Database and Information Systems

Data Mining

Data Mining Tasks

- Classification
- Prediction
- Clustering
- Summarization
- Dependency Modelling
- Change and Deviation Detection

Classification

- well understood
    - decision theory
    - many heuristic solutions
- applications in
    - customer relationship management: tailored marketing
    - banking: credit authorization
    - document management: e-mail routing

Classification

- given
  - a data base $D = \{t_1, t_2, ..., t_n\}$
  - of tupels $t_i = \vec{x}$ and
  - a set of classes $C = \{c_1, c_2, ..., c_m\}$,
- find a mapping $f : D \rightarrow C$
  - such that f partitions D.

Classification

- classes are predefined:
  supervised learning, learning with a teacher
- notation
  - $c_t(t_i)$: class assignment in the training data
  - $c(t_i)$: class assignment by the classifier
- usually: $|D| \gg |C|$
- class is a set of tuples: $c_j = \{t_i | f(t_i) = c_j\}$
- no tuple belongs to several classes

Classification

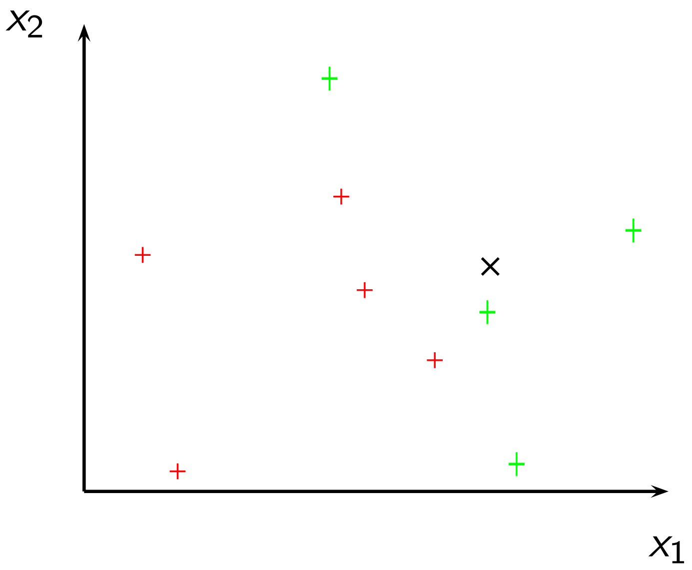
- Nearest-Neighbor Classifier
- Threshold-based Classifiers
- Decision Trees
- Neural Networks
- Stochastic Classification
- Evaluation

Nearest-Neighbor Classifier

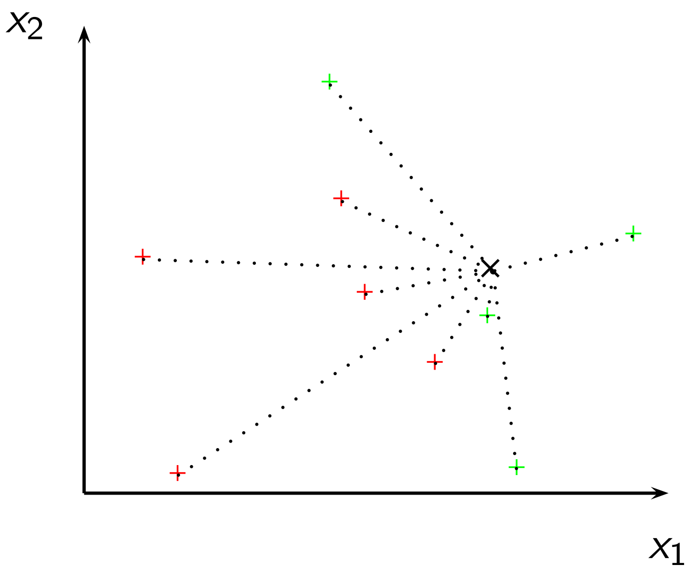
- direct approach: training data $T = \{(\vec{x}_i, k)\}$ are
  - directly stored in the classifier and
  - used for classification
- nearest neighbor

$$c(\vec{x}) = \arg_{c_k}(\vec{x}_j, k), \quad j = \arg\min_i d(\vec{x}, \vec{x}_i)$$

