Ensemble Methods, Random Forests and AdaBoost

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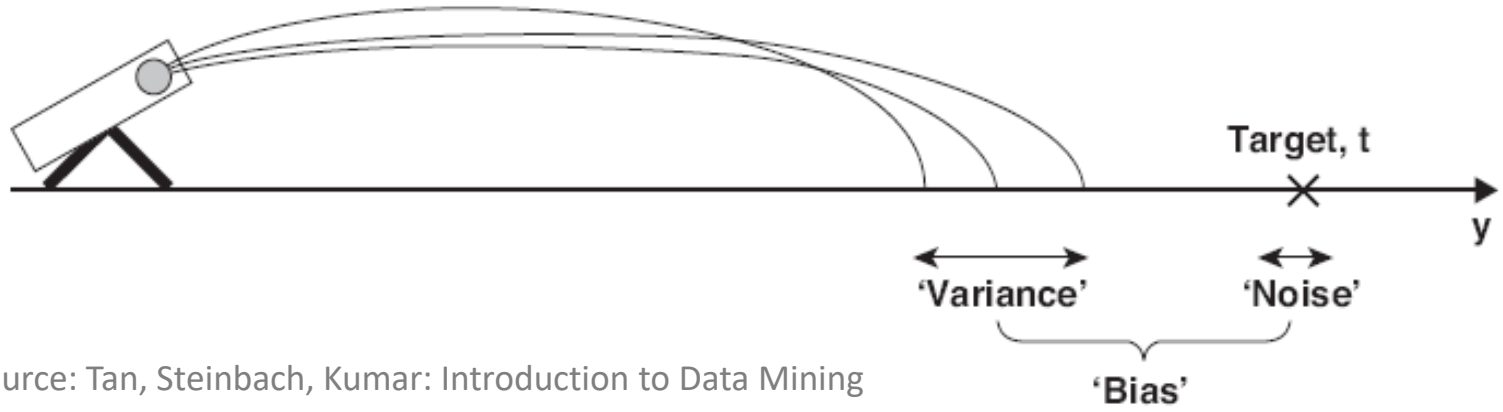
Outline

- Ensemble Methods
- Random Forests
- AdaBoost
- Stacking
- Summary

Variance, Bias and Noise



Source: Tan, Steinbach, Kumar: Introduction to Data Mining

Variance, bias and noise are different components of the error

$$err = Bias_{\alpha} + Varianz_{f} + Noise$$

In this example:

Bias: depending on firing angle α (systematic error)

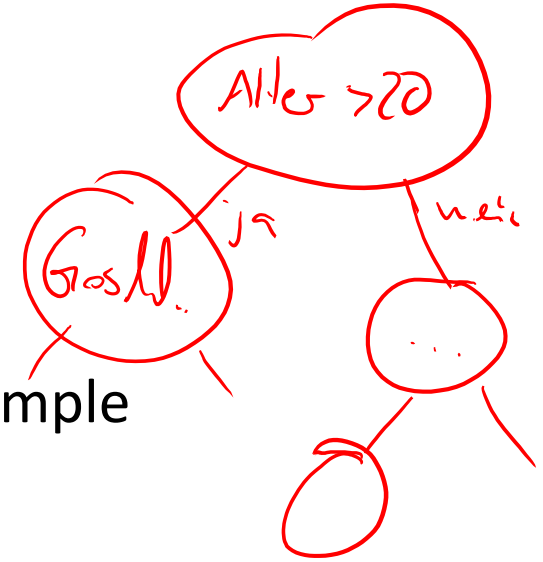
Variance: depending on the applied force f (data)

Noise: Fuzziness of the target (noise)

Bias and Variance Decomposition

Bias

the part of the error that is caused by the model



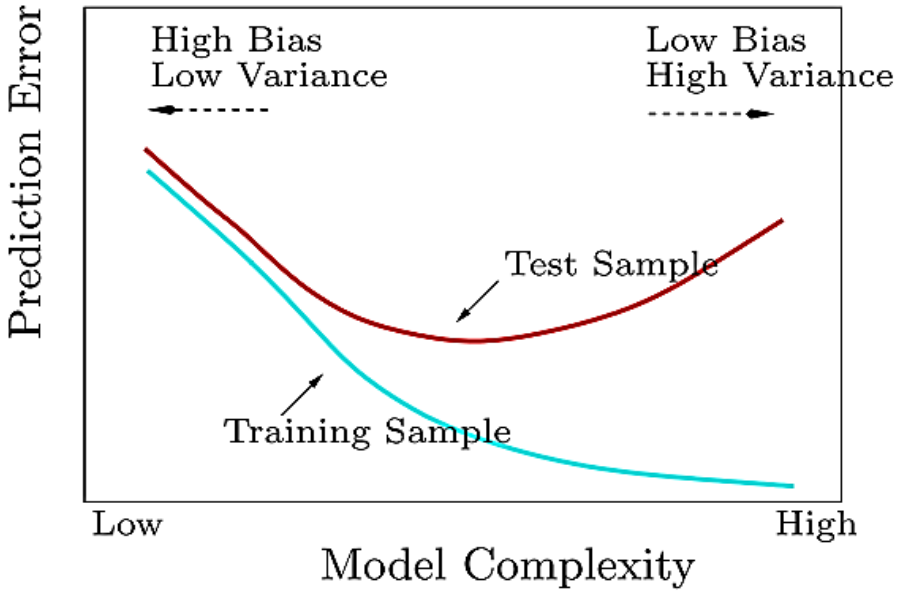
Variance

the part of the error that is caused by the data sample

Bias-Variance Trade-off

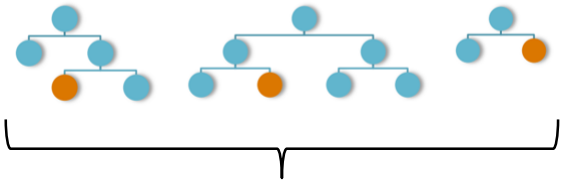
- Algorithms that can easily adapt to any given decision boundary are very sensitive to small variations in the data and vice versa
- Models with a low bias often have a high variance
  - e.g., nearest neighbor, unpruned decision trees
- Models with a low variance often have a high bias
  - e.g., decision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

Bias-Variance Trade-off



Random Forest

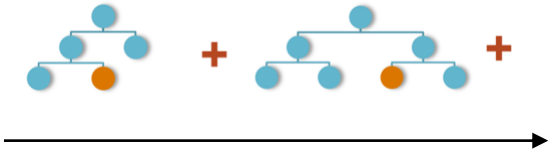
Variance ↓



Voting

Booosting

Bias ↓



Weighted Sum

Ensemble Classifiers

Idea

Combine the predictions of multiple classifiers

Objectives

→ 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

Important

formation of an ensemble of diverse classifiers from a single training set

Why does ensembles work?

