Database and Information Systems

Data Mining

- Data-Mining: The Task
- Data-Mining as a Process
- Data Preprocessing
- Data Mining Tasks

Data Mining Tasks

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

Classification

- well understood
  - decision theory
  - many heuristic solutions
- many problems can be mapped to a classification task
- 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

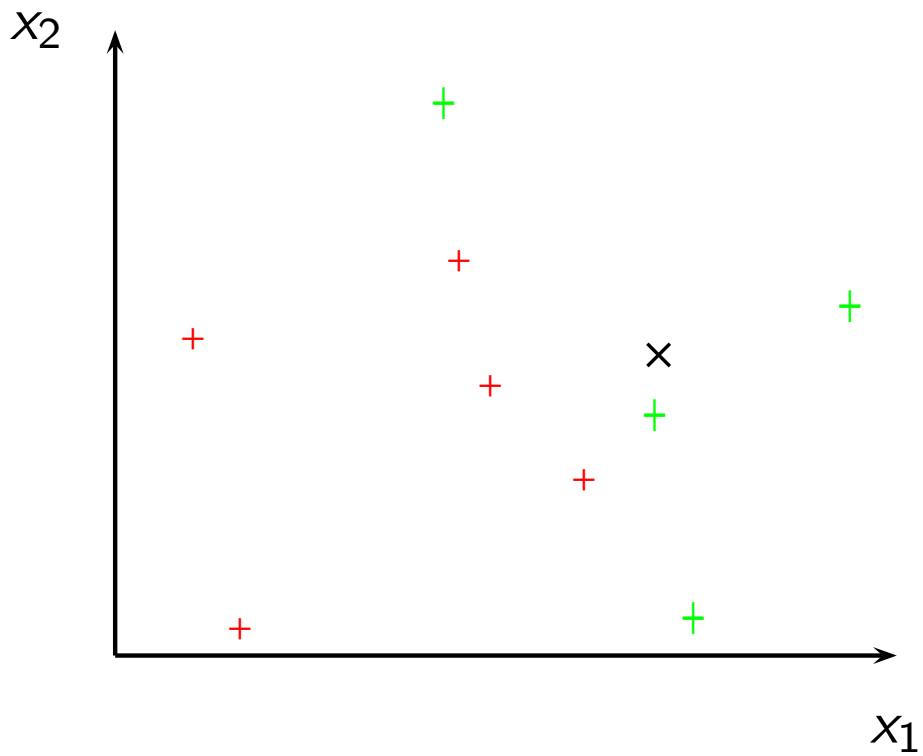
- Nearest-Neighbor Classifier
- Threshold-based Classifiers
- Decision Trees
- Random Forests
- Neural Networks
- Stochastic Classification
- Evaluation

Nearest-Neighbor Classifier

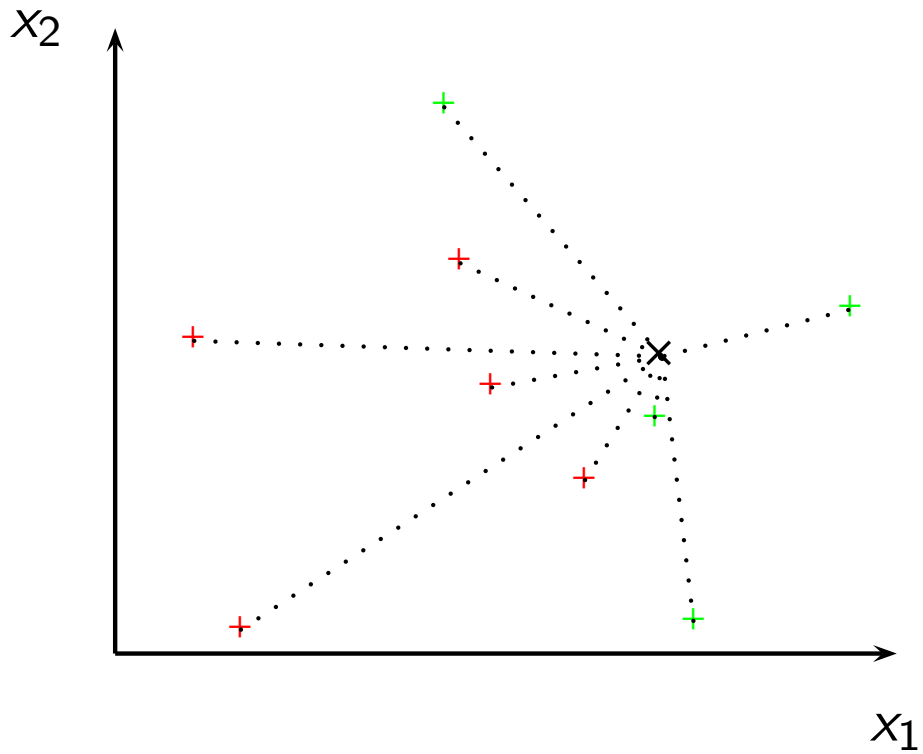
- direct approach: training data $T = \{(\vec{x}_i, k)\}$ are
  - directly stored in the classifier and
  - used for classification
- nearest neighbor