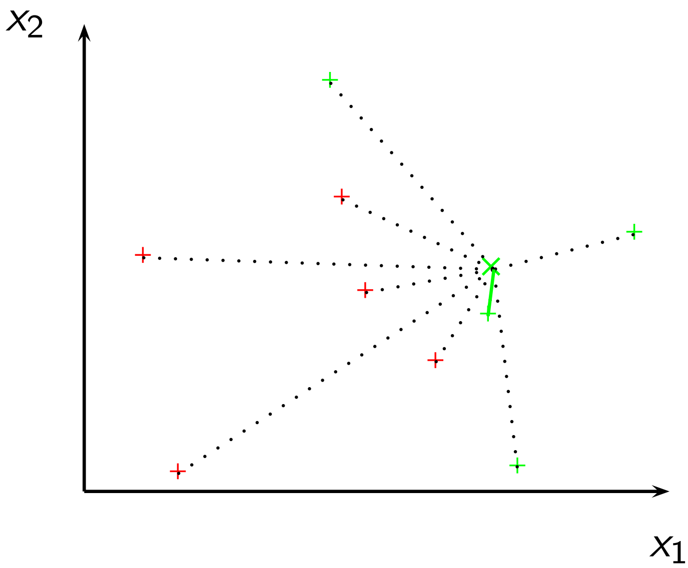
Nearest-Neighbor Classifier



Nearest-Neighbor Classifier



Nearest-Neighbor Classifier



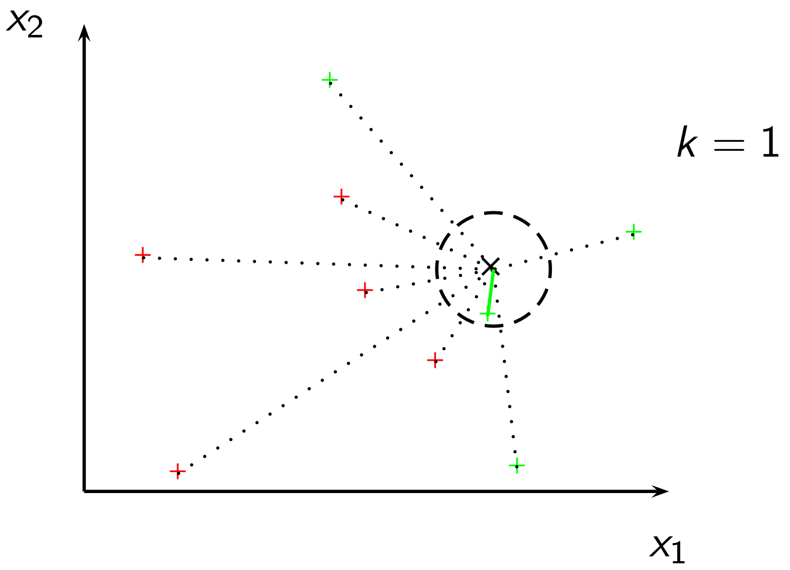
Nearest-Neighbor Classifier

- k-nearest neighbors
  - determine the set N of the k nearest neighbors of $\vec{x}$ in T
  - choose the class with the maximum number of data points in N

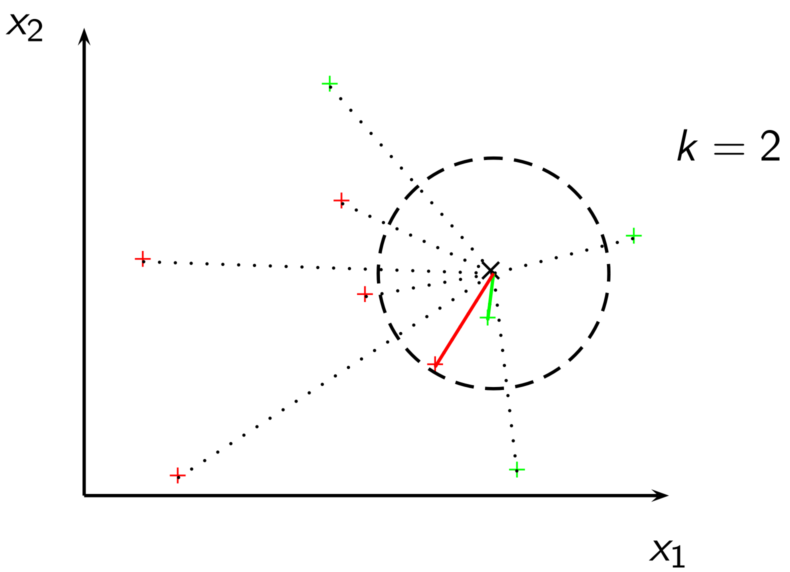
$$c(\vec{x}) = \arg\max_{c_k} |\{c_k | c_k \in N\}|$$

