Data Mining und Maschinelles Lernen

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Ensemble Methods

- Bias-Variance Trade-off
- Basic Idea of Ensembles
- Bagging
  - Basic Algorithm
  - Bagging with Costs

- Randomization
  - Random Forests
- Boosting
- Stacking
- Error-Correcting Output Codes (ECOC)

Bias and Variance Decomposition

- Bias:
  - the part of the error that is caused by bad model
- Variance:
  - the part of the error that is caused by the data sample

- Bias-Variance Trade-off:
  - algorithms that can easily adapt to any given decision boundary are very sensitive to small variations in the data
    - and vice versa
  - Models with a low bias often have a high variance
    - e.g., nearest neighbor, unpruned decision trees
  - Models with a low variance often have a high bias
    - e.g., decision stump, linear model

Ensemble Classifiers

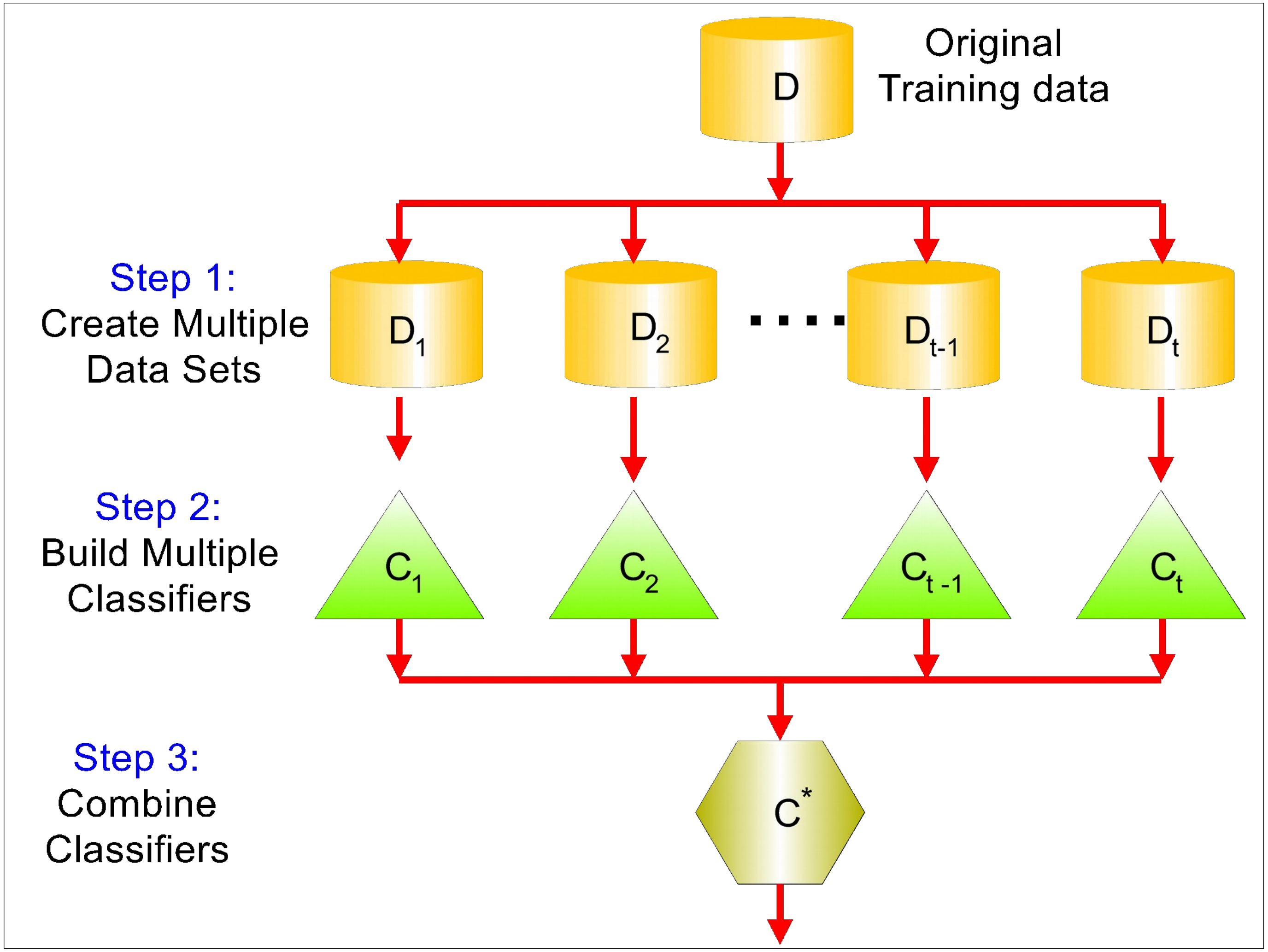
- IDEA:
  - do not learn a *single* classifier but learn a *set of classifiers*
  - *combine the predictions* of multiple classifiers
- MOTIVATION:
  - reduce variance: results are less dependent on peculiarities of a single training set
  - reduce bias: a combination of multiple classifiers may learn a more expressive concept class than a single classifier
- KEY STEP:
  - formation of an ensemble of *diverse* classifiers from a single training set

Why do ensembles work?

- Suppose there are 25 base classifiers
  - Each classifier has error rate, $\varepsilon = 0.35$
  - Assume classifiers are independent
    - i.e., probability that a classifier makes a mistake does not depend on whether other classifiers made a mistake
    - **Note:** in practice they are not independent!
- Probability that the ensemble classifier makes a wrong prediction
  - The ensemble makes a wrong prediction if the majority of the classifiers makes a wrong prediction
  - The probability that 13 or more classifiers err is

$$\sum_{i=13}^{25} \binom{25}{i} \varepsilon^i (1-\varepsilon)^{25-i} \approx 0.06 \ll \varepsilon$$

Bagging: General Idea



Generate Bootstrap Samples

- Generate new training sets using sampling with replacement (bootstrap samples)

Original Data	1	2	3	4	5	6	7	8	9	10
Bagging (Round 1)	7	8	10	8	2	5	10	10	5	9
Bagging (Round 2)	1	4	9	1	2	3	2	7	3	2
Bagging (Round 3)	1	8	5	10	5	5	9	6	3	7

