpha)$ is a proper substructure of $E$
  - The root node or more than the root node

# Extracting Classification Rules from Trees

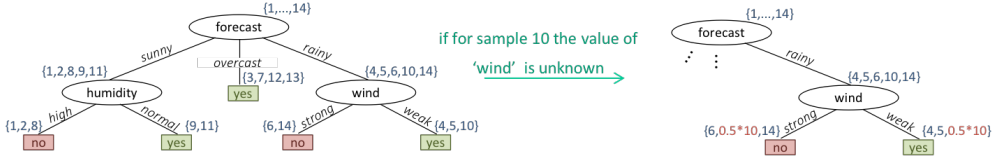
- Represent the knowledge in the form of IF-THEN rules
- One rule is created for each path from the root to a leaf
- Each attribute-value pair along a path forms a conjunction
- The leaf node holds the class prediction
- Rules are easier for humans to understand

## Example

**if** forecast = "overcast" **then** playing_tennis = "yes"
**if** forecast = "sunny" **and** humidity = "high" **then** playing_tennis = "no"
**if** forecast = "sunny" **and** humidity = "normal" **then** playing_tennis = "yes"
**if** forecast = "rainy" **and** wind = "strong" **then** playing_tennis = "no"
**if** forecast = "rainy" **and** wind = "weak" **then** playing_tennis = "yes"

# Enhancement: Handle Missing Attribute Values

- If node $n$ tests attribute $A$:
  - Assign most common value of $A$ among other examples sorted to node $n$
  - Assign the most common value of the attribute among other examples with the same target value sorted to node $n$
  - Assign probability $p_i$ to each of the possible values $v_i$ of attribute $A$ among other examples sorted to node $n$
    - Assign fraction $p_i$ of example to each descendant in tree
    - Classify new examples in the same fashion: Classification decision is the one with the highest probability (sum over all instance fragments of each class decision)



# Decision Tree Classifiers: Summary

## Pro

- Relatively fast learning speed (in comparison to other classification methods)
- Fast classification speed
- Convertible to simple and easy to understand classification rules
- Often comparable classification accuracy with other classification methods

## Contra

- Not very stable, small changes of the data can lead to large changes of the tree

# Agenda

# Nearest Neighbor Classifiers

## Motivation

- Assume data in a non-vector representation: graphs, forms, XML-files, etc.
- No simple way to use linear classifiers or decision trees

## Solutions

- Use appropriate kernel function for kernel machines (e.g. kernel SVM)
  $\rightsquigarrow$ Not always clear how to define a kernel
- Transformation of objects to some vector space (e.g. representation learning)
  $\rightsquigarrow$ Difficult to determine appropriate transformation & vector space
- *Here*: Nearest neighbor classifier
  $\rightsquigarrow$ Direct usage of the similarity of objects for classification

# Nearest Neighbor Classifiers

## Procedure

Assign query object $q$ to the class $c_j$ of the closest training object $x \in D$:

$$class(q) = class(NN(q)) \qquad NN(q) = \{x \in D \mid \forall x' \in D : d(q,x) \leq d(q,x')\}$$

$\rightsquigarrow$ Instance-Based Learning

## Example


Classifier decides that query object $q$ is a dog.

# Instance-Based Methods

## Eager Evaluation

- Create models from data (training phase) and then use these models for classification (test phase)
- Examples: Decision tree, Bayes classifier

## *Instance*-Based Learning

- Store training examples and delay the processing ("lazy evaluation") until a new instance must be classified
- Typical Approaches: $k$-nearest neighbor approach:
  - Instances represented as points in a metric space (e.g. Euclidean)
  - Classification by label of NN $\rightsquigarrow$ requires fast NN queries
  - $\rightsquigarrow$ Training phase = Index construction (e.g. R-tree)

# Nearest Neighbor Classifiers: Notions

## Notions

- Distance Function: Defines the (dis-)similarity for pairs of objects
- *Decision Set*: The set of $k$ nearest neighboring objects to be used in the decision rule

## Decision Rule

Given the class labels of the objects from the decision set, how to determine the class label to be assigned to the query object?