  - more robust against singular data points
  - but more expensive

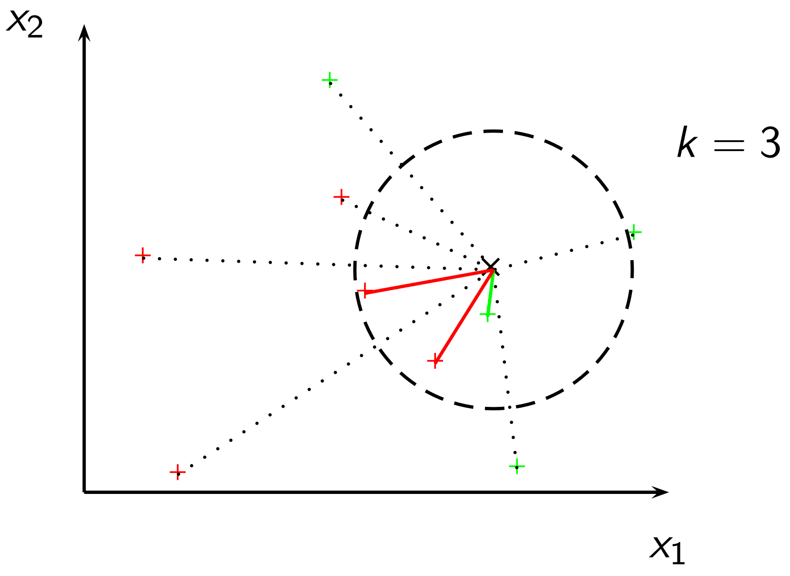
Nearest-Neighbor Classifier



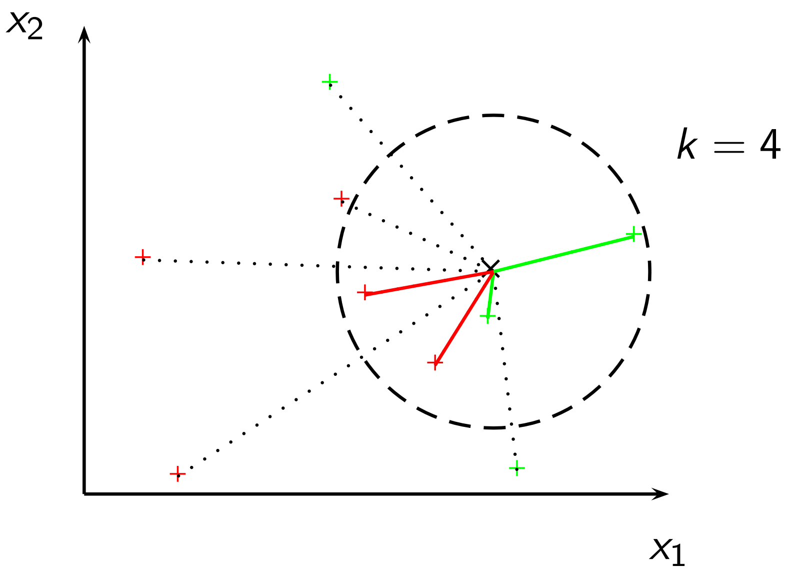
Nearest-Neighbor Classifier



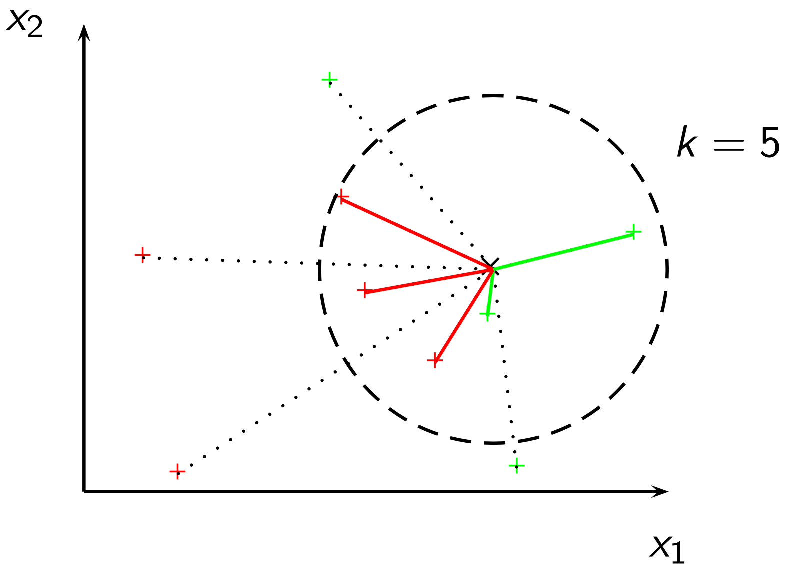
Nearest-Neighbor Classifier



Nearest-Neighbor Classifier



Nearest-Neighbor Classifier



Nearest-Neighbor Classifier

- NN-classifier is instance-based
  - model size and classification effort grow linearly with amount of training data
  - no generalization of the available training data
- generalizing models required
  - use class representatives as data points
  - e.g. mean of class or class-dependent clusters

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Threshold-Based Classifiers

- simple generalizing model
- a threshold divides the data space into two subspaces

$$c(\vec{x}_i) = \begin{cases} 1 & x_j > \theta_j \\ 2 & else \end{cases}$$

- analogue separation criteria for non-numeric data

Threshold-Based Classifiers

- choice of the optimal threshold:
  - minimizing the classification error on the training data

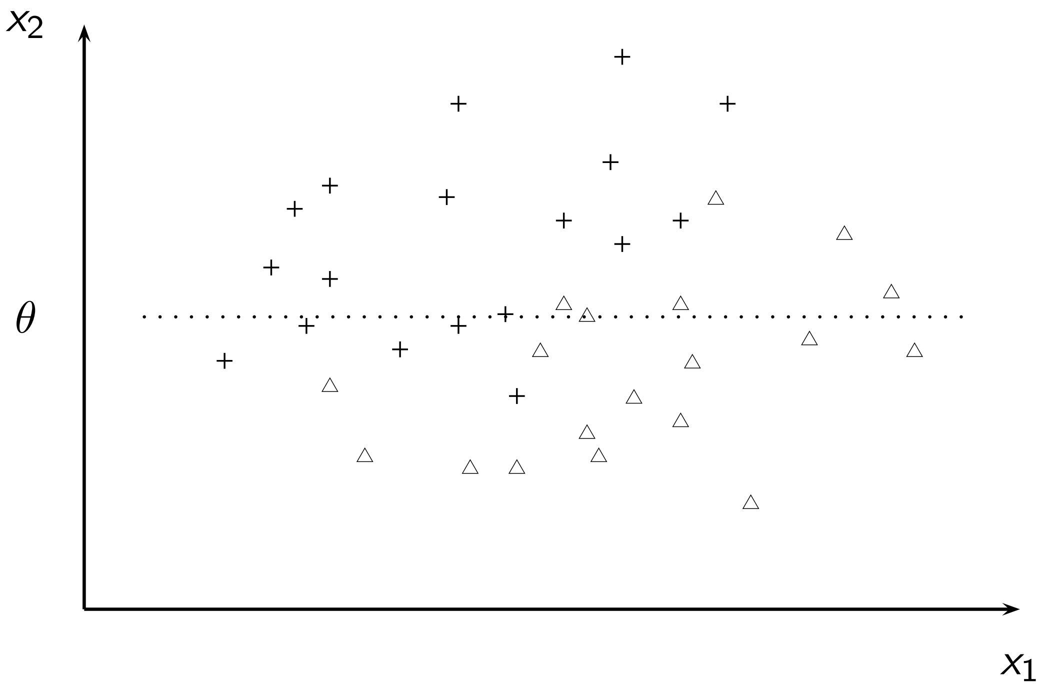
$$\theta = \arg\min_{\theta} |\{t_i | c(t_i) \neq c_t(t_i)\}|$$

  - for numeric data approximated by minimizing the distance of misclassified samples to the threshold