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

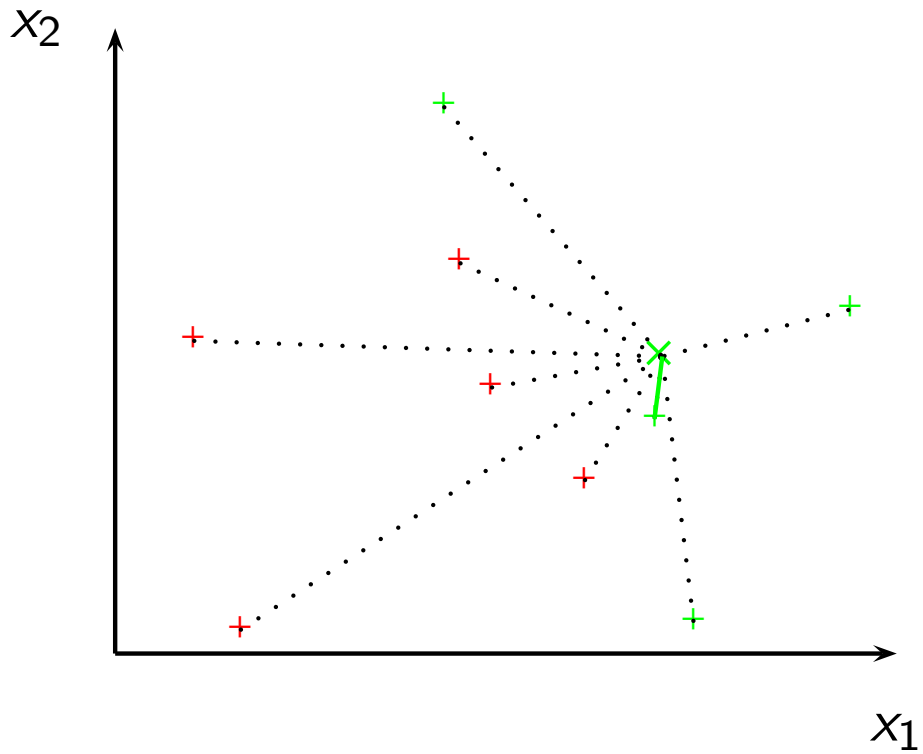
Nearest-Neighbor Classifier



Nearest-Neighbor Classifier



Nearest-Neighbor Classifier



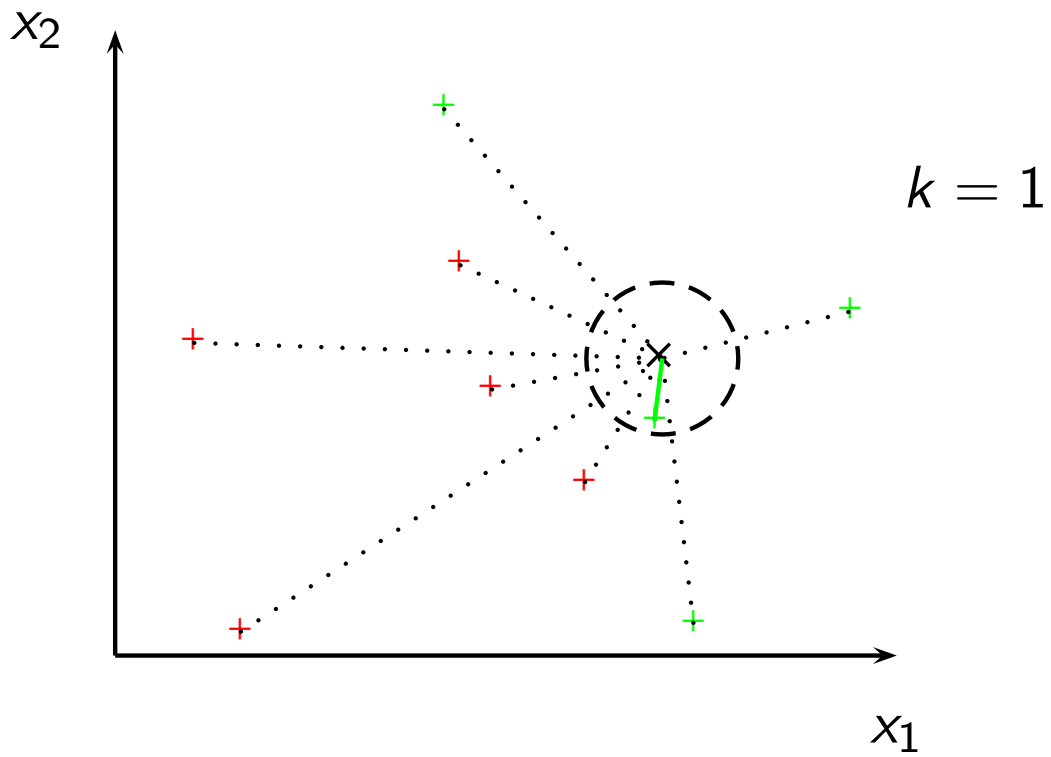
Nearest-Neighbor Classifier

- 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

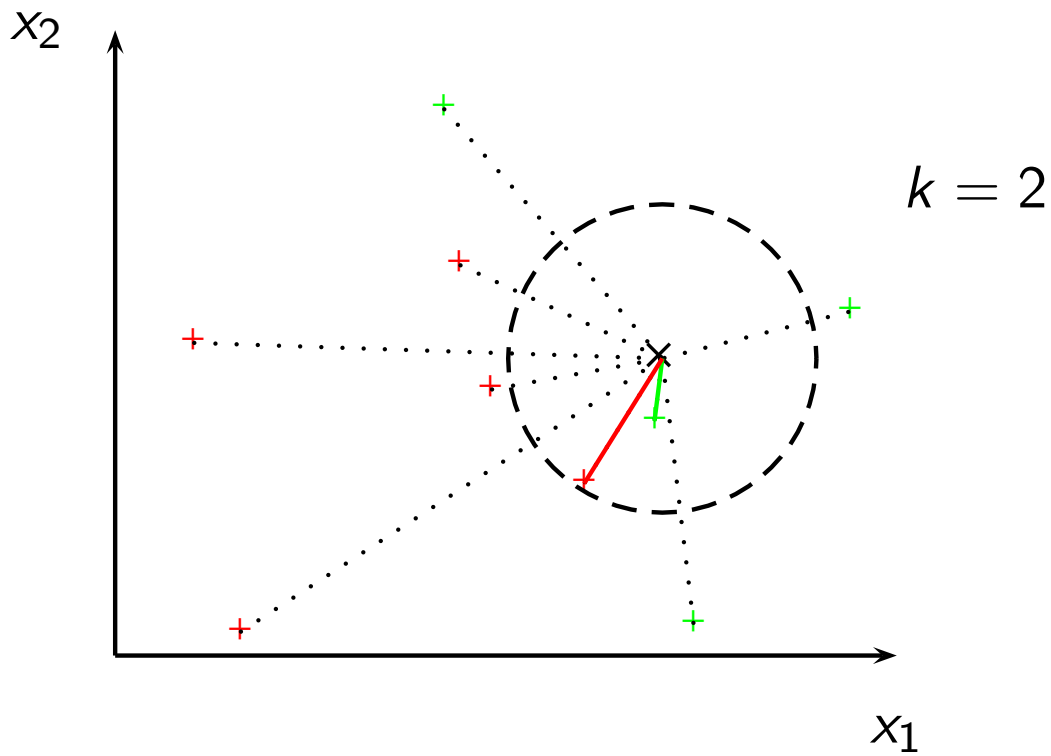
$$c(\vec{x}) = \arg\max_{c_k} |\{c_k | c_k \in N\}|$$