Suppose there are 25 base classifiers

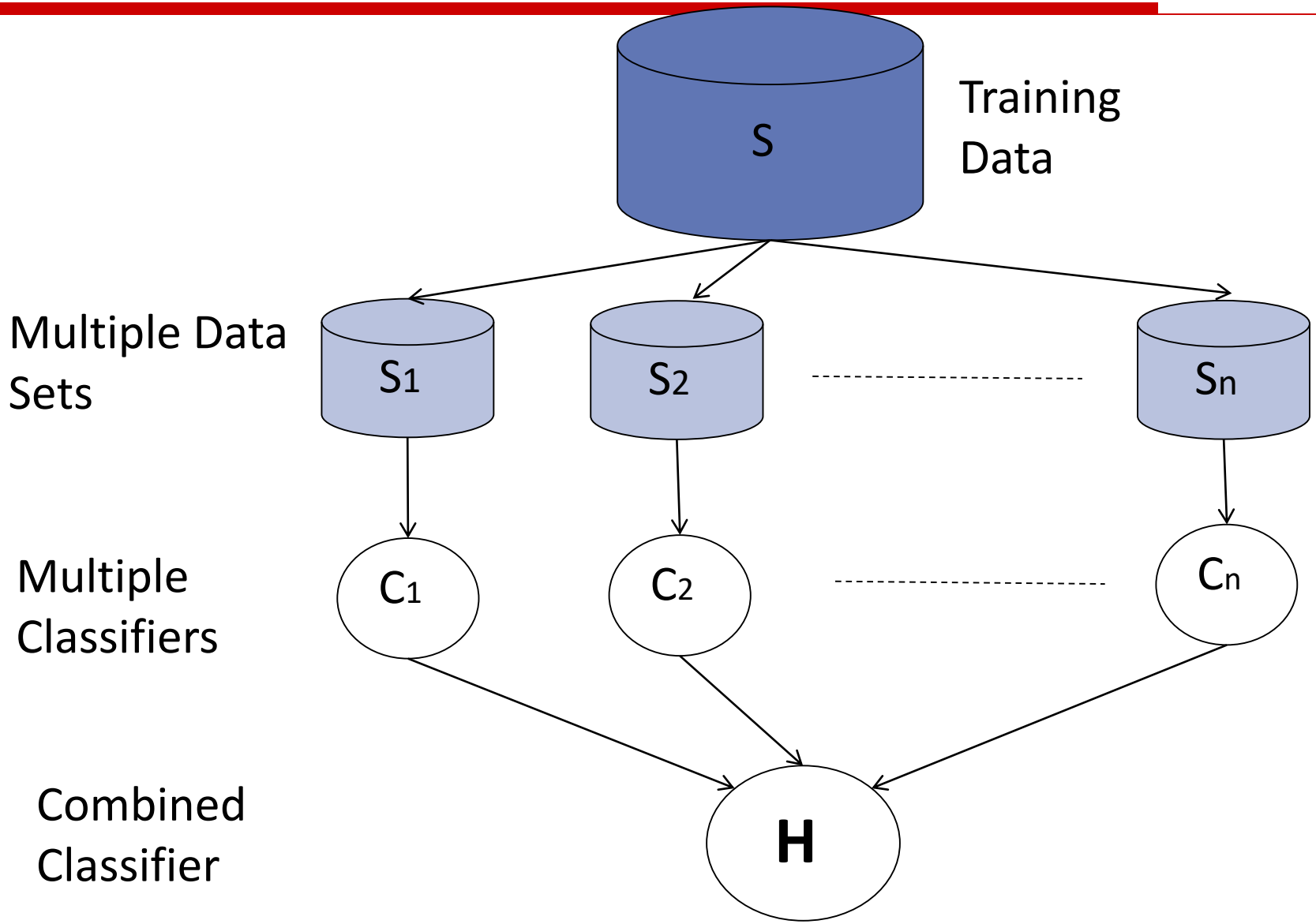
- Each classifier has error rate, $\varepsilon = 0.35$
- Assume classifiers are independent
  i.e., probability that a classifier makes a mistake does not depend on whether other classifiers made a mistake

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

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

Basic Idea of Meta Learning



Ensemble Methods

- Bootstrapping → Aufteilung der Daten
- Bagging (Breiman 1994)
- Boosting (Schapire 1989)
- Adaboost (Schapire 1995)
- Random Forest (Breiman 2001)

Prediction of classes by combining several models that have been trained.

Problem

- Biases in data samples may mislead classifiers
  - overfitting problem
  - model is overfit to single noise points

- If we had different samples
  - e.g., data sets collected at different times, in different places, …
  - ...and trained a single model on each of those data sets...
  - only one model would overfit to each noise point
  - voting could help address these issues

- But usually, we only have one dataset!

Bootstrap – also called 0.632 Bootstrap

Given a record with n instances (observations).
Bootstrap sample: draw a sample of the same length from the original dataset with replacement.

Original Data	1	2	3	4	5	6	7	8	9	10
Bootstrap 1	7	8	10	8	2	5	10	10	5	9
Bootstrap 2	1	4	9	1	2	3	2	7	3	2
Bootstrap 3	1	8	5	10	5	5	9	6	3	7
…										

For each set of size n, the probability that a given example appears in it is $\Pr(x \in B_i) = 1 - \left(1 - \frac{1}{n}\right)^n \xrightarrow[n\to\infty]{} 0.6322$

On average, less than 2/3 of the examples appear in any single bootstrap sample.

Estimate the error rate at Bootstrap

- Error estimation from the test data is very pessimistic
- Training was done on only ~63% of all instances
- To compensate this, we combine the test-set error rate with the resubstitution error on the instances in the training set.
- The error rate is offset against the resubstitution error:

$$\text{error} = 0.632 * error_{test\ instances} + 0.368 * error_{training\ instances}$$

- The resubstitution error (on the training data) is given less weight than the error on the test data.
- The process is repeated several times and the mean value of the error rates is calculated.
- Works well for very small datasets.