$$\theta = \arg\min_{\theta} \sum_{t_i, c(t_i) \neq c_t(t_i)} |x_j - \theta_k|$$

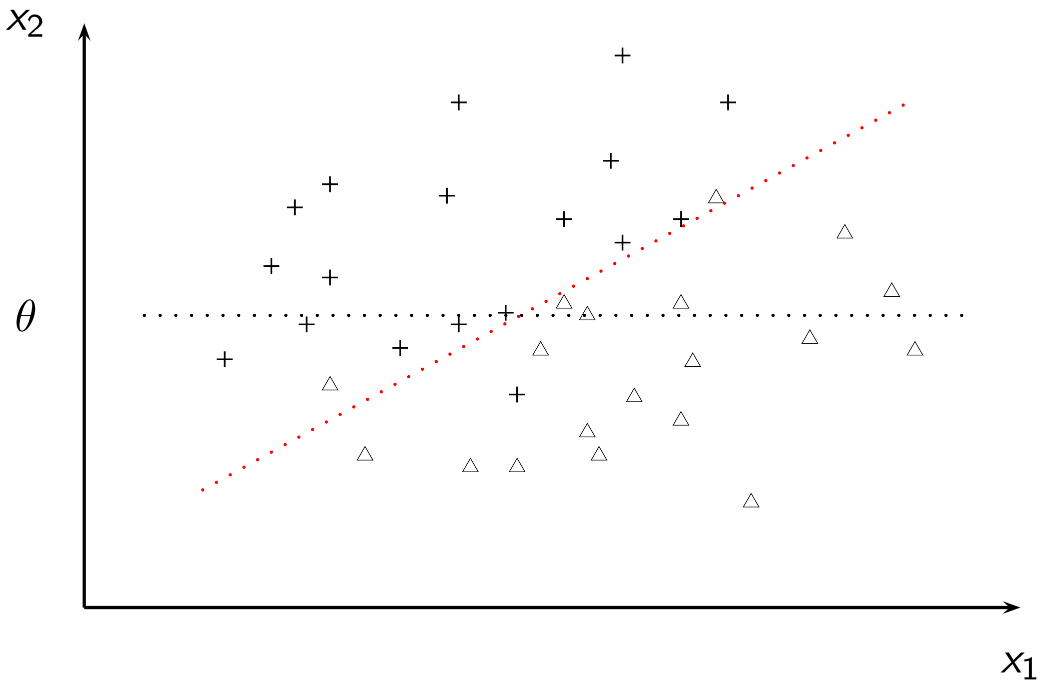
Threshold-Based Classifiers

- insufficient to separate more difficult distributions



Threshold-Based Classifiers

- better class separation



Threshold-Based Classifiers

- algorithm for finding an optimal threshold
  1. sort the values $[v_1, ..., v_m]$
  2. extract $m - 1$ potential thresholds by either
     - computing the mean of all neighboring values or
     - choosing the smaller one of two neighboring values
  3. evaluate all potential thresholds and select the one with the maximum gain

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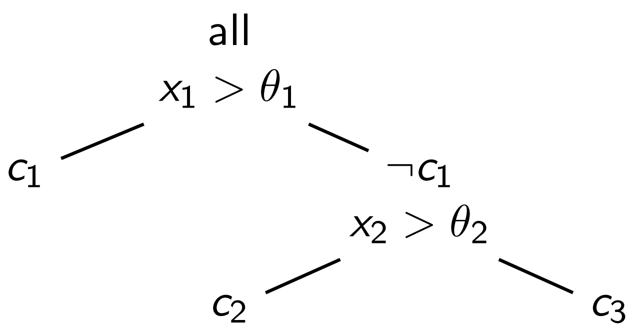
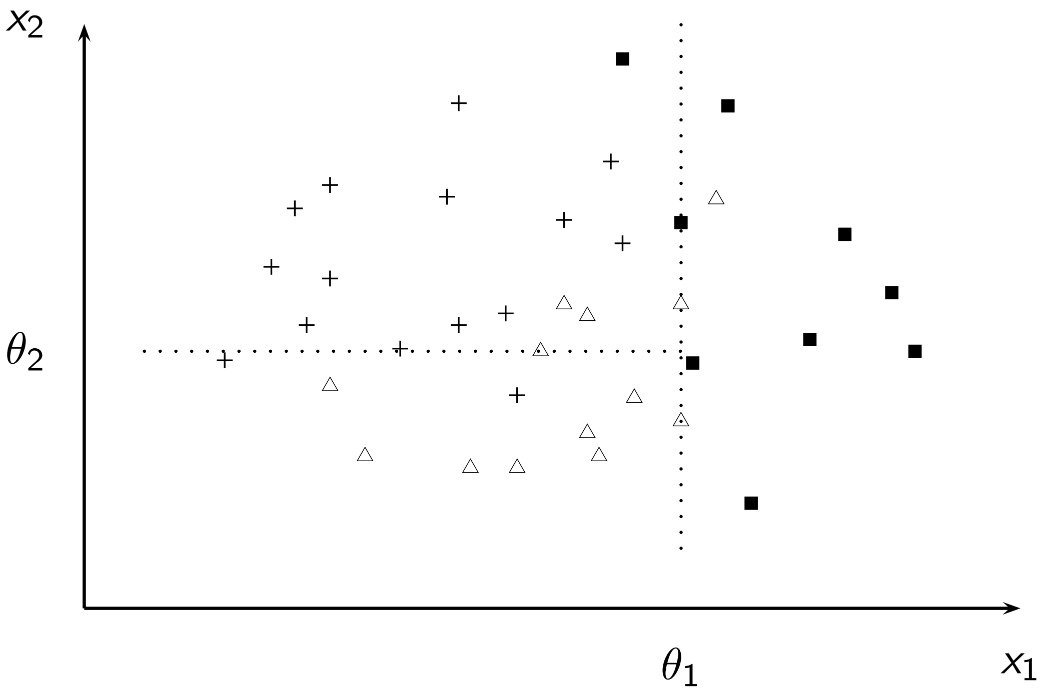
Decision trees

- extension of threshold-based classifiers to multiple classes:
  - multi-branch splits
  - decomposition into a sequence of sub-decisions



- finding the optimal decision tree is NP complete
  $\rightarrow$ deterministic (non-backtracking), greedy algorithms

Decision trees



Decision trees

- ID3: split along a dimension as to maximise information gain
- entropy of a set S partitioned into k classes

$$E(S) = -\sum_{i=1}^{k} p(c_i) \cdot \log p(c_i)$$

- entropy of a test set T partitioned into n subsets by an attribute test X with n possible outcomes

$$E_X(T) = -\sum_{i=1}^{n} \frac{|T_i|}{|T|} \cdot E(T_i)$$

- information gain of the attribute test

$$G(X) = E(T) - E_X(T)$$

Decision trees

- C4.5: extension of ID3 to numerical data
  - split along a dimension so that the resulting subsets have lowest class entropy
    i.e. contain data points of as few classes as possible
- problem of overfitting
  - splitting until no data point is misclassified usually means to adapt the classifier too much to the training data
    - "learning off by heart"
    - degrading performance on held out test data
  - cut-off criterion required, or post-pruning