  - more robust against singular data points
  - but more expensive

Nearest-Neighbor Classifier



Nearest-Neighbor Classifier



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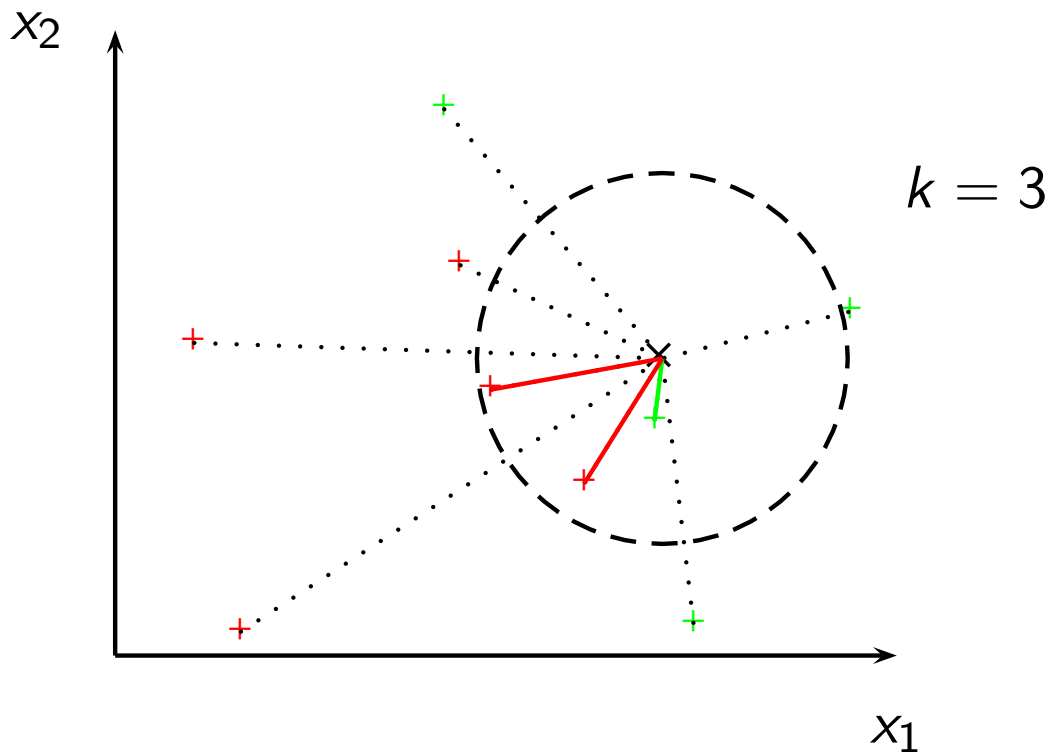
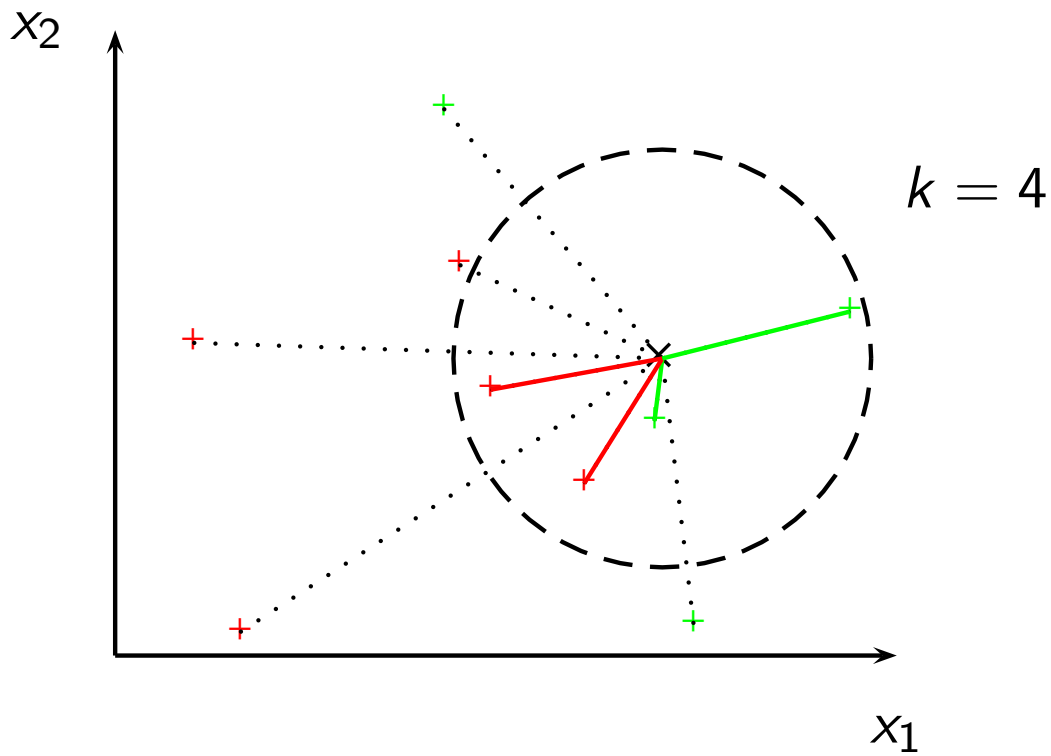
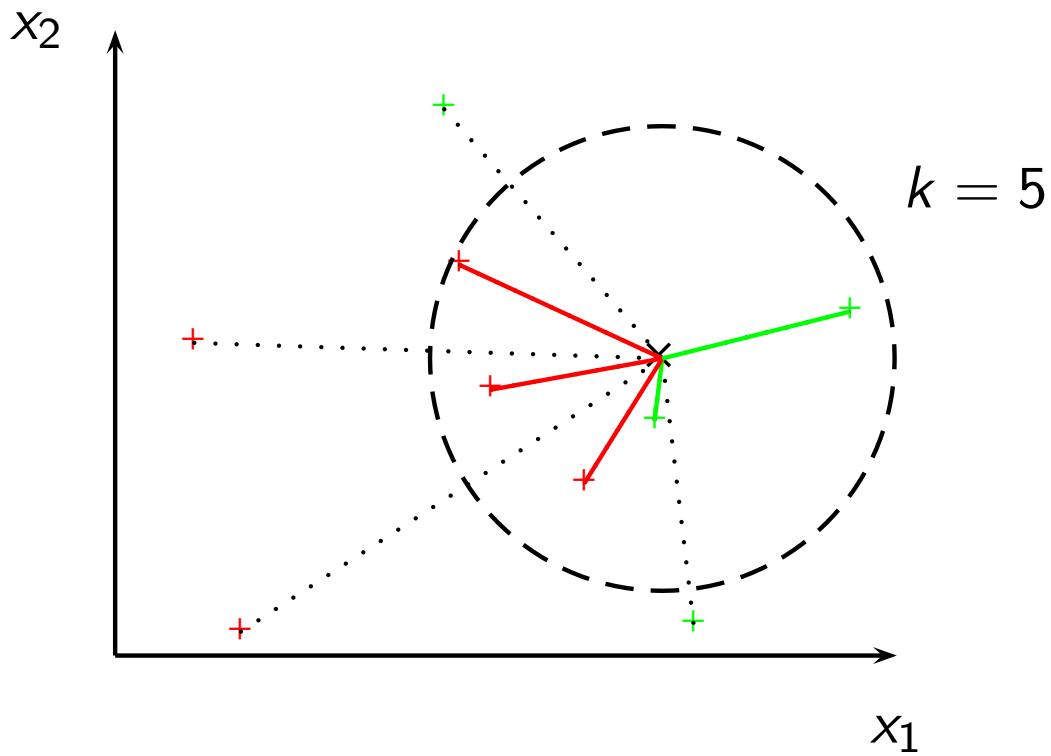