Bagging - Aggregate Bootstrapping
Models may differ when learned on different data samples

- Idea of bagging:
  - create samples by picking examples with replacement
  - learn a model on each sample
  - combine models
- Samples
  - differ in the subset of examples
  - replacement randomly re-weights instances
- Uses usually the same base learner of B bootstrap versions of the original dataset and calculates mean value from the predictions of the models
- Reduces the variability of the prediction
- Works better with predictions that show small bias but have a higher variance. E. g. decision trees

Bagging: Basic approach

1. for m = 1 to t // t ... number of iterations
   a) draw with replacement a bootstrap sample D_m of 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

Variant of Bagging: Randomization

- Randomize the learning algorithm instead of the input data
- Some algorithms already have a random component
  e.g. 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
  - E.g.: test selection in decision trees or rule learning
- Can be combined with bagging

Boosting

- Idea of boosting
  - train a set of classifiers, one after another
  - 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
    - so they 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

Random Forest
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

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Motivation

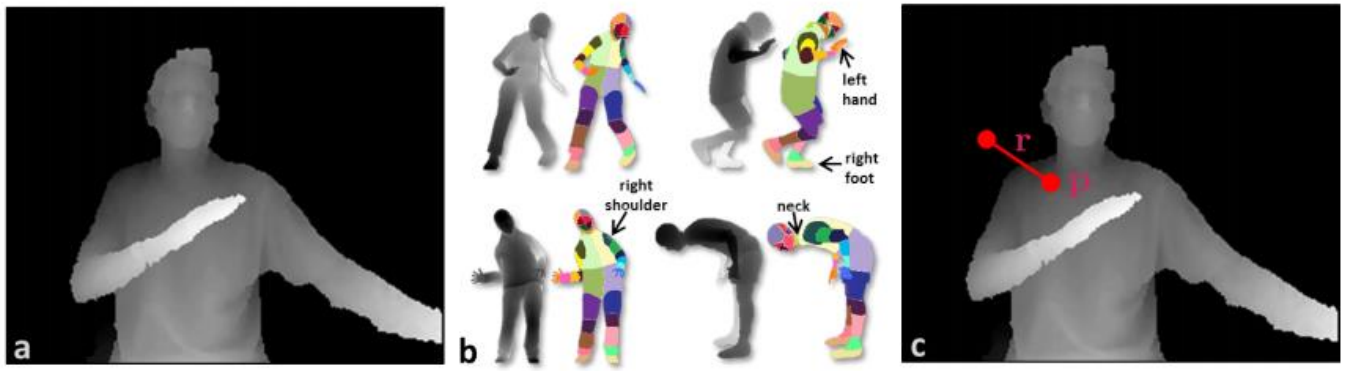


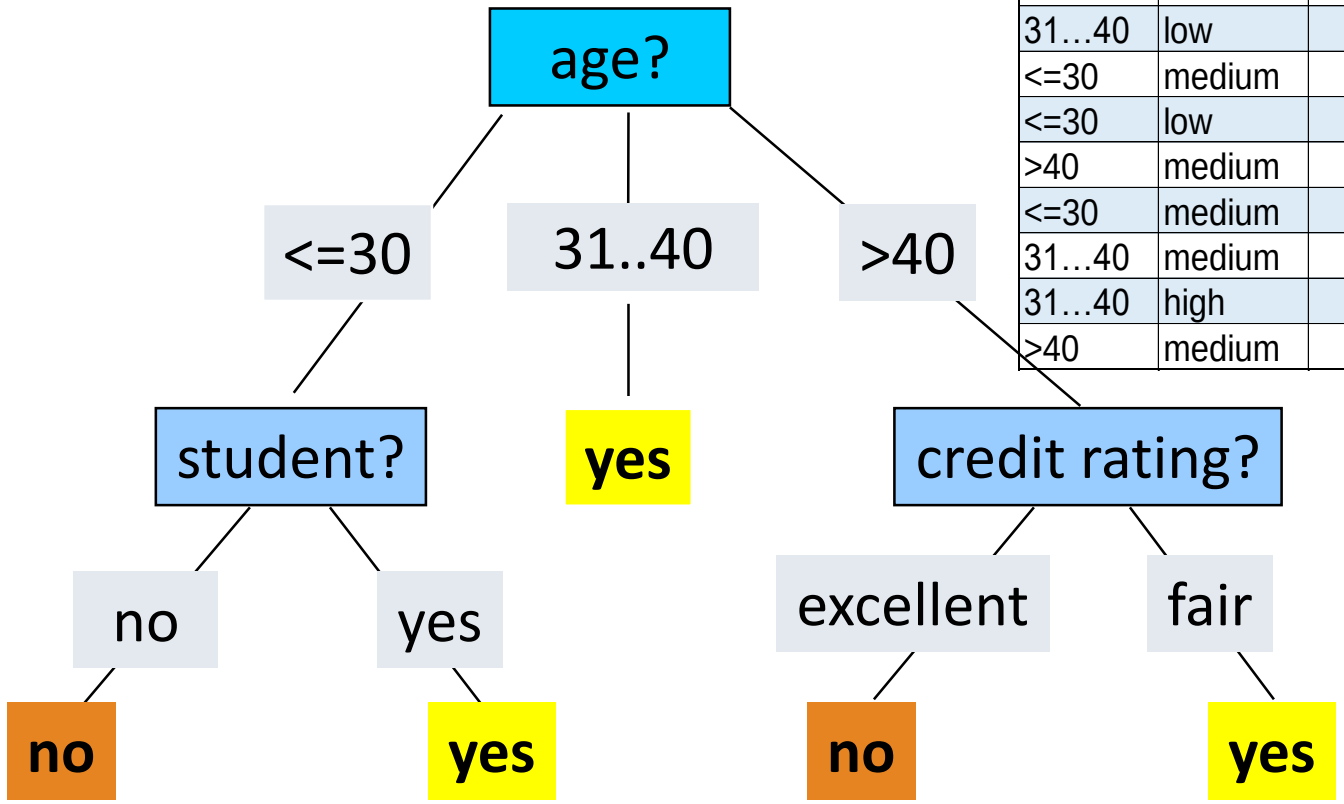
Fig. 3.15: **Classification forests in Microsoft Kinect for XBox**