Decision trees

- decision rules can be extracted from a decision tree
  - IF part: combine all tests on the path from the root node to the leave node
  - THEN part: the final classification

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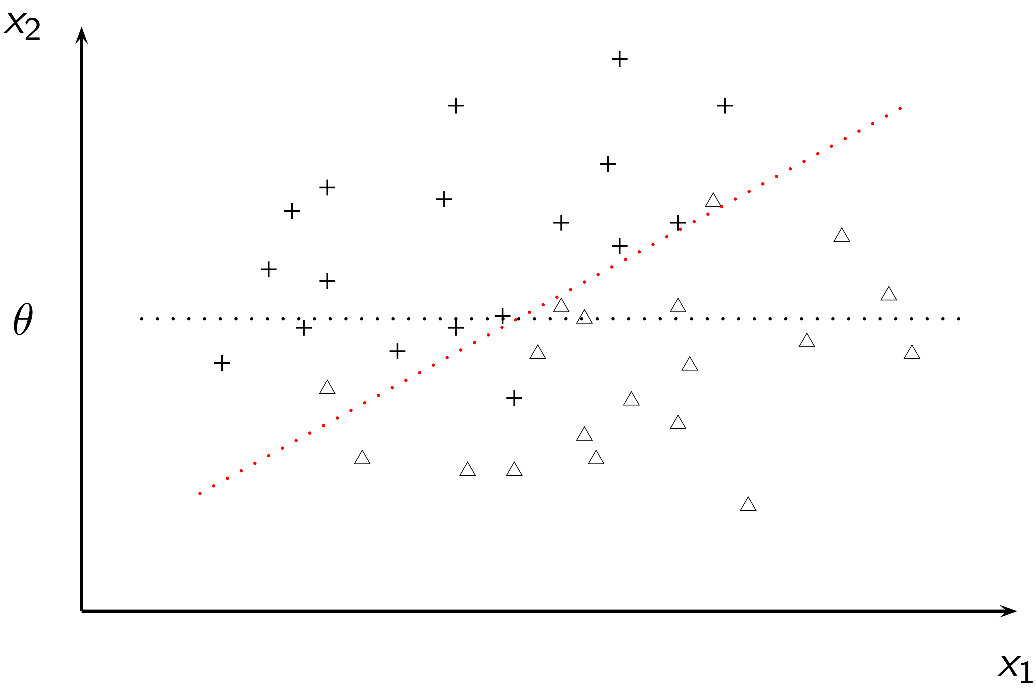
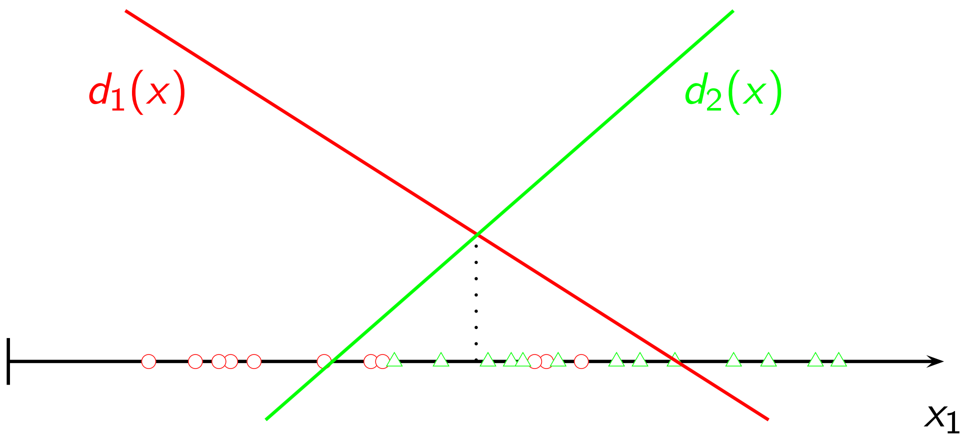
Neural Networks

- sometimes linear functions can be used to separate two classes



Neural Networks

- classes are represented by means of linear discrimination functions $d_k(\vec{x})$



$\longrightarrow$ linear discriminance analysis (LDA)

Neural Networks

- class decision is reduced to a maximum detection

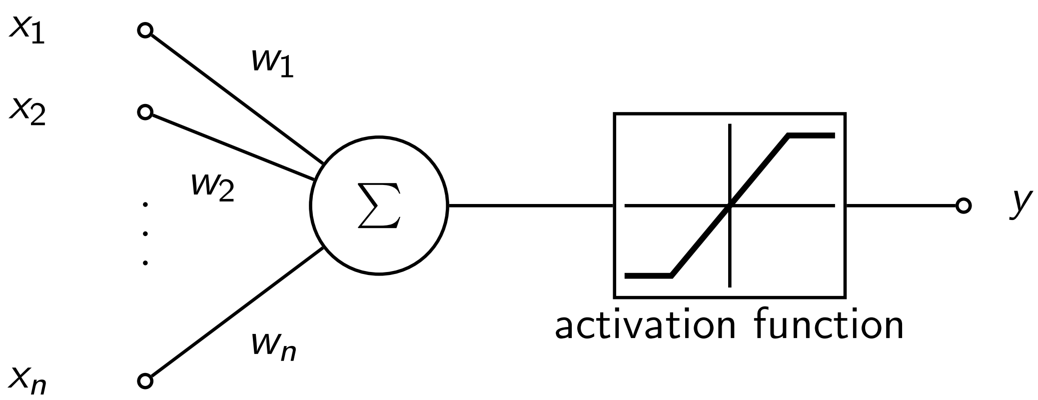
$$c(\vec{x}) = \arg\max_{c_k} d_k(\vec{x})$$