# Decision Rules

## Majority Vote (Default)

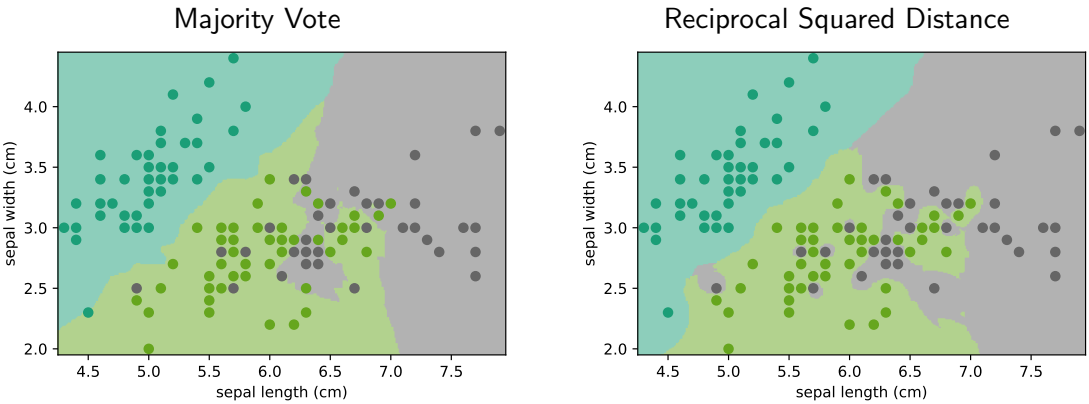
Choose majority class in the decision set, i.e. the class with the most representatives in the decision set

## Weighted Decision Rules

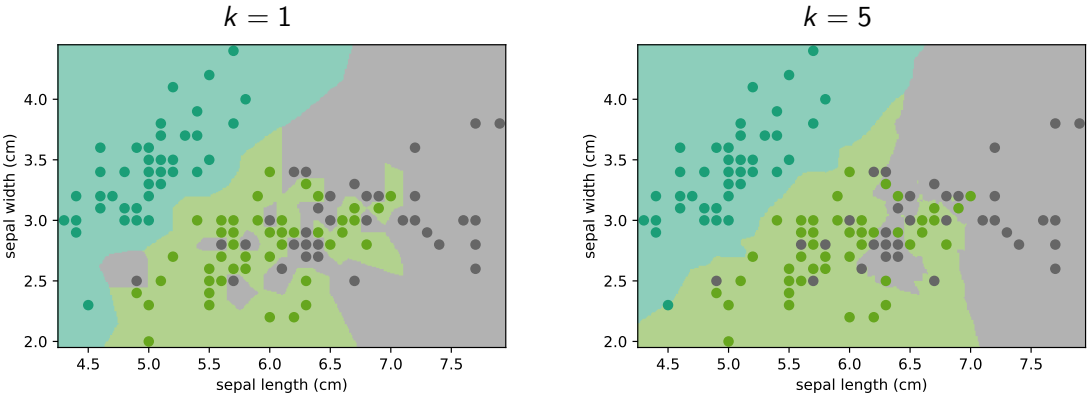
Choose *weighted* majority of decision set class labels. Weight variants:

- *Reciprocal squared distance*: $d(q, x)^{-2}$
- *Inverse A-Priori Probability*: Use inverse frequency of classes in the training set

# Example: $k = 5$ – Influence of Weighting



# Example: Majority Vote – Influence of $k$



# NN Classifier: Parameter $k$

Choosing an appropriate $k$: Tradeoff between *overfitting* and *generalization*:

## Influence of $k$

- $k$ too small: High sensitivity against outliers
- $k$ too large: Decision set contains many objects from other classes

## Rules of Thumb

- Based on theoretical considerations: Choose $k$, such that it grows slowly with $n$, e.g. $k \approx \sqrt{n}$ or $k \approx \log n$
- Empirically, $1 \ll k < 10$ yields a high classification accuracy in many cases

# NN Classifier: Variants

- *k-NN* Classifier: Consider the $k$ nearest neighbors for the class assignment decision
- *Weighted k-NN* Classifier: Use weights for the classes of the $k$ nearest neighbors
- *Mean-based NN* Classifier: Determine mean vector $m_i$ for each class $c_j$ (in training phase); Assign query object to the class $c_j$ of the nearest mean vector $m_i$
- *Generalization*: Representative-based NN Classifier; Use more than one representative per class

# NN Classifier: Discussion

## Pro

- *Applicability*: Training data and distance function required only
- High classification *accuracy* in many applications
- Easy *incremental* adaptation to new training objects useful also for prediction
- *Robust* to noisy data by averaging $k$-nearest neighbors

## Contra

- Naïve implementation is inefficient: Requires $k$-nearest neighbor query processing $\rightsquigarrow$ support by database techniques may help to reduce from $\mathcal{O}(n)$ to $\mathcal{O}(\log n)$
- Does not produce explicit knowledge about classes, *but* provides some explanation information
- Curse of dimensionality: Distance between neighbors could be dominated by irrelevant attributes $\rightsquigarrow$ Apply dimensionality reduction first