Decision Tree Induction: An Example

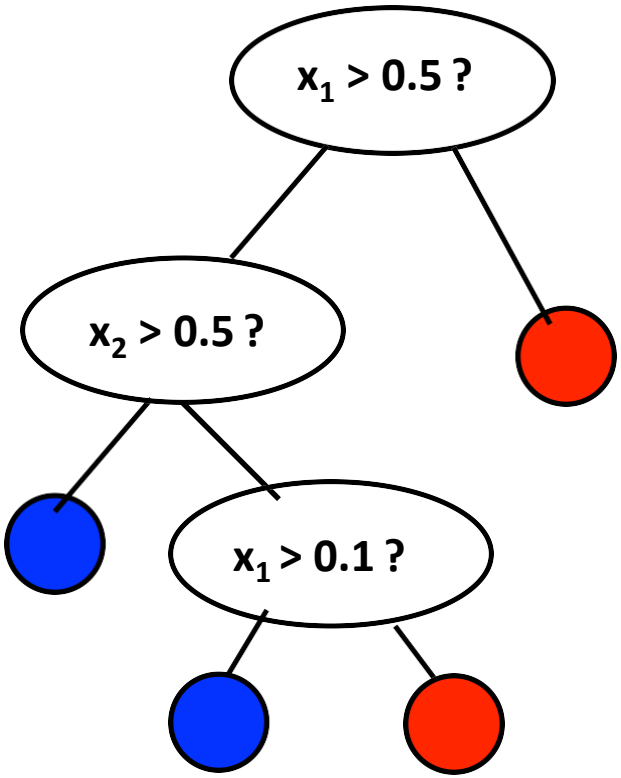
Training data set: Buys_computer

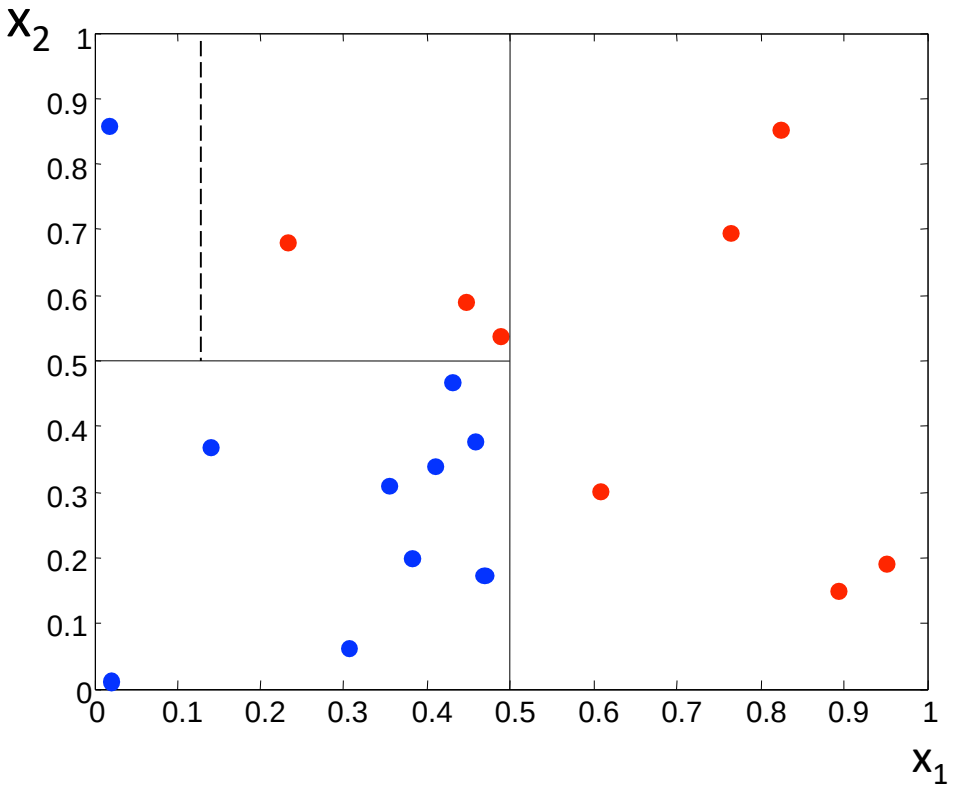
age	income	student	credit_rating	buys_computer
<=30	high	no	fair	no
<=30	high	no	excellent	no
31…40	high	no	fair	yes
>40	medium	no	fair	yes
>40	low	yes	fair	yes
>40	low	yes	excellent	no
31…40	low	yes	excellent	yes
<=30	medium	no	fair	no
<=30	low	yes	fair	yes
>40	medium	yes	fair	yes
<=30	medium	yes	excellent	yes
31…40	medium	no	excellent	yes
31…40	high	yes	fair	yes
>40	medium	no	excellent	no

Resulting tree:

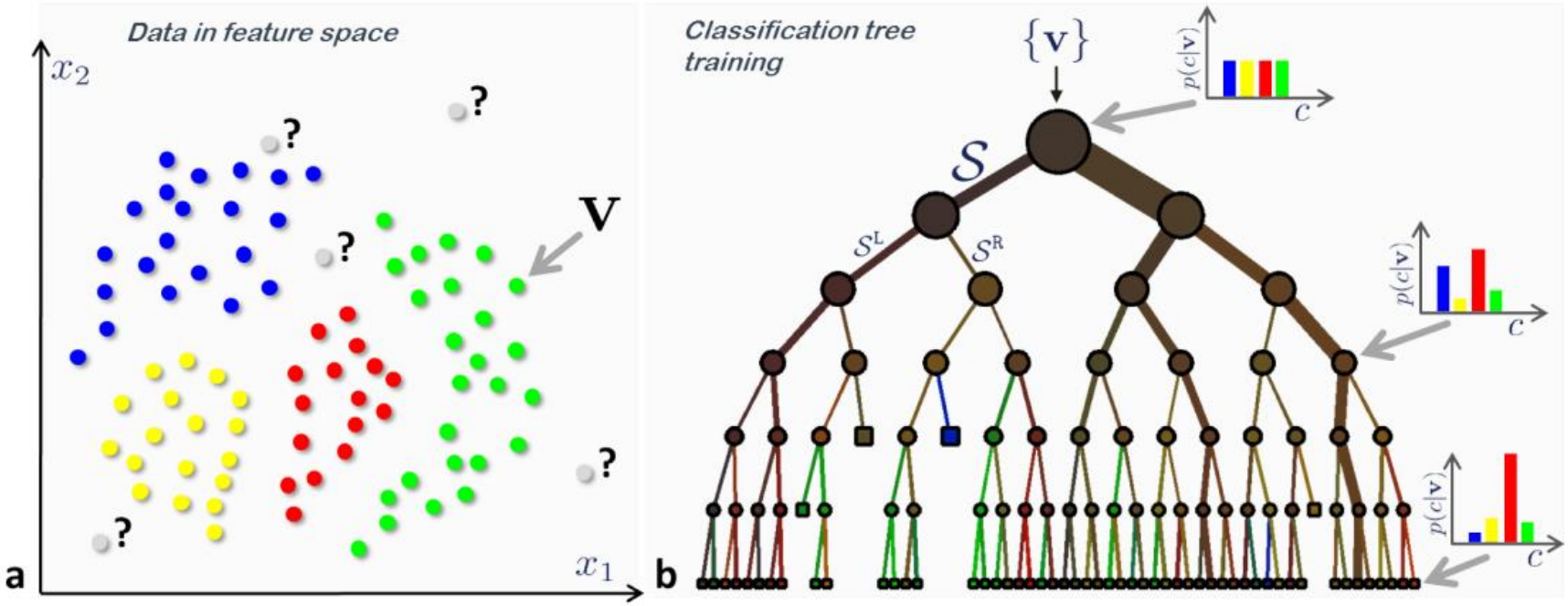


Decision Tree splits input data into cases





Decision Tree splits input data into cases



Criminisi, A., Shotton, J., and Konukoglu, E., "Decision Forests for Classification, Regression, Density Estimation, Manifold Learning and Semi-Supervised Learning," MSR-TR-2011-114, 2011.