- discriminating functions are (in the simplest case) linear combinations of the components of a data point

$$d_k(\vec{x}) = w_0 + \sum w_i x_i$$

Neural Networks

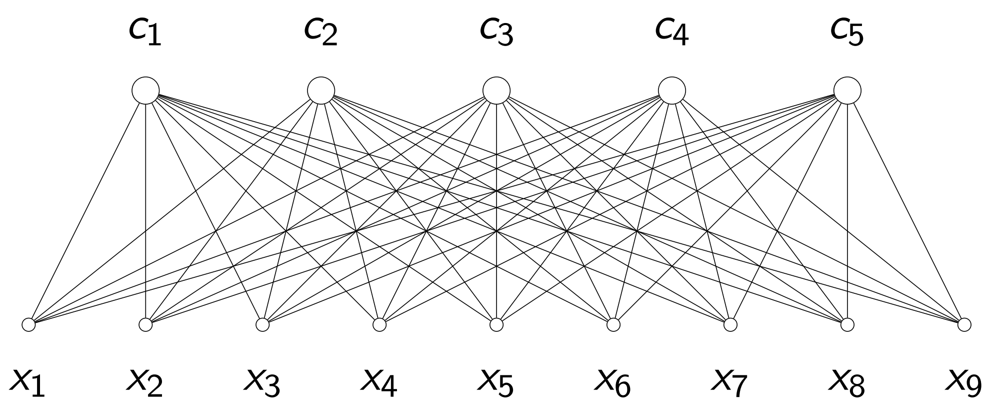
- corresponds to first part of a perceptron



- single perceptron: classification only for
  - two class problems and
  - linear separable classes

Neural Networks

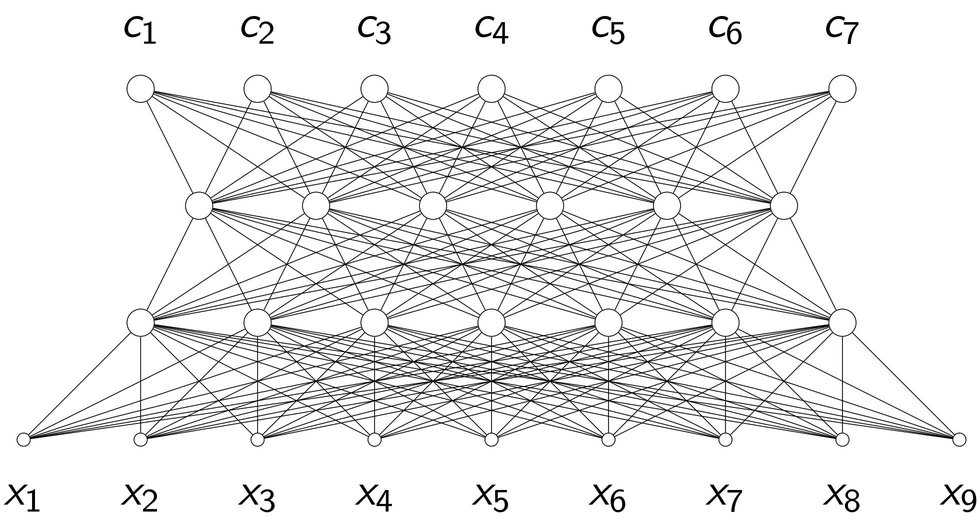
- extension to multiple classes: single-layer networks



- class decision: maximum detection ("the winner takes all")

Neural Networks

- multiple perceptrons simulate a piecewise-linear discrimination function
- single layer networks only for simple problems
  → usually multiple-layer networks required

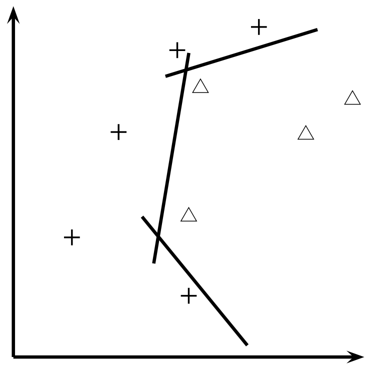


Neural Networks

- optimal architecture has to be determined experimentally
- only few heuristic criteria available

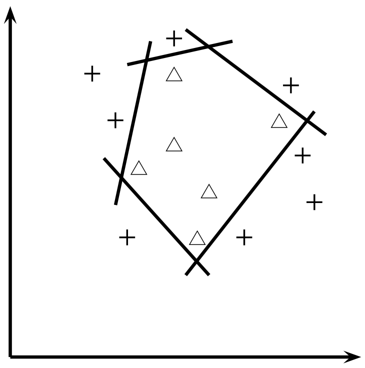
Neural Networks

- How many layers are necessary?



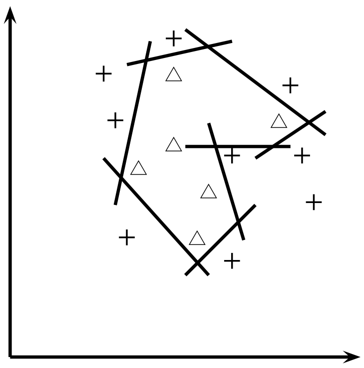
single-layer network

no islands



two-layer network

only convex islands



three-layer network

also concave islands

Neural Networks

- How many nodes per layer are required?
  - the more nodes, the smoother the class separation
  - the more nodes, the more training data and training cycles are required

Neural Networks

- training of neuronal networks
- error driven learning
  - assume an initial (random) assignment of synaptic weights w_{ij}
  - determine the error of the output value of a node i: $e_i = \frac{(y_i - d_i)^2}{2}$
  - change the weights w_{ij} according to a learning rule
  - continue with the next training sample
- backpropagation of the error signal from the output layer to the input layer

Neural Networks

- examples of learning rules
  - Hebb rule

    $$\Delta w_{ij} = \eta \, x_{ij} \, y_j$$

    η: learning rate (approx $1/|T|$)
    does not consider the desired output
  - delta rule

    $$\Delta w_{ij} = \eta \, x_{ij} \, (d_j - y_j)$$

  - learning rules with momentum

    $$\Delta w_{ij}(n) = \eta \, x_{ij} \, (d_j - y_j) + \alpha \, \Delta w_{ij}(n-1)$$