  - some examples may appear in more than one set
  - some examples will appear more than once in a set
  - for each set of size n, the probability that a given example appears in it is

$$\Pr(x \in D_i) = 1 - \left(1 - \frac{1}{n}\right)^n \to 0.6322$$

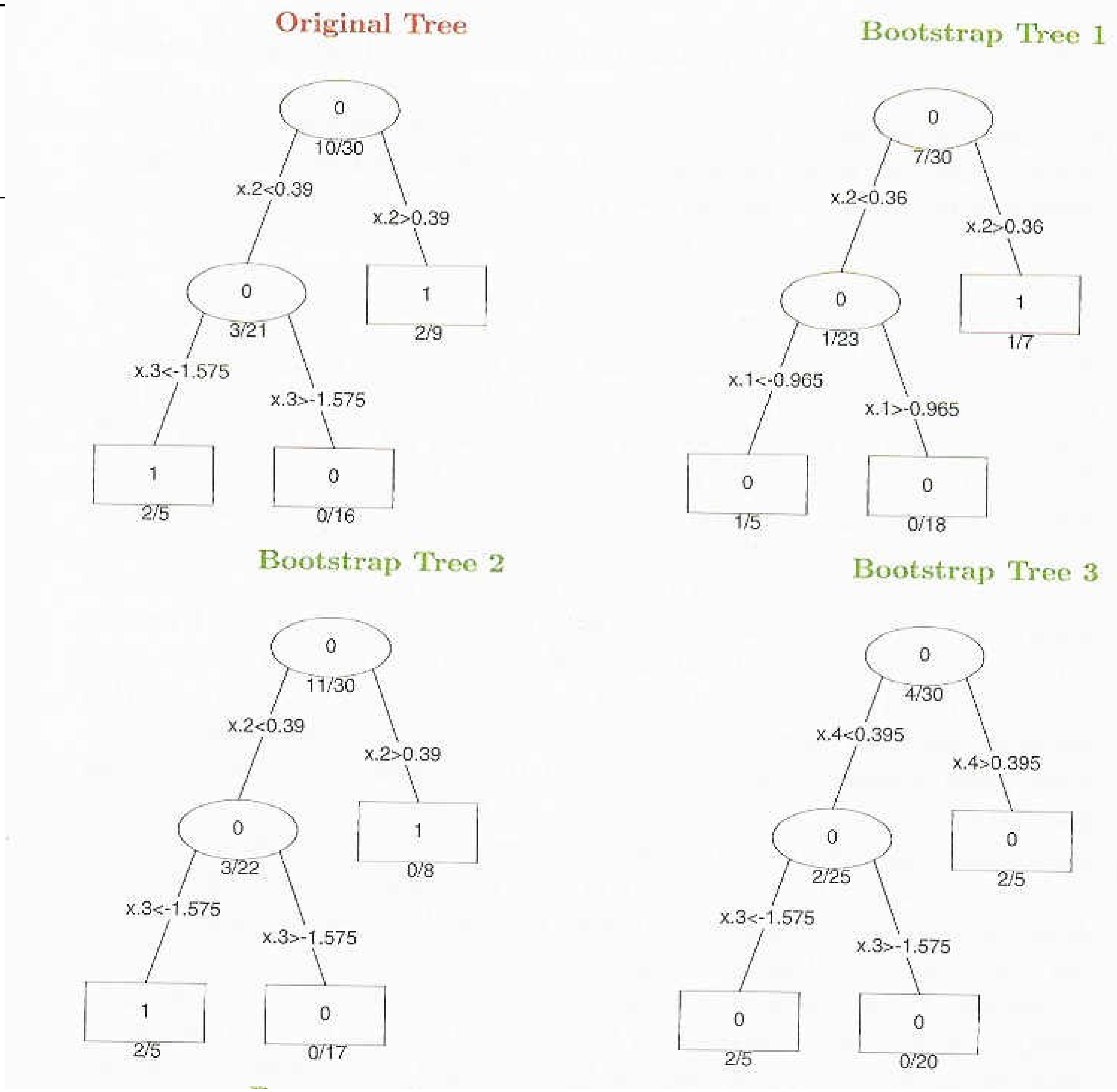
    - i.e., on average, less than 2/3 of the examples appear in any single bootstrap sample

Bagging Algorithm

1. for $m = 1$ to t // t ... number of iterations
   a) draw (with replacement) a bootstrap sample D_m of the data
   b) learn a classifier C_m from D_m
2. for each test example
   a) try all classifiers C_m
   b) predict the class that receives the highest number of votes