Nearest-Neighbor Classifier



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

Classification

- Nearest-Neighbor Classifier
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Threshold-Based Classifiers

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

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

- analogue separation criteria for non-numeric data

Threshold-Based Classifiers

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

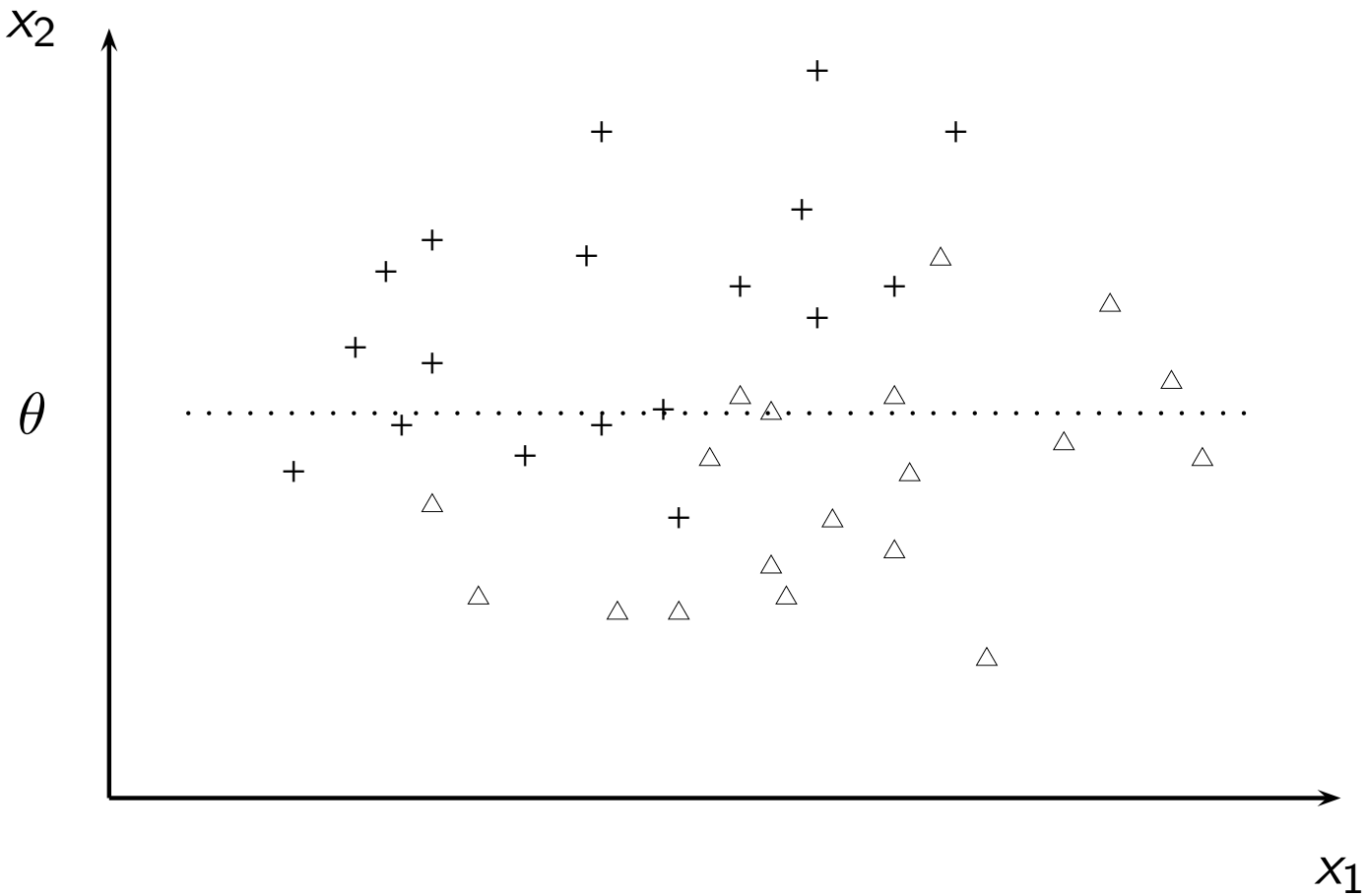
$$\theta = \arg\min_{\theta} |\{t_i | c(t_i) \neq c_t(t_i)\}|$$