Neural Networks

- gradient descent search: all weights are changed until no significant change of the global error measure can be observed
  - high number of training iterations is required
  - local search: optimum is not guaranteed
  - not even convergence of the algorithm is guaranteed

Neural Networks

- problems
  - many parameters have to be determined empirically
    - number of layers, number of nodes per layer
    - learning rate, momentum
    - initialization
    - termination criterion
  - overfitting may occur
    - stop training early enough
    - choose the most simple architecture possible

Neural Networks

- decision rules can be extracted from a neural network
  - cluster the node activations
  - generate rules from high synaptic links
  - combine the rules across layers

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Stochastic Classification

- Bayesian inference
  - given: a prior data distribution
  - observe data
  - infer a posterior distribution
- Bayes' theorem

$$p(c_k|\vec{x}) = \frac{p(\vec{x}|c_k) \cdot p(c_k)}{p(\vec{x})}$$

  - $p(\vec{x})$ does not influence a class decision
  - $p(\vec{x}|c_k)$ and $p(c_k)$ have to be estimated using the available training data

Stochastic Classification

- $p(c_k)$: class probability

$$p(c_k) = \frac{|c_k|}{|S|}$$

- $p(\vec{x}|c_k)$: data generation (or emission) model
  - more difficult to estimate
  - simplifying assumption:
    conditional independence between attributes

  $\rightarrow$ naïve / simple Bayesian classifier

$$p(\vec{x}|c_k) = \prod_{i=1}^{n} p(x_i|c_k)$$

- training method: maximum likelihood (ML) estimation

Stochastic Classification

- classification rule

$$k = \arg\max_k p(c_k|\vec{x}) = \arg\max_k p(\vec{x}|c_k) \cdot p(c_k)$$

- Bayes classifier has optimal error rates
- but: in practice worse because of the independence assumption

Stochastic Classification

- problems with non-trivial input output dependencies
  - strongly correlated variables
  - time series analysis
- Bayesian networks
- emission probabilities are conditioned on the state of the model
- state of the model is not directly observable $\rightarrow$ hidden variable
- simplifying assumption: state probabilities depend only on the preceding state
- ML training requires direct counting of observations
- alternative: expectation maximization (EM)
  - start with an initial probability estimation
  - modify the current probabilities as to better fit the training data
- resulting probabilities are only approximations

Comparison of classifiers

	Nearest Neighbor	Decision Trees	(Linear) Discriminance	Stochastic Models
model	sample set	ranking of tests	class boundaries	probabilistic generation
generalization	no	forced	yes	yes
robust against				
incons. data	no	now	yes	yes
outliers	only k-NN	low	yes	yes
perspicuity	high	high	low	low
scalability	very low	low	good	very good
additional assumptions	metrics	no	architecture learning rule	(architecture) distribution

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Evaluation

- goal: predicting future model performance
  - estimation of an error rate on a sample of test cases
- testing on the training data is too optimistic
  - error rate is significantly lower compared to a real application scenario

  $\longrightarrow$ evaluation only on separate data: test set
- but: available test set data is usually limited
  - manual data cleansing
  - manual class assignment
- using data for training and testing: resampling

Resampling Methods

- held out data
  - 30% ... 50% of the data are reserved for testing
  - training and test data are independent
  - error estimation is pessimistic and depends on the partitioning
    $\longrightarrow$ repeat the measurement with different partitionings and average
- leave one out
  - use $n - 1$ samples for training and evaluate on the n-th one
  - repeat with all n samples
  - extremely expensive

Resampling Methods

- n-fold cross validation
  - combines hold-out and leave-one-out
  - divide data set into p partions
  - use $p-1$ partitions for training; evaluate on the remaning one
- bootstrapping
  - generate artificial training data by replacing data items
  - obtain bootstrap estimations of the error rates on these data sets
  - useful if few data are available

Quality Measures

- error rate

$$e = \frac{|M|}{|S|}$$

  S: test set, $M \subseteq S$: misclassified data
- accuracy

$$a = 1 - e = \frac{|S| - |M|}{|S|}$$

- only for atomic data!

Quality Measures

- contrastive analysis:
  - absolute improvement/degradation: comparison with a baseline case

$$\Delta_{abs} a = a_n - a_{n+1}$$

  - relative improvement/degradation

$$\Delta_{rel} a = \frac{a_n - a_{n+1}}{a_n}$$

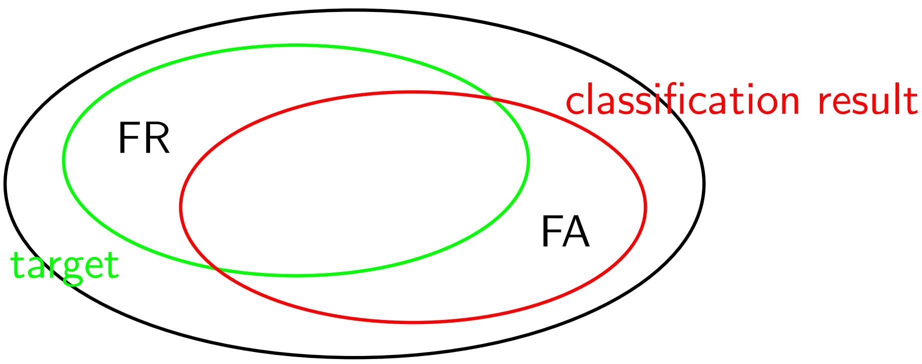
Quality Measures

- special case: 2 classes (true/false) $\rightarrow$ 2 error cases
- false positives/acceptance: false acception rate (sensitivity)

$$FAR = \frac{|\{x|c(x) = \text{true} \neq c_t(x)\}|}{|\{x|c(x) = \text{true}\}|}$$

- false negatives/rejection: false rejection rate (specificity)

$$FRR = \frac{|\{x|c(x) = \text{false} \neq c_t(x)\}|}{|\{x|c(x) = \text{false}\}|}$$