# Agenda

# Ensemble Classification

## Problem

- No single classifier performs good on every problem
- For some techniques, small changes in the training set lead to very different classifiers

## Idea

Improve performance by combining different classifiers $\rightsquigarrow$ ensemble classification.
Different possibilities exist. Discussed here:

- Bagging (Bootstrap aggregation)
- Boosting

# Bagging

## How to obtain different classifiers?

Easiest way: Train the *same classifier* K on *different datasets*

## Bagging (or Bootstrap Aggregation)

- Randomly select $m$ different subsets from the training set
- On each subset, independently train a classifier $K_i$ $(i = 1, \ldots, m)$
- Overall decision:

$$K(x) = sign\left(\frac{1}{m}\sum_{i=1}^{m} K_i(x)\right)$$

# Boosting

## Boosting

- Linear combination of several *weak* learners (different classifiers)
- Given $m$ weak learners $K_i$ and weights $\alpha_i$ for $i = 1, \ldots, m$
- Overall decision

$$K(x) = sign\left(\sum_{i=1}^{m} \alpha_i K_i(x)\right)$$

- *Important difference*: classifiers are trained in sequence!
- Repeatedly misclassified points are weighted stronger

# AdaBoost

Widely used boosting method: AdaBoost [21]: Meta-algorithm that iteratively generates a chain of weak learners

## General Idea

- Assume $(t-1)$ weak learners are already given. The $t$th learner should focus on instances that were previously misclassified.
- Assign a weight $w_i$ to each instance $x_i$ to represent its importance
- Start with equal weight for each instance, adapt weights according to the performance of previously trained classifiers

[21] Yoav Freund and Robert E. Schapire. A decision-theoretic generalization of on-line learning and an application to boosting. Journal of Computer and System Sciences, 55(1):119–139, 1996.

# AdaBoost – Algorithm

Given: $n$ data points $x_1, \ldots, x_n$, labels $y_1, \ldots, y_n$
Initialize $w_1 = \ldots = w_n = \frac{1}{n}$
**for** $i = 1, \ldots, m$ **do**
Fit a classifier $K_i(x)$ to the training data by minimizing weighted error function

$$J_i = \sum_{j=1}^{n} w_j \mathbb{I}(K_i(x_j) \neq y_j)$$

where $\mathbb{I}$ is the indicator function
Compute weighting coefficient

$$\alpha_i = \ln\left(\frac{1-\epsilon_i}{\epsilon_i}\right) \qquad \text{where } \epsilon_i = \frac{J_i}{\sum_{j=1}^{n} w_j}$$

Update all data weights:

$$w_j := w_j \exp\left(\alpha_i \mathbb{I}(K_i(x_j) \neq y_j)\right)$$

Final Model

$$K(x) = \mathit{sign}\left(\sum_{i=1}^{m} \alpha_i K_i(x)\right)$$

# Classification: Summary

| | Model | Compactness | Model Interpretability | Decision Interpretability |
|---|---|---|---|---|
| **Linear Model** | hyperplane | compact (# dims) | medium/low | low |
| **SVM** | hyperplane/non-linear(kernel) | compact (# SV) | medium/low | low |
| **Decision Tree** | set of (axis-parallel) hyperplanes | compact (pruned) | good | good (rules) |
| ***k*NN** | no model | no model | no model | medium/good (example) |
| **Bayes** | statistical density distribution | model dependent | model dependent | medium/good (probabilities) |

| | Data Types | Robustness | Training Time | Test Time |
|---|---|---|---|---|
| **Linear Model** | arbitrary (kernel) | low | high | low/high (for high-dim) |
| **SVM** | arbitrary (kernel) | high | medium | low/medium |
| **Decision Tree** | categorical & vector | low | low/medium | low |
| ***k*NN** | arbitrary (distance) | high | no training | low (index)/ very high |
| **Bayes** | arbitrary (probability distribution) | high | model-dependent | model-dependent; often low |

# Classification: Conclusion

- Classification is an extensively studied problem (mainly in statistics and machine learning)
- Classification is probably one of the most widely used data mining techniques with a lot of extensions
- Scalability is an important issue for database applications: thus combining classification with database techniques should be a promising topic
- Research directions: classification of complex data, e.g., text, spatial, multimedia, etc.;
  *Example*: $k$NN-classifiers rely on distances but do not require vector representations of data
- Results can be improved by ensemble classification