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

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

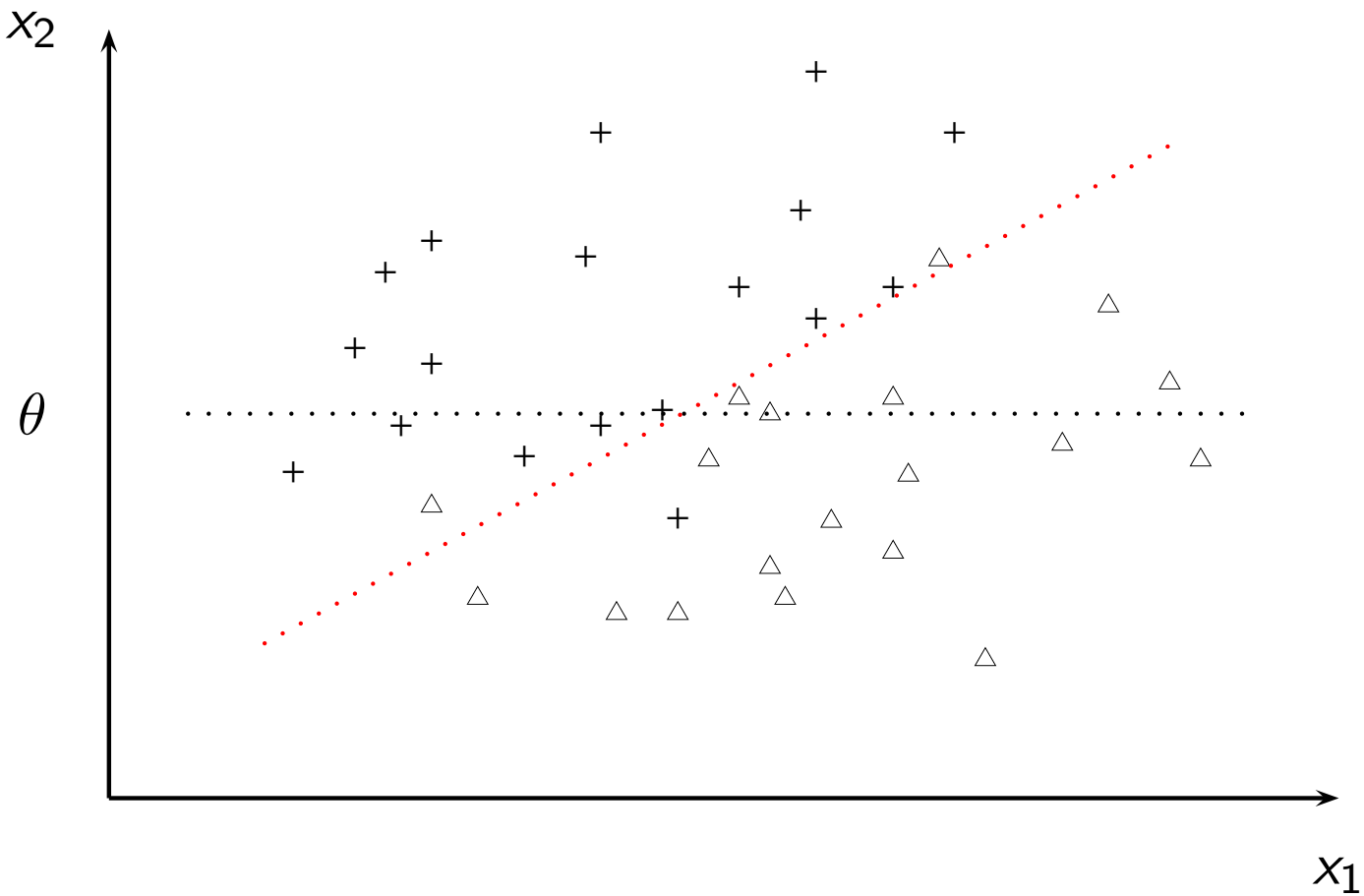
Threshold-Based Classifiers

- 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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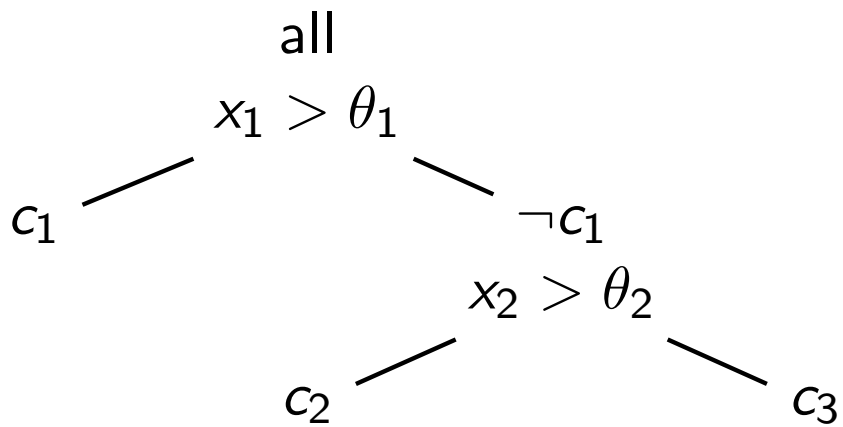
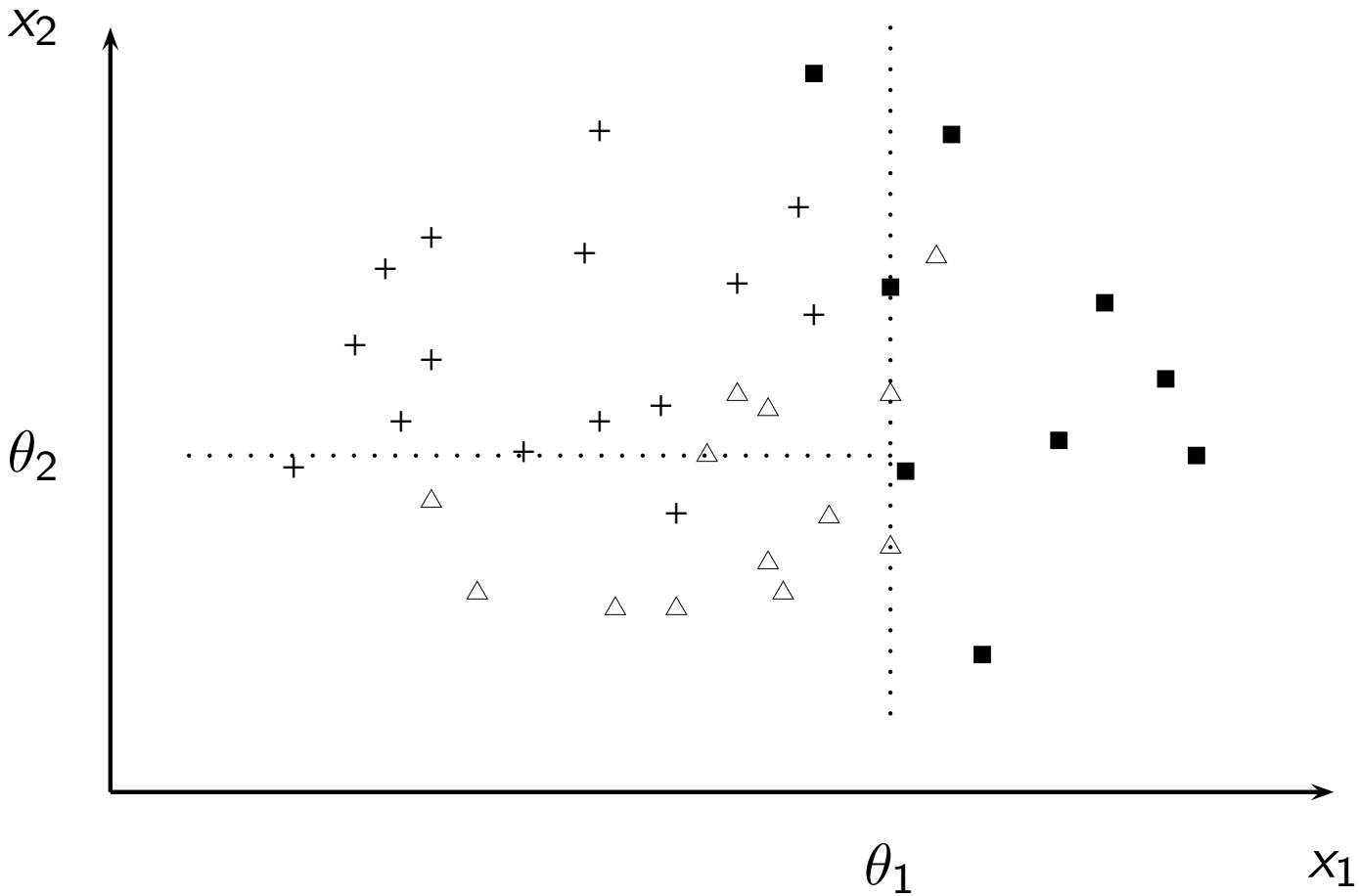
Decision trees

- 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 leaf node
  - THEN part: the final classification

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Random Forests

- ensemble based method
- goal: reducing the effect of "almost" random split decisions
- forcing the training to consider alternative splits

- given: N training instances with M variables
- T random samples (with replacement) with a sample size $S \approx 0.66N$; the remaining instances are used for estimating the prediction error (out-of-bag evaluation)
- for each node of the tree $m \ll M$ variables are selected randomly to take the decision at that node
- no pruning is applied

- classification: (weighted) majority vote among the results of the individual trees

Random Forests

- highly accurate classifiers without much prior knowledge
- fast training
- highly parallel classification
- can deal with very large problems (training data, number of variables, number of classes)
- estimates the importance of the different variables
- build-in evaluation; no separate test data required

Random Forests

- prone to overfitting, in particular for noisy data sets
- does not handle large amounts of irrelevant features
- sensitive to correlations between trials: "small heterogeneous is better than large homogeneous" (Gashler et al. 2008)
  - growing too many trees might reduce the accuracy