ID3 Algorithm – Iterative Dichotomizer 3

Input: Example set S
Output: Decision Tree DT

If all examples in S belong to the same class c
return a new leaf and label it with c

Else

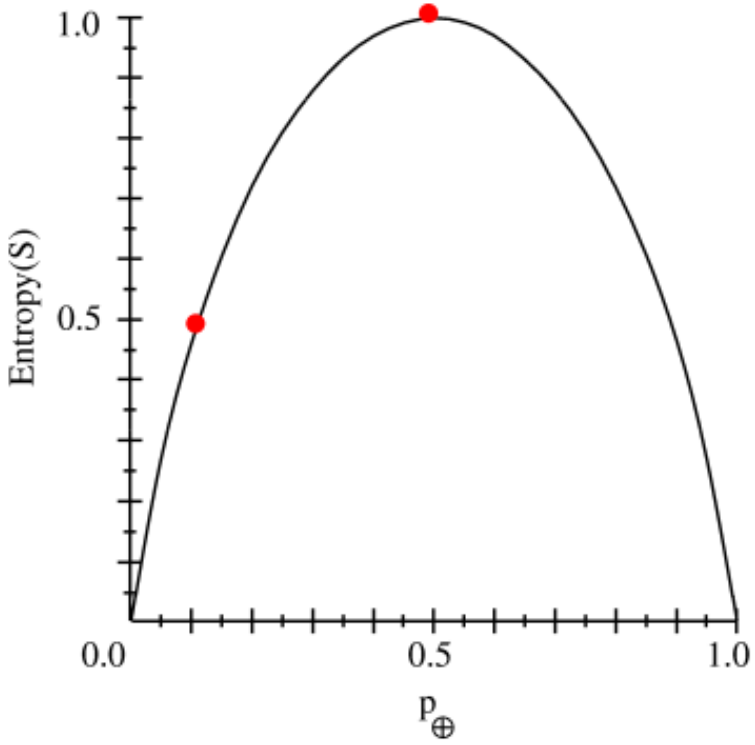
i. Select an attribute A according to some heuristic function
ii. Generate a new node DT with A as test
iii. For each Value v_i of A
   a) Let S_i = all examples in S with $A = v_i$
   b) Use ID3 to construct a decision tree DT_i for example set S_i
   c) Generate an edge that connects DT and DT_i

Entropy

Let v_i a possible value of a particular attribute A and let p_j be the fraction of data points belonging to the class $j \in \{1, \ldots, k\}$ for attribute value v_i

$$\text{Info}(v_i) = \text{H}(v_i) = -\sum_{j=1}^{k} p_j \log_2 p_j$$

Two Classes



Low values:

High values:

Information Gain as Split Criteria (ID3/C4.5)

Let p_i be the probability that an arbitrary tuple in T belongs to class C_i, estimated by $|C_{i,T}|/|T|$

$$\text{Info}(T) = H(T) = -\sum_{j=1}^{k} p_j \log_2 p_j$$

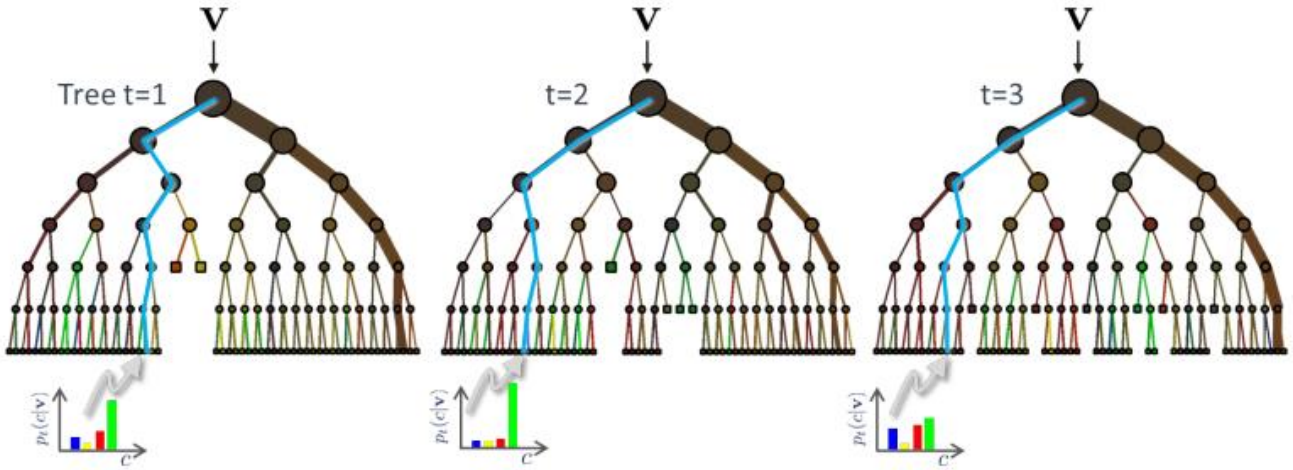
The overall entropy for a r-way split of set T into sets T_1, …, T_r by attribute A is computed as the weighted average:

$$\text{Info}(T, A) = \text{Entropy-Split}(T \Rightarrow T_1 \ldots T_r) = \sum_{i=1}^{r} \frac{|T_i|}{|T|} \cdot H(T_i)$$

Information Gain is computed as difference of the entropy before split and after split.

$$InfoGain(T, A) = Info(T) - Info(T,A) = \text{H}(T) - \sum_{i=1}^{r} \frac{|T_i|}{|T|} \cdot \text{H}(T_i)$$

Random Forest



- Random Forest consists of many "Trees", hence "Forest".
- Random “because the trees are randomly generated”
- It is not the whole dataset, but bootstrap learning samples are used
- At each node only random selection of attributes
- Assigning a value to each record based on the decision of each tree → majority

Random Forest for Classification or Regression

1. For b = 1 to B
   a) Draw a bootstrap sample **Z*** of size *N* from the training data.
   b) Grow a random forest tree T_b to the bootstrapped data, by recursively repeating the following steps for each terminal node of the tree, until the minimum node size n_{min} is reached.
      i. Select *m* variables at random from the *p* variables.
      ii. Pick the best variable/split-point among the *m*.
      iii. Split the node into two daughter nodes.
2. Output the ensemble of trees $\{T_b\}_1^B$

Classification:

Let $\hat{C}_b(x)$ be the class prediction of the *b*th random-forest tree.