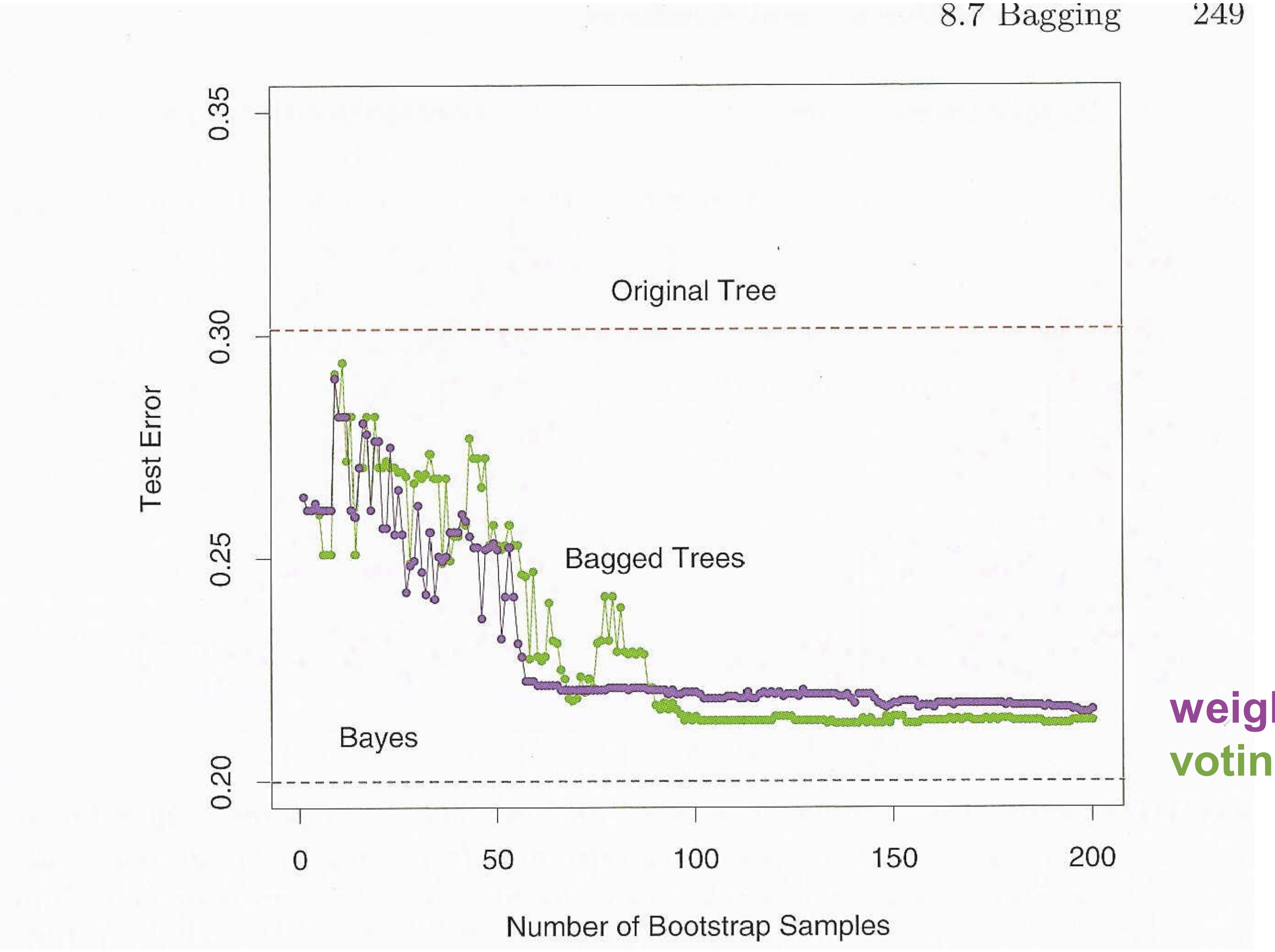
- variations are possible
  - e.g., size of subset, sampling w/o replacement, etc.
- many related variants
  - sampling of features, not instances
  - learn a set of classifiers with different algorithms

Bagged Decision Trees



from Hastie, Tibshirani, Friedman: The Elements of Statistical Learning, Springer Verlag 2001

Bagged Trees



weighted voting

voting

from Hastie, Tibshirani, Friedman: The Elements of Statistical Learning, Springer Verlag 2001

Bagging with costs

- Bagging unpruned decision trees is known to produce good probability estimates
  - Where, instead of voting, the individual classifiers' probability estimates $\Pr_n(j \mid x)$ are averaged

$$\Pr(j|x) = \frac{1}{t} \sum_{n=1}^{t} \Pr_n(j|x)$$

  - Note: this can also improve the error rate
- We can use this with minimum-expected cost approach for learning problems with costs
  - predict class c with $c = \arg\min_i \sum_j C(i|j) \Pr(j|x)$
- Problem: not interpretable
  - *MetaCost* re-labels training data using bagging with costs and then builds single tree (Domingos, 1997)

Randomization

- Randomize the learning algorithm instead of the input data
- Some algorithms already have a random component
  - eg. initial weights in neural net
- Most algorithms can be randomized, e.g. greedy algorithms:
  - Pick from the N best options at random instead of always picking the best options
  - Eg.: test selection in decision trees or rule learning
- Can be combined with bagging

Random Forests

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- Combines bagging and random attribute subset selection:
  - Build the tree from a bootstrap sample
  - Instead of choosing the best split among all attributes, select the best split among a random subset of k attributes
    - is equal to bagging when k equals the number of attributes
- There is a bias/variance tradeoff with k:
  - The smaller k, the greater the reduction of variance but also the higher the increase of bias

Boosting

- Basic Idea:
  - later classifiers focus on examples that were misclassified by earlier classifiers
  - weight the predictions of the classifiers with their error
- Realization
  - perform multiple iterations
    - each time using different example weights
  - weight update between iterations
    - increase the weight of incorrectly classified examples
    - this ensures that they will become more important in the next iterations (misclassification errors for these examples count more heavily)
  - combine results of all iterations
    - weighted by their respective error measures

Boosting – Algorithm AdaBoost.M1

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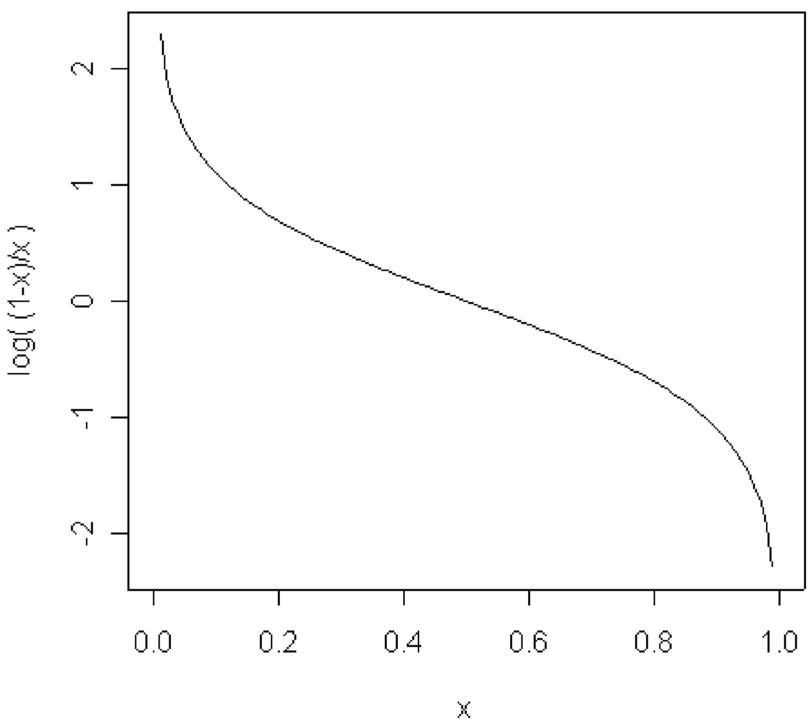
1. initialize example weights $w_i = 1/N \quad (i = 1..N)$
2. for $m = 1$ to t // t ... number of iterations
   a) learn a classifier C_m using the current example weights
   b) compute a weighted error estimate $$err_m = \frac{\sum w_i \text{ of all incorrectly classified } e_i}{\sum_{i=1}^{N} w_i}$$
   c) compute a classifier weight $$\alpha_m = \frac{1}{2} \ln\left(\frac{1-err_m}{err_m}\right)$$
   d) for all correctly classified examples e_i: $w_i \leftarrow w_i e^{-\alpha_m}$
   e) for all incorrectly classified examples e_i: $w_i \leftarrow w_i e^{\alpha_m}$
   f) normalize the weights w_i so that they sum to 1
3. for each test example
   a) try all classifiers C_m
   b) predict the class that receives the highest sum of weights α_m