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	no	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

  $\rightarrow$ 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
    $\rightarrow$ 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

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

$$\Delta_{abs} e = e_n - e_{n-1}$$

  - relative improvement/degradation

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

$$\Delta_{rel} e = \frac{e_n - e_{n-1}}{e_n}$$

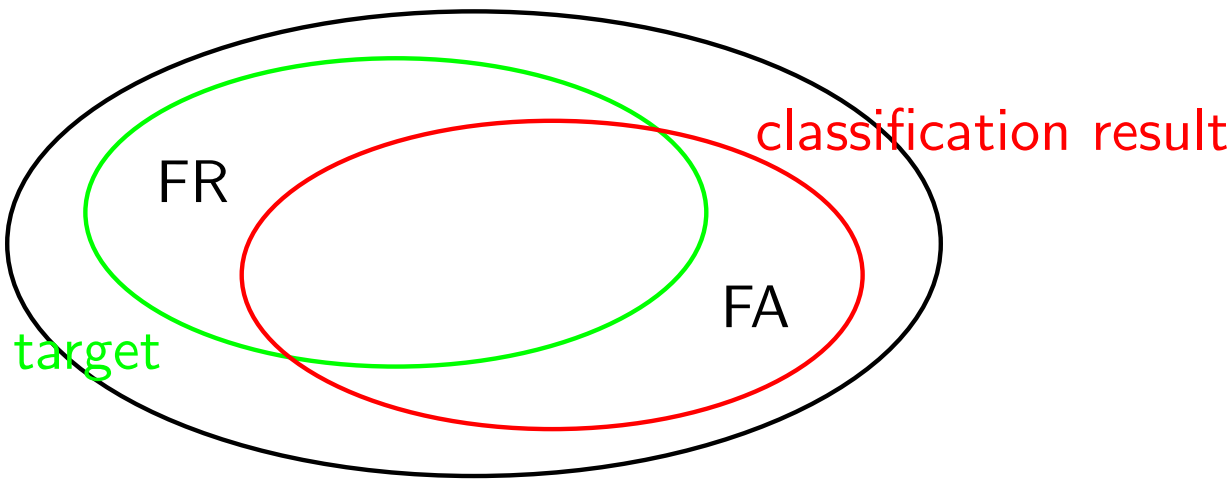
Quality Measures

- 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)

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



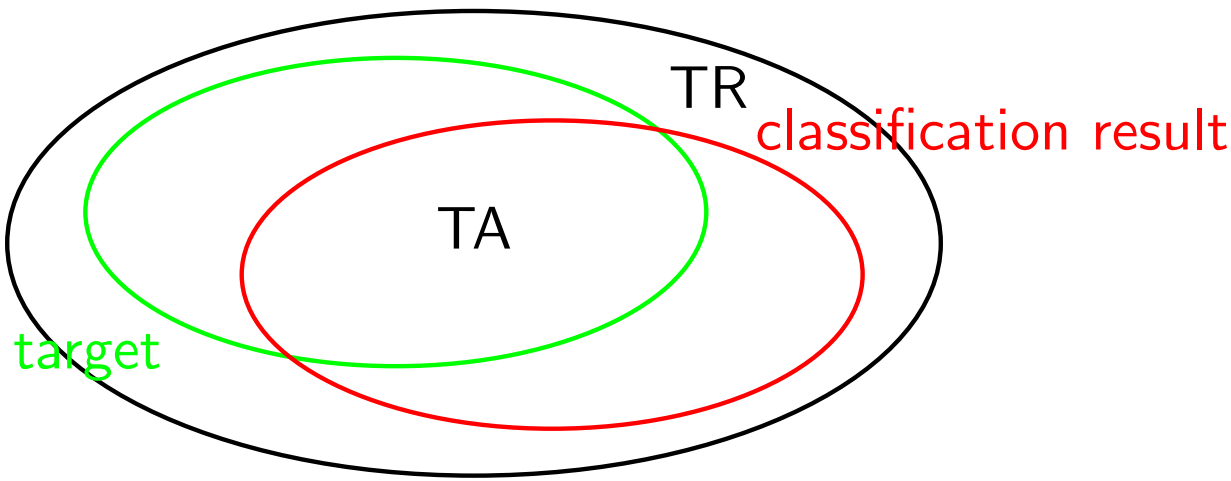
Quality Measures

- true positives/acceptance: true acception rate

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

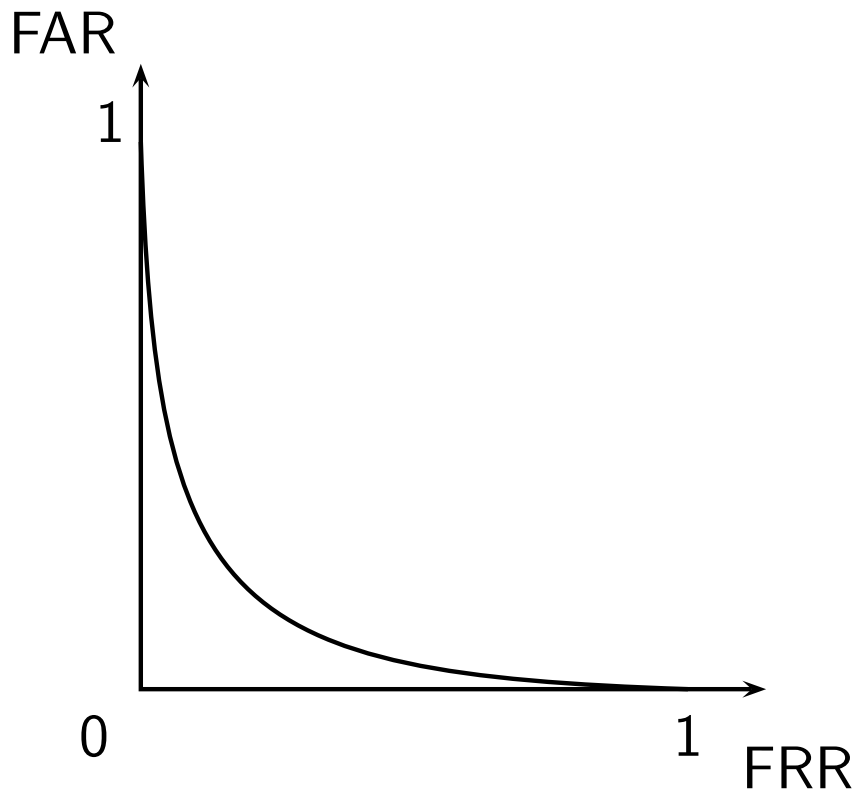
- true negatives/rejection: true rejection rate