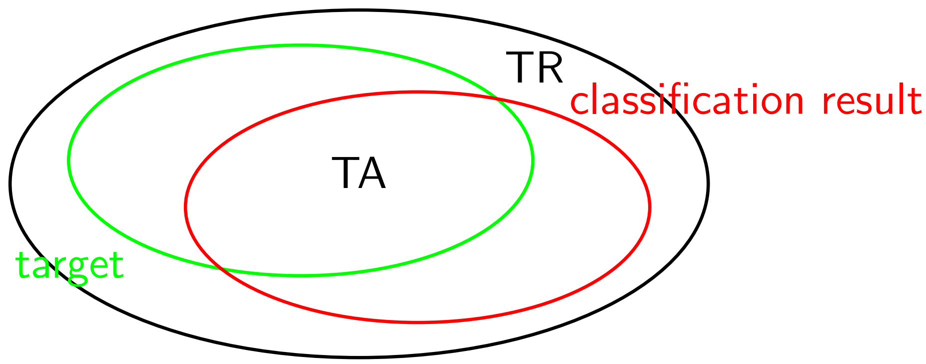
Quality Measures

- true positives/acceptance: true acception rate

$$TAR = \frac{|\{x|c(x) = \text{true} = c_t(x)\}|}{|\{x|c(x) = \text{true}\}|}$$

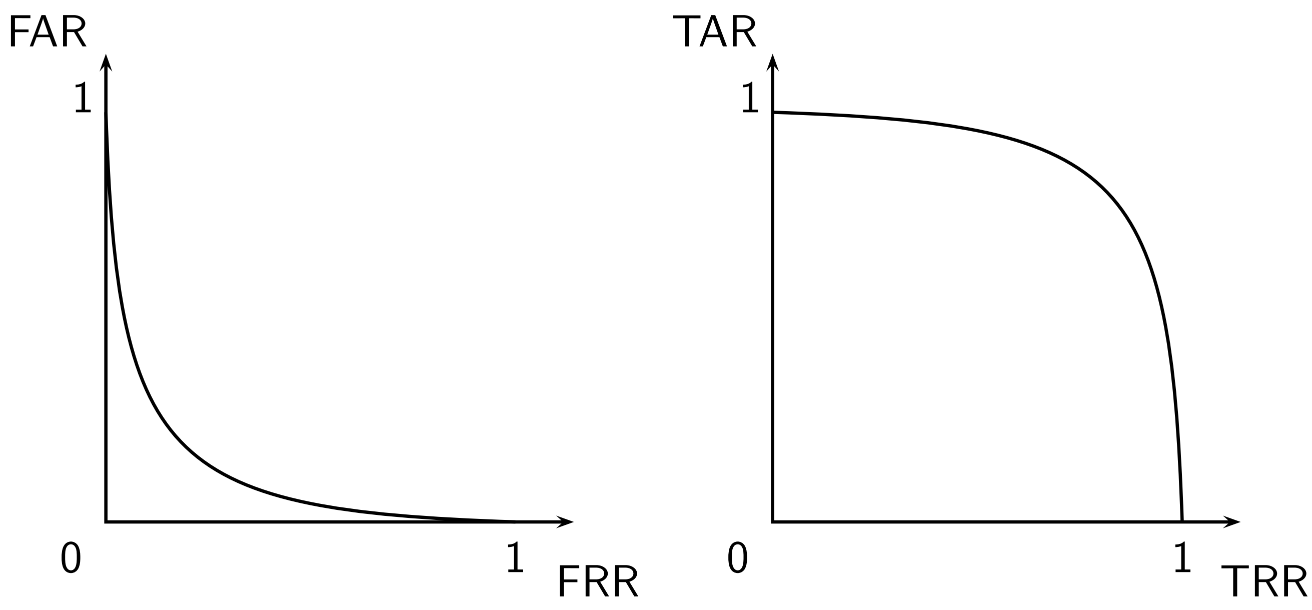
- true negatives/rejection: true rejection rate

$$TRR = \frac{|\{x|c(x) = \text{false} = c_t(x)\}|}{|\{x|c(x) = \text{false}\}|}$$



Quality Measures

- trade-off between FAR and FRR / TAR and TRR

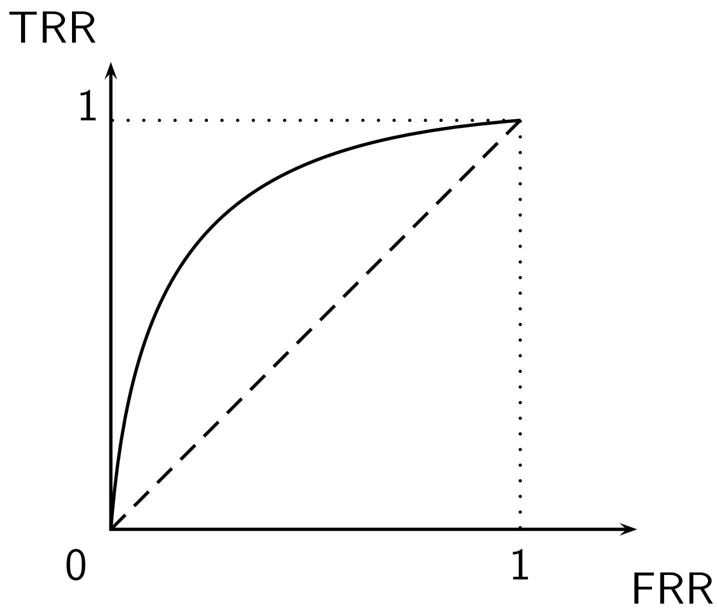


- trivial classifier: upper threshold for the error rate

$$e_{max} = \min(p(\text{true}), p(\text{false}))$$

Quality Measures

- receiver operating characteristic (ROC): TRR vs. FRR



- quality: area under the ROC-curve

Quality Measures

- in general $k^2 - k$ (k: number of classes) error types
- description of the error type distribution as a confusion matrix
- biased error consequences: weighted error measures
  - error types e_{ij} are associated with costs c_{ij}

$$e_w = \frac{\sum_{i=1}^{m} \sum_{j=1}^{m} e_{ij} \cdot c_{ij}}{|S|}$$