= 1 because weights are normalized

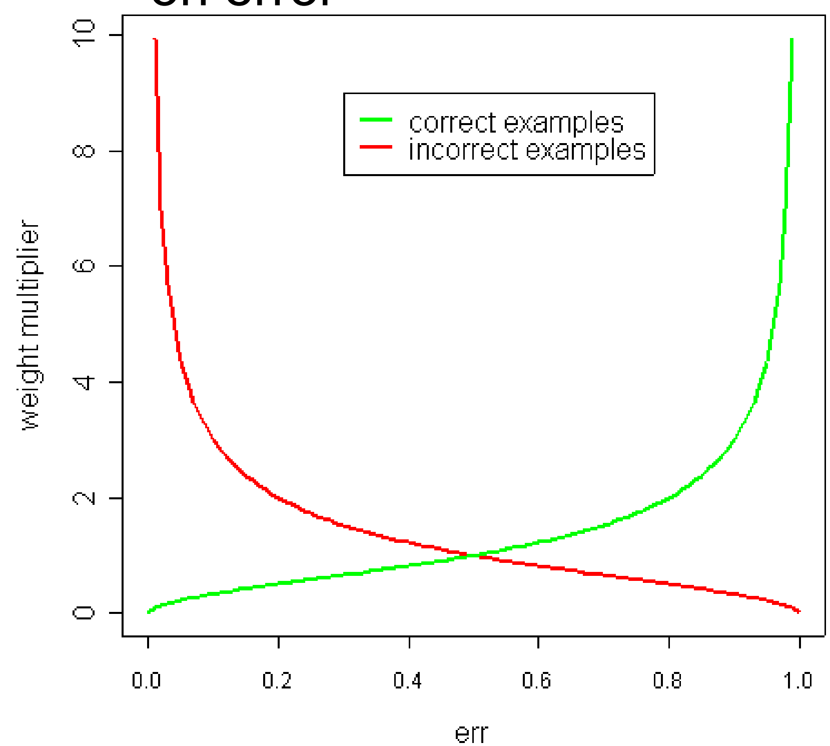
update weights so that sum of correctly classified examples equals sum of incorrectly classified examples

Illustration of the Weights

- Classifier Weights α_m
  - differences near 0 or 1 are emphasized

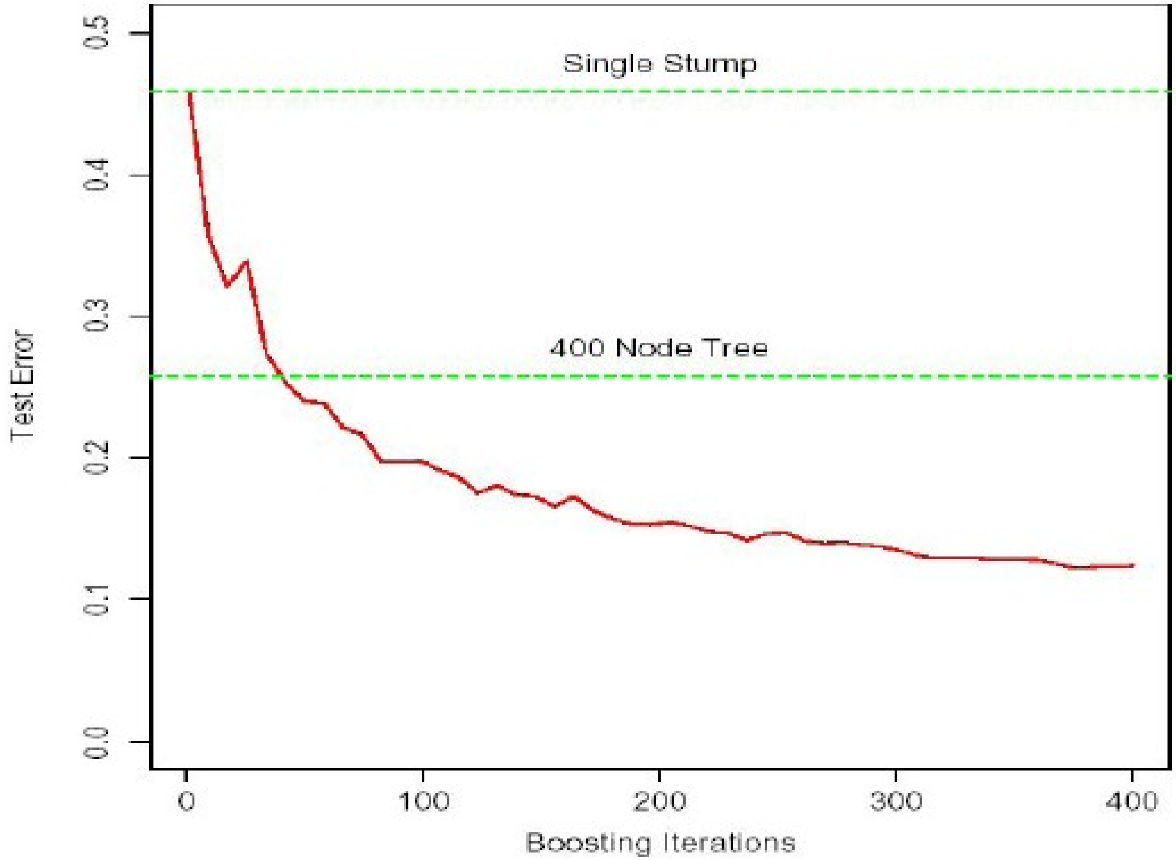


- Example Weights w_i
  - multiplier for correct and incorrect examples, depending on error



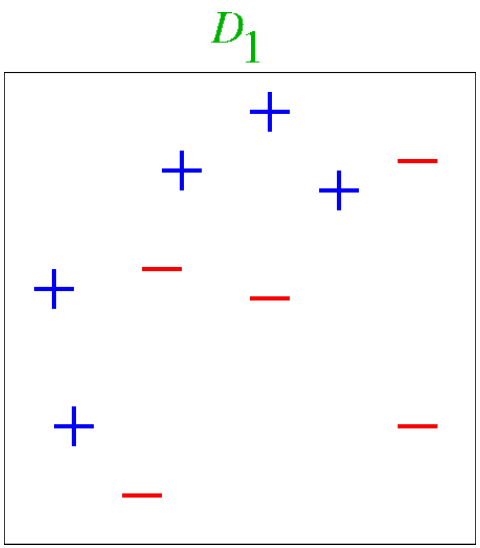
Boosting – Error rate example

- boosting of decision stumps on simulated data



from Hastie, Tibshirani, Friedman: The Elements of Statistical Learning, Springer Verlag 2001

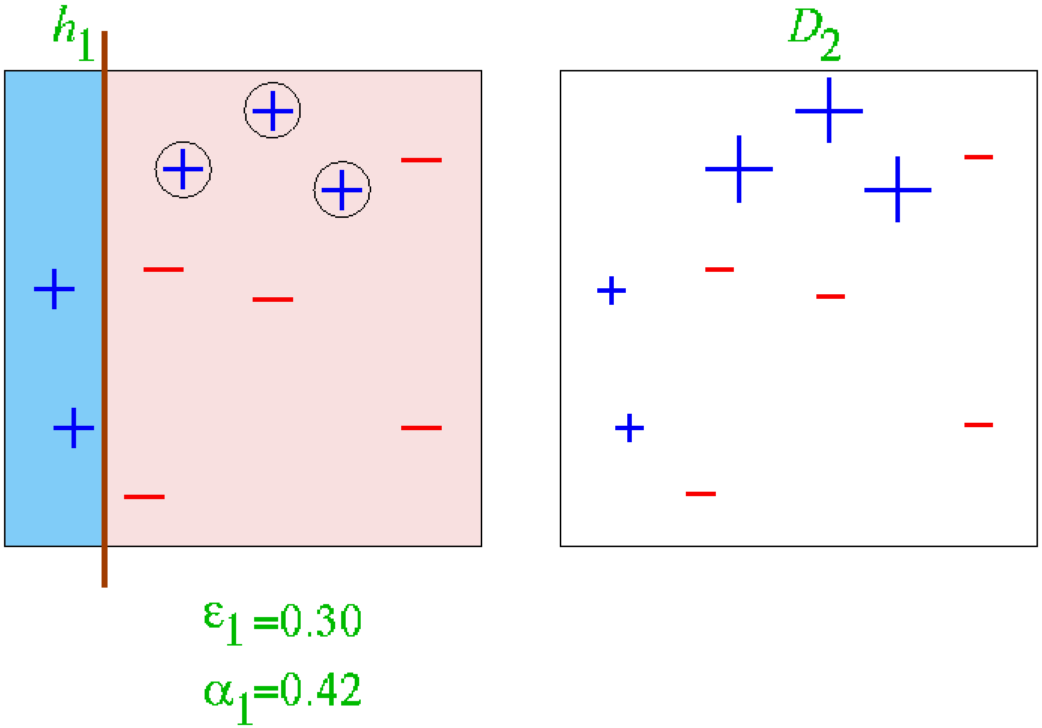
Toy Example



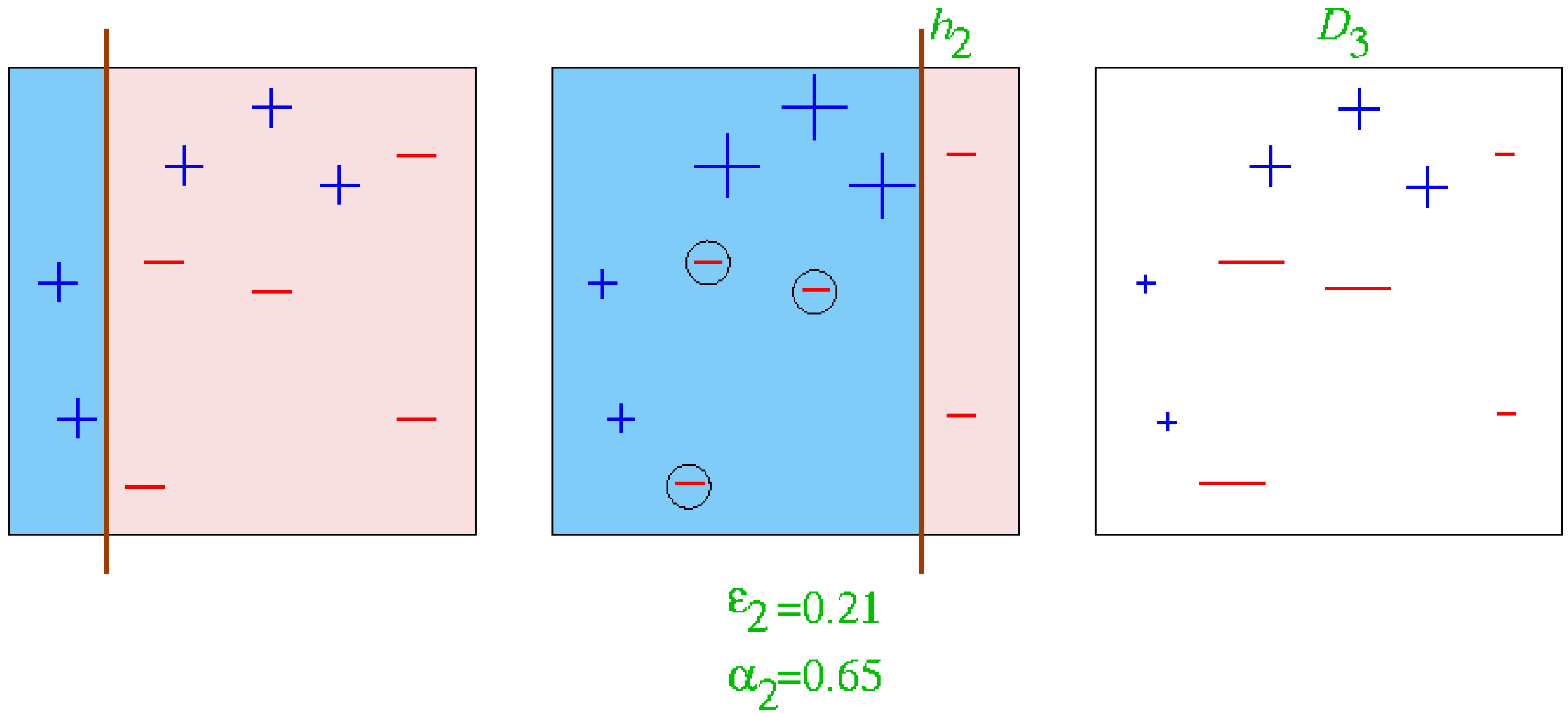
(taken from Verma & Thrun, Slides to CALD Course CMU 15-781, Machine Learning, Fall 2000)

- An Applet demonstrating AdaBoost
  - http://www.cse.ucsd.edu/~yfreund/adaboost/

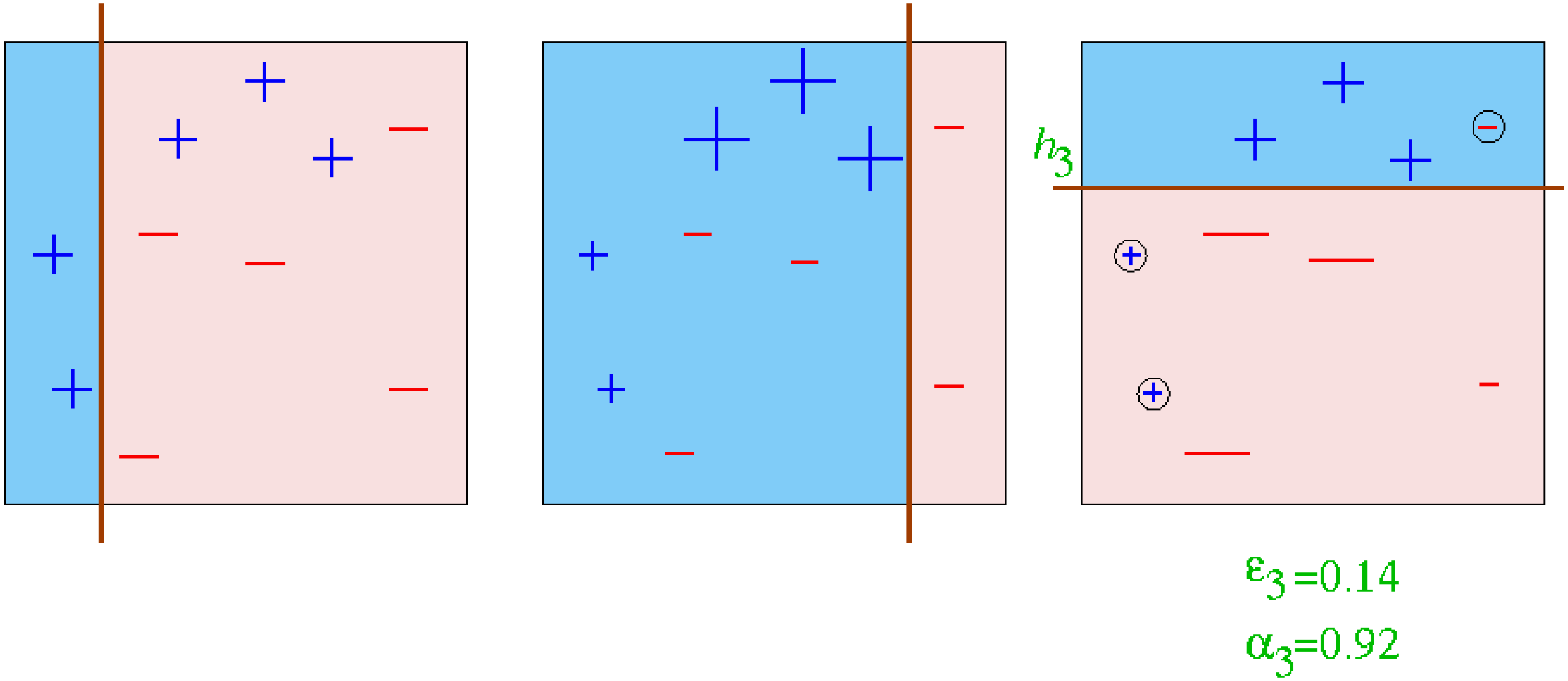
Round 1



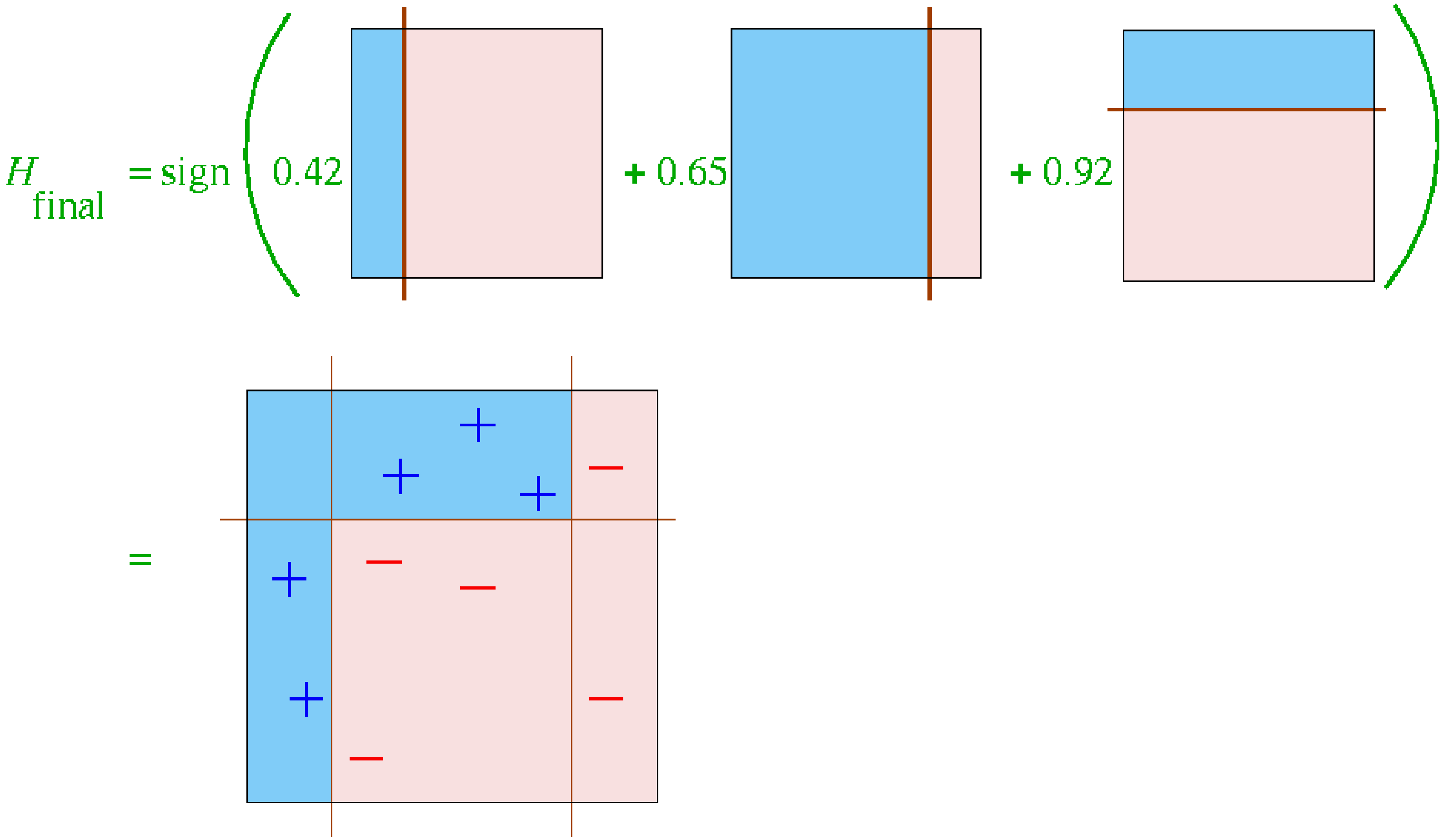
Round 2



Round 3



Final Hypothesis



Dealing with Weighted Examples

Two possibilities (→ cost-sensitive learning)

- directly
  - example e_i has weight w_i
  - number of examples $n \Rightarrow$ total example weight $\sum_{i=1}^{n} w_i$
- via sampling
  - interpret the weights as probabilities
  - examples with larger weights are more likely to be sampled
  - assumptions
    - sampling with replacement
    - weights are well distributed in [0,1]
    - learning algorithm sensible to varying numbers of identical examples in training data
  - boosting can thus be used in very much the same way as bagging

Comparison Bagging/Boosting

- Bagging
  - noise-tolerant
  - produces better class probability estimates
  - not so accurate
  - statistical basis
  - related to random sampling
- Boosting
  - very susceptible to noise in the data
  - produces rather bad class probability estimates
  - if it works, it works really well
  - based on learning theory (statistical interpretations are possible)
  - related to windowing

Example

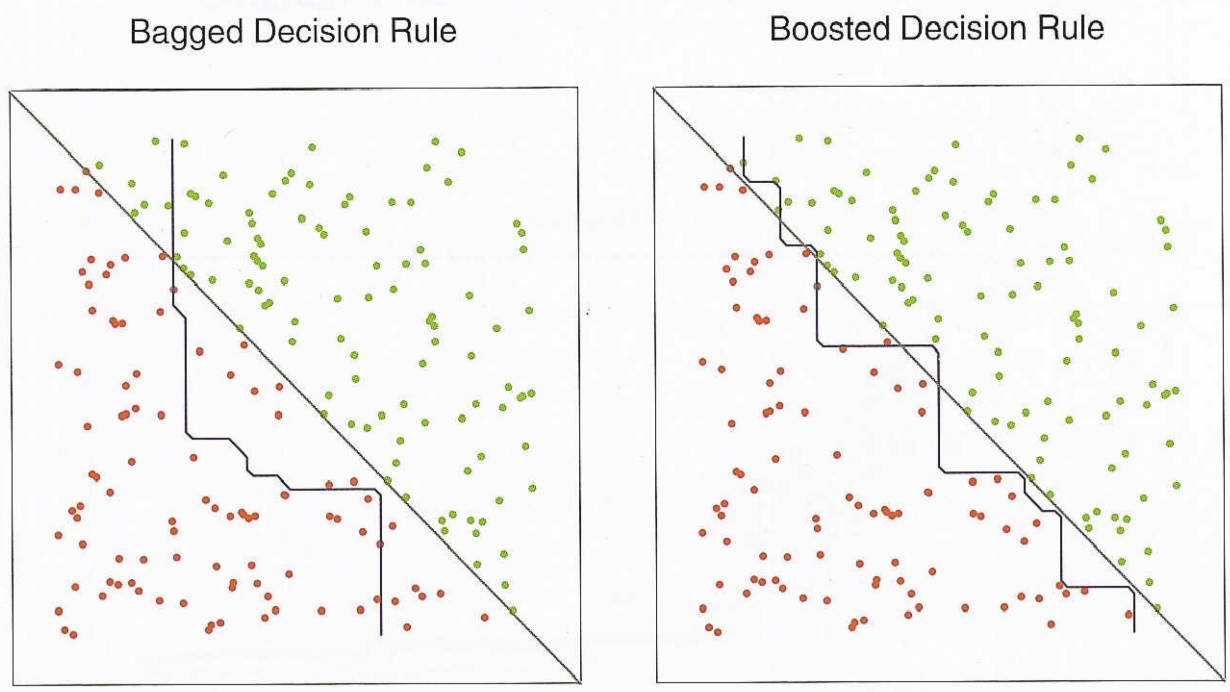


FIGURE 8.11. *Data with two features and two classes, separated by a linear boundary. Left panel: decision boundary estimated from bagging the decision rule from a single split, axis-oriented classifier. Right panel: decision boundary from boosting the decision rule of the same classifier. The test error rates are* 0.166, *and* 0.065 *respectively. Boosting is described in Chapter 10.*

from Hastie, Tibshirani, Friedman: The Elements of Statistical Learning, Springer Verlag 2001

Additive regression

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- It turns out that boosting is a greedy algorithm for fitting additive models
- More specifically, implements forward stagewise additive modeling
- Same kind of algorithm for numeric prediction:

1. Build standard regression model (e.g. tree)
2. Gather residuals
3. learn model predicting residuals (e.g. tree)
4. goto 2.

- To predict, simply sum up individual predictions from all models

Combining Predictions

- voting
  - each ensemble member votes for one of the classes
  - predict the class with the highest number of vote (e.g., bagging)
- weighted voting
  - make a *weighted* sum of the votes of the ensemble members
  - weights typically depend
    - on the classifiers confidence in its prediction (e.g., the estimated probability of the predicted class)
    - on error estimates of the classifier (e.g., boosting)
- stacking
  - Why not use a classifier for making the final decision?
  - training material are the class labels of the training data and the (cross-validated) predictions of the ensemble members

Stacking

- Basic Idea:
  - learn a function that combines the predictions of the individual classifiers
- Algorithm:
  - train n different classifiers $C_1 \ldots C_n$ (the *base classifiers*)
  - obtain predictions of the classifiers for the training examples
  - form a new data set (the *meta data*)
    - **classes**
      - the same as the original dataset
    - **attributes**
      - one attribute for each base classifier
      - value is the prediction of this classifier on the example
  - train a separate classifier M (the *meta classifier*)

This is better done with cross-validation!

Stacking (2)

- Example:

Attributes			Class
x_{11}	...	x_{1n_a}	t
x_{21}	...	x_{2n_a}	f
...	...	...	...
x_{n_e1}	...	$x_{n_en_a}$	t

training set

C_1	C_2	...	C_{n_c}
t	t	...	f
f	t	...	t
...	...	...	...
f	f	...	t

predictions of the classfiers

C_1	C_2	...	C_{n_c}	Class
t	t	...	f	t
f	t	...	t	f
...	...	...	...	...
f	f	...	t	t

training set for stacking

- Using a stacked classifier:
  - try each of the classifiers $C_1 \ldots C_n$
  - form a feature vector consisting of their predictions
  - submit these feature vectors to the meta classifier M

Error-correcting output codes
(Dietterich & Bakiri, 1995)

- Class Binarization technique
  - Multiclass problem → binary problems
  - Simple scheme: One-vs-all coding
- Idea: use error-correcting codes instead
  - one code vector per class
- Prediction:
  - base classifiers predict 1011111, true class = ??
- Use code words that have large pairwise Hamming distance d
  - Can correct up to $(d-1)/2$ single-bit errors

class	class vector
a	1 0 0 0
b	0 1 0 0
c	0 0 1 0
d	0 0 0 1

class	class vector
a	1 1 1 1 1 1 1
b	0 0 0 0 1 1 1
c	0 0 1 1 0 0 1
d	0 1 0 1 0 1 0

7 binary classifiers

More on ECOCs

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- Two criteria :
  - Row separation:
    minimum distance between rows
  - Column separation:
    minimum distance between columns
    - (and columns' complements)
    - Why? Because if columns are identical, base classifiers will likely make the same errors
    - Error-correction is weakened if errors are correlated
- 3 classes → only 2^3 possible columns
  - (and 4 out of the 8 are complements)
  - Cannot achieve row and column separation
- Only works for problems with > 3 classes

Exhaustive ECOCs

- Exhaustive code for k classes:
  - Columns comprise every possible k-string …
  - … except for complements and all-zero/one strings
  - Each code word contains $2^{k-1} - 1$ bits
- Class 1: code word is all ones
- Class 2: 2^{k-2} zeroes followed by $2^{k-2}-1$ ones
- Class i : alternating runs of 2^{k-i} 0s and 1s
  - last run is one bit shorter than the others

Exhaustive code, $k = 4$

class	class vector
a	1111111
b	0000111
c	0011001
d	0101010

Extensions of ECOCs

- Many different coding strategies have been proposed
  - exhaustive codes infeasible for large numbers of classes
    - Number of columns increases exponentially
  - Random code words have good error-correcting properties on average!
- Ternary ECOCs (Allwein et al., 2000)
  - use three-valued codes -1/0/1, i.e., positive / ignore / negative
  - this can, e.g., also model pairwise classification
- ECOCs don't work with NN classifier
  - because the same neighbor(s) are used in all binary classifiers for making the prediction
  - But: works if different attribute subsets are used to predict each output bit

Summary: Forming an Ensemble

- Modifying the data
  - Subsampling
    - bagging
    - boosting
  - feature subsets
    - randomly feature samples
- Modifying the learning task
  - pairwise classification / round robin learning
  - error-correcting output codes
- Exploiting the algorithm characterisitics
  - algorithms with random components
    - neural networks
  - randomizing algorithms
    - randomized decision trees
  - use multiple algorithms with different characteristics
- Exploiting problem characteristics
  - e.g., hyperlink ensembles