Then $\hat{C}_{rf}^B(x) = \text{majority vote}\{\hat{C}_b(x)\}_1^B$

Regression: $\hat{f}_{rf}^B(x) = \frac{1}{B}\sum_{b=1}^B T_b(x)$

Why does Random Forest work?

$$Var\left(\frac{1}{B}\sum_{i=1}^{B} T_i(c)\right) = \frac{1}{B^2}\sum_{i=1}^{B}\sum_{j=1}^{B} Cov(T_i(x), T_j(x))$$

$$= \frac{1}{B^2}\sum_{i=1}^{B}\left(\sum_{j\neq i}^{B} Cov(T_i(x), T_j(x)) + Var(T_i(x))\right)$$

$$= \frac{1}{B^2}\sum_{i=1}^{B}\left((B-1)\sigma^2 \cdot \rho + \sigma^2\right)$$

$$= \frac{B(B-1)\rho\sigma^2 + B\sigma^2}{B^2}$$

$$= \frac{(B-1)\rho\sigma^2}{B} + \frac{\sigma^2}{B}$$

$$= \rho\sigma^2 - \frac{\rho\sigma^2}{B} + \frac{\sigma^2}{B}$$

$$= \rho\sigma^2 + \sigma^2\frac{1-\rho}{B}$$

i=j

$\rho_{i,j} = \frac{Cov(T_i, T_j)}{\sigma_i \sigma_j}$

Hint:

$$\mathrm{Var}\left(\sum_{i=1}^{n} X_i\right) = \sum_{i,j=1}^{n} \mathrm{Cov}(X_i, X_j)$$

$$= \sum_{i=1}^{n} \mathrm{Var}(X_i) + \sum_{i,j=1, i\neq j}^{n} \mathrm{Cov}(X_i, X_j)$$

$$= \sum_{i=1}^{n} \mathrm{Var}(X_i) + 2\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} \mathrm{Cov}(X_i, X_j).$$

De-correlation results in higher accuracy!

Before each split, select m < p of the attributes randomly as candidates for split.

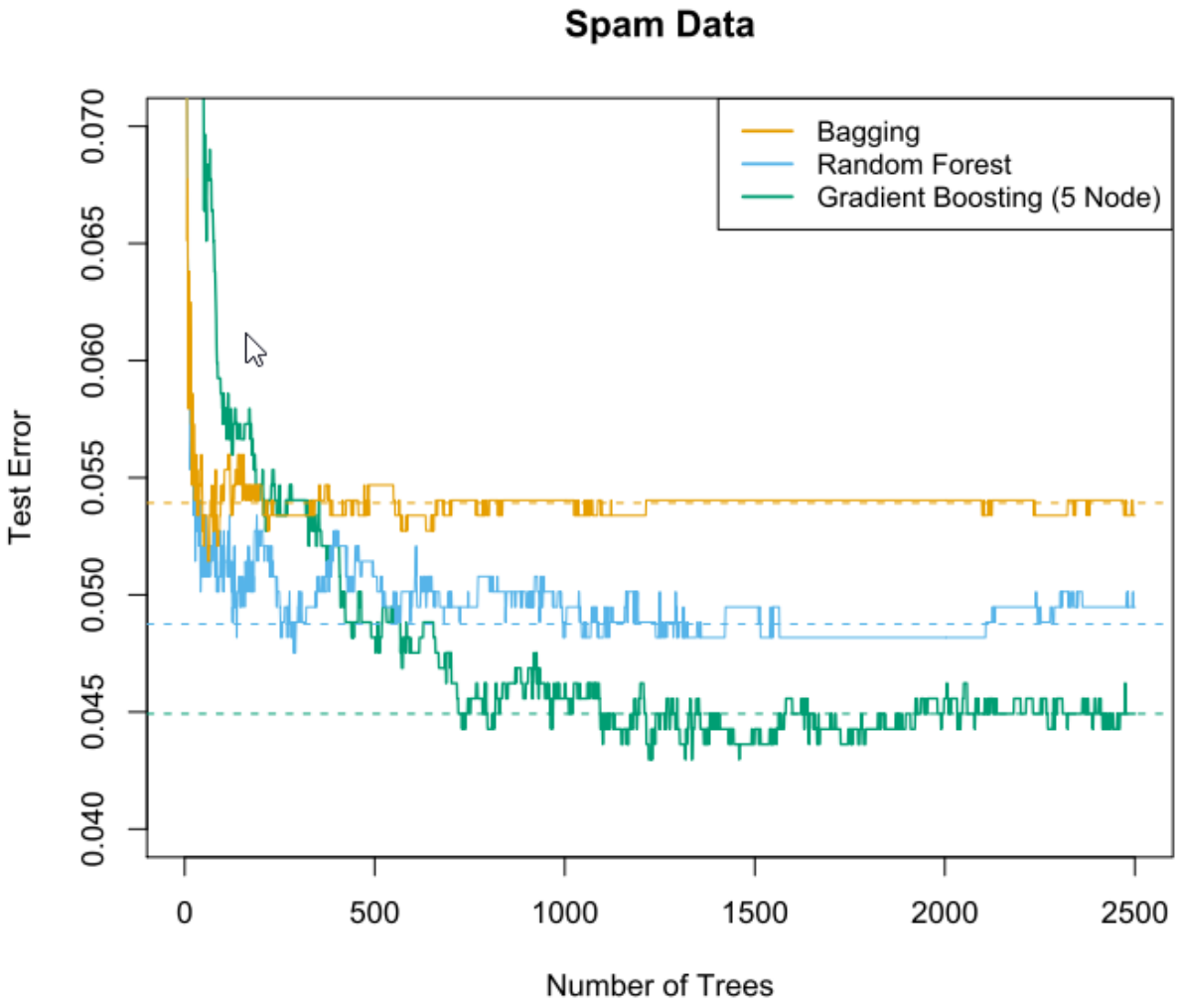


FIGURE 15.1. Bagging, random forest, and gradient boosting, applied to the spam data. For boosting, 5-node trees were used, and the number of trees were chosen by 10-fold cross-validation (2500 trees). Each "step" in the figure corresponds to a change in a single misclassification (in a test set of 1536).

Source: ESL_II

Bootstrap: Out-Of-Bag (OOB)

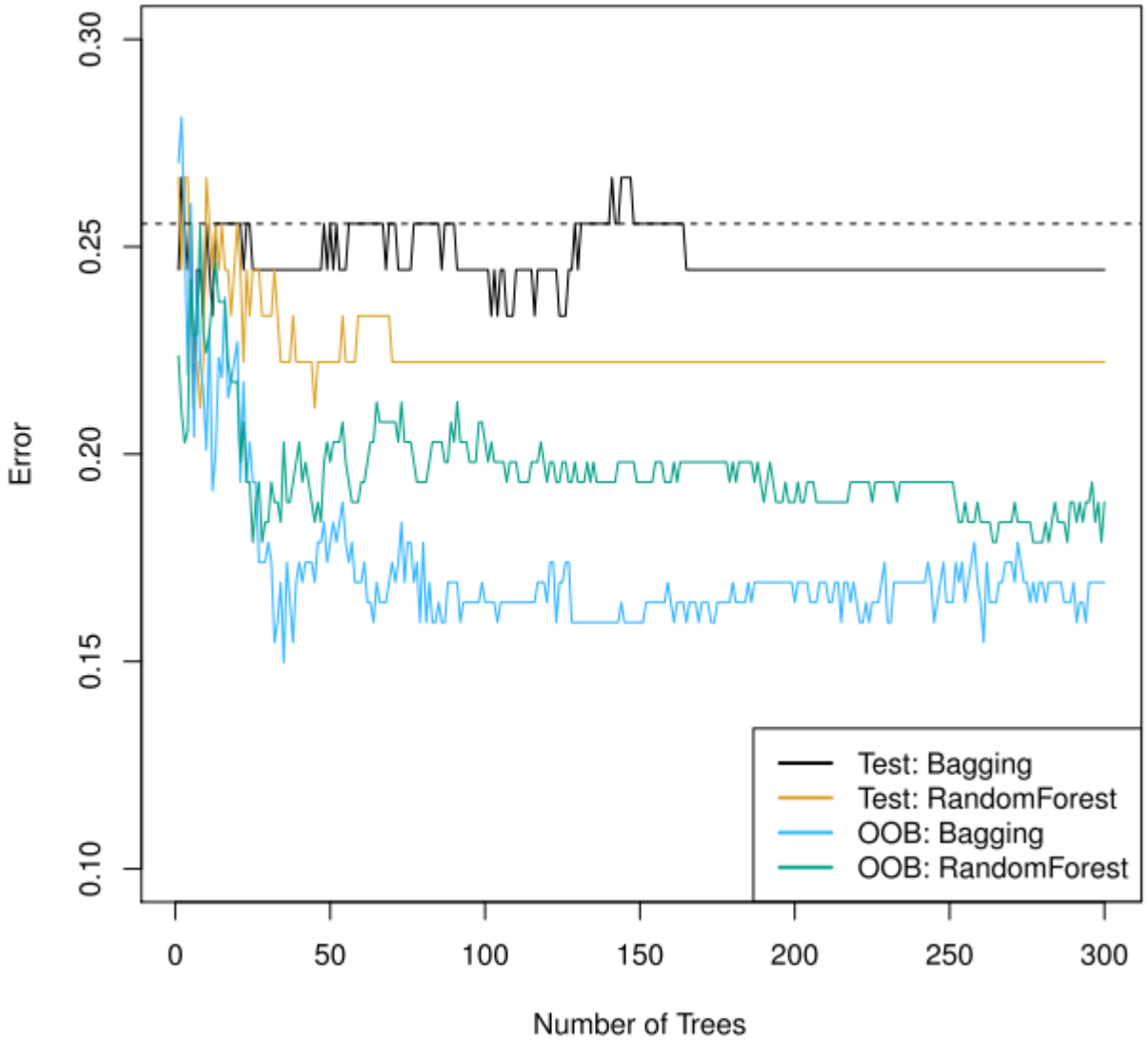
Observations that are not included in the bootstrap sample are called Out-Of-Bag (OOB).

Out-of-Bag error rate can be calculated for any observation over whole forest and corresponds to leave-one-out error rate.

Unlike most models, cross-validation is performed while Random Forest is being adapted.

→ no cross-validation necessary

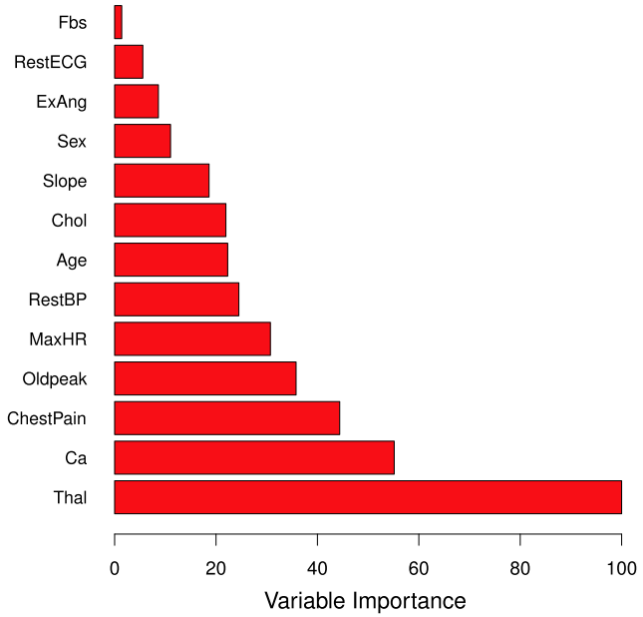
Bagging-Error and Out-Of-Bag-Error

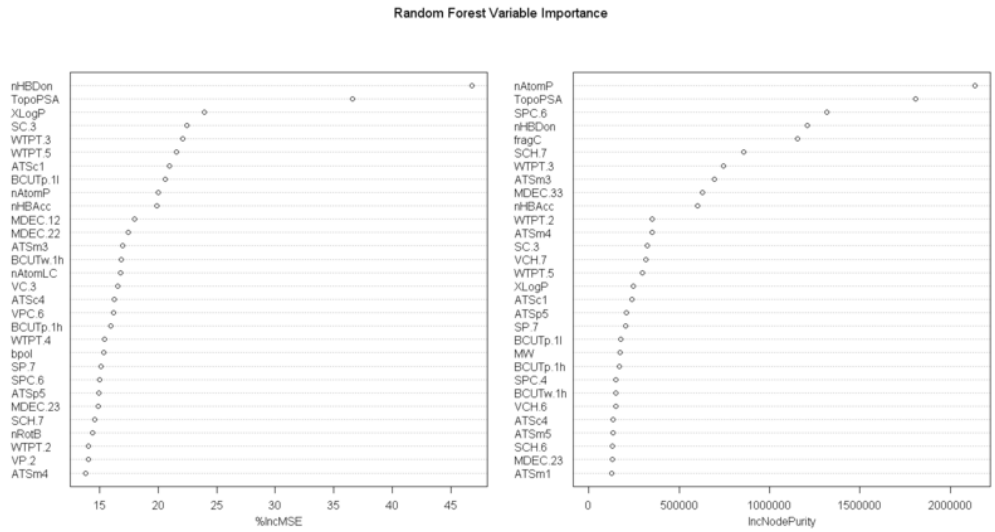


Ranking of features

For each split, you can calculate the improvement in the split criterion for split characteristics.

The influence of a characteristic is calculated as the sum of the improvements in the split criterion over the whole forest
→ feature ranking





Advantages of Random Forest

- Suitable for high-dimensional data where the number of attributes exceeds the number of objects observed
- yet robust against overfitting
- Quantifies the importance of individual variables
- Good performance compared to classics such as support vector machines and neural networks
- Straightforward estimation of the error rate
- Consistent estimation of target values
- Problem with a single tree:
  has high variance → wrong decision in "high" nodes runs through subsequent nodes → many trees reduce this effect

Differences to an standard Decision Tree

- Each tree is trained with a “bootstrap resample of data”. “Bootstrap resample of data set with N samples: Make new data set by drawing with replacement N samples; i.e., some samples will probably occur multiple times in new data set”
- For each split, randomly select m attributes from the total p attributes ($m = \sqrt{p}$)
- No Pruning

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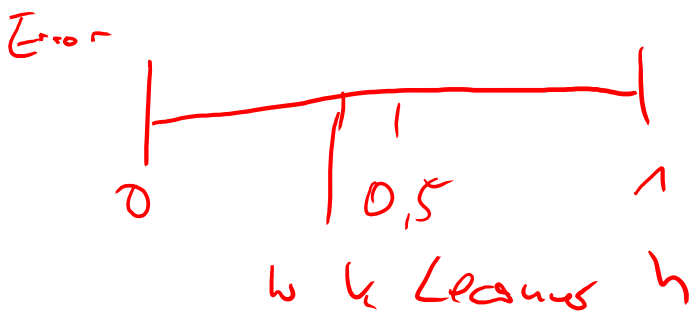
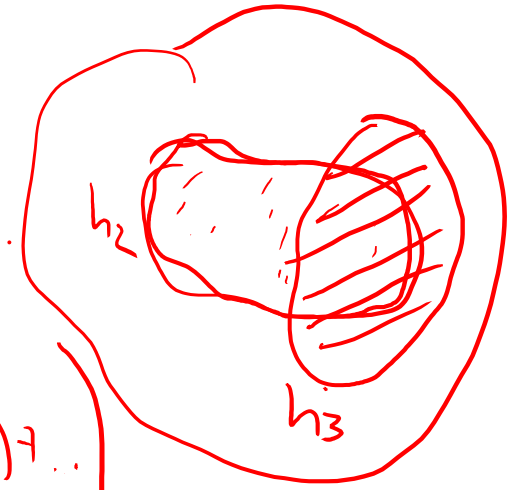
Boosting

- Ensembles
  - Weighted combinations of classifiers
  - “Committee” decisions
  - Equal weights (majority vote) in a simple case
  - Might want to weight unevenly – up-weight good experts
- **Boosting**
  - Focus new experts on examples that others get wrong
  - Train experts sequentially
  - Errors of early experts indicate the “hard” examples
  - Focus later classifiers on getting these examples right
  - Combine the whole set in the end
  - Convert many “weak” learners into a complex classifier

Idea

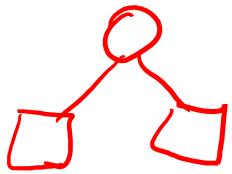
Binary Classification



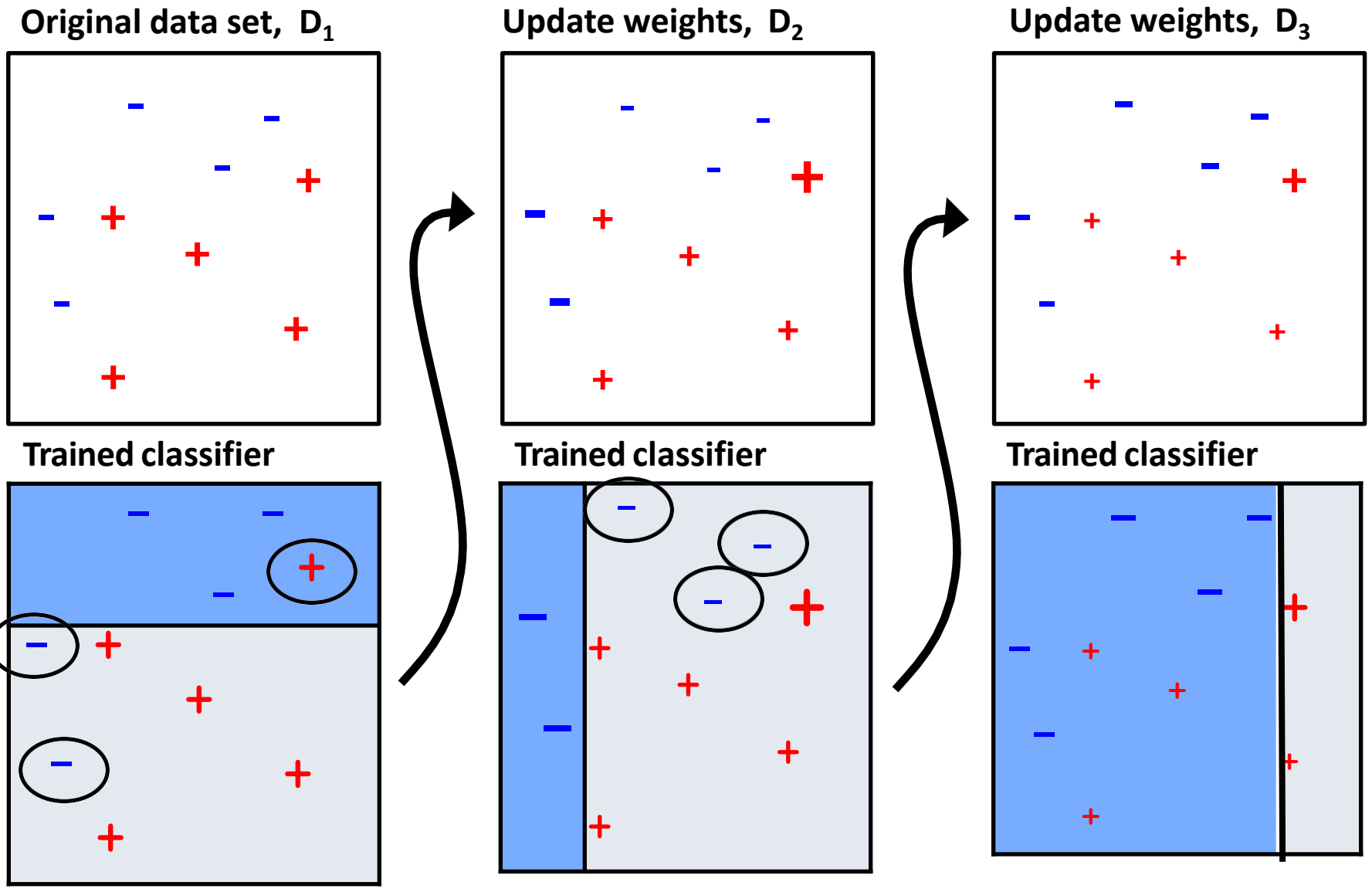