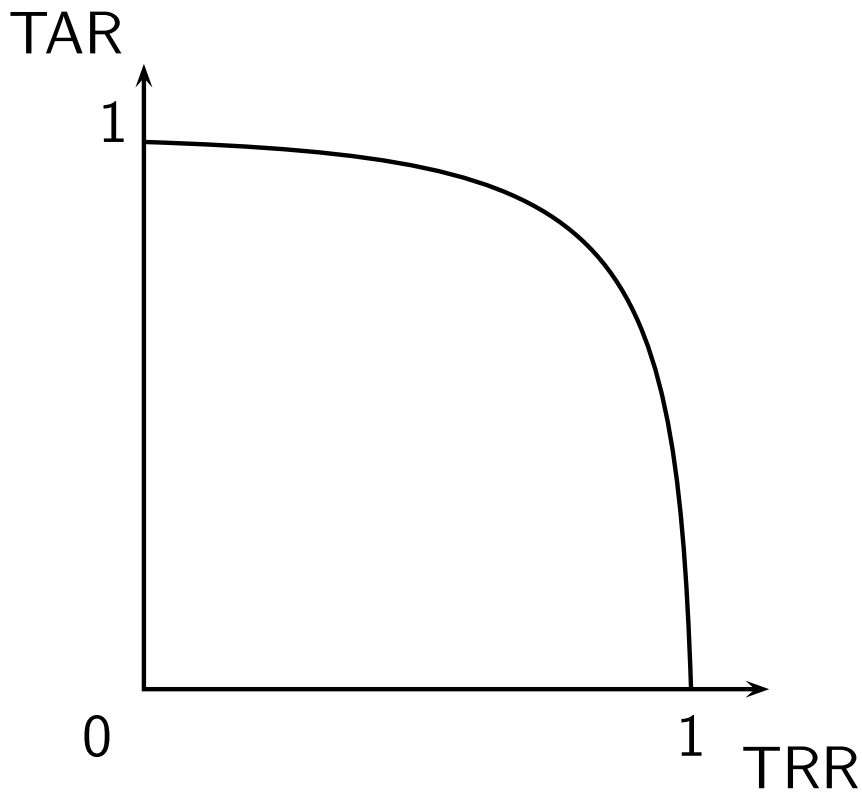
$$TRR = \frac{|\{x|c(x) = \text{false} = c_t(x)\}|}{|\{x|c(x) = \text{false}\}|}$$



Quality Measures

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



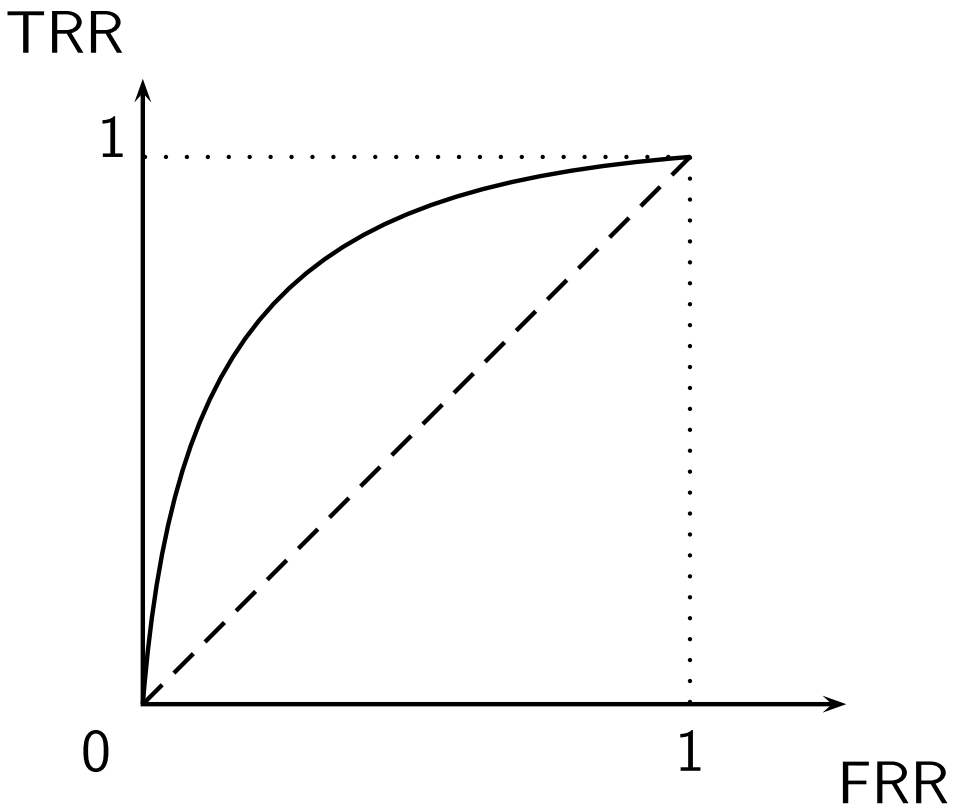


- trivial classifier: upper threshold for the error rate

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

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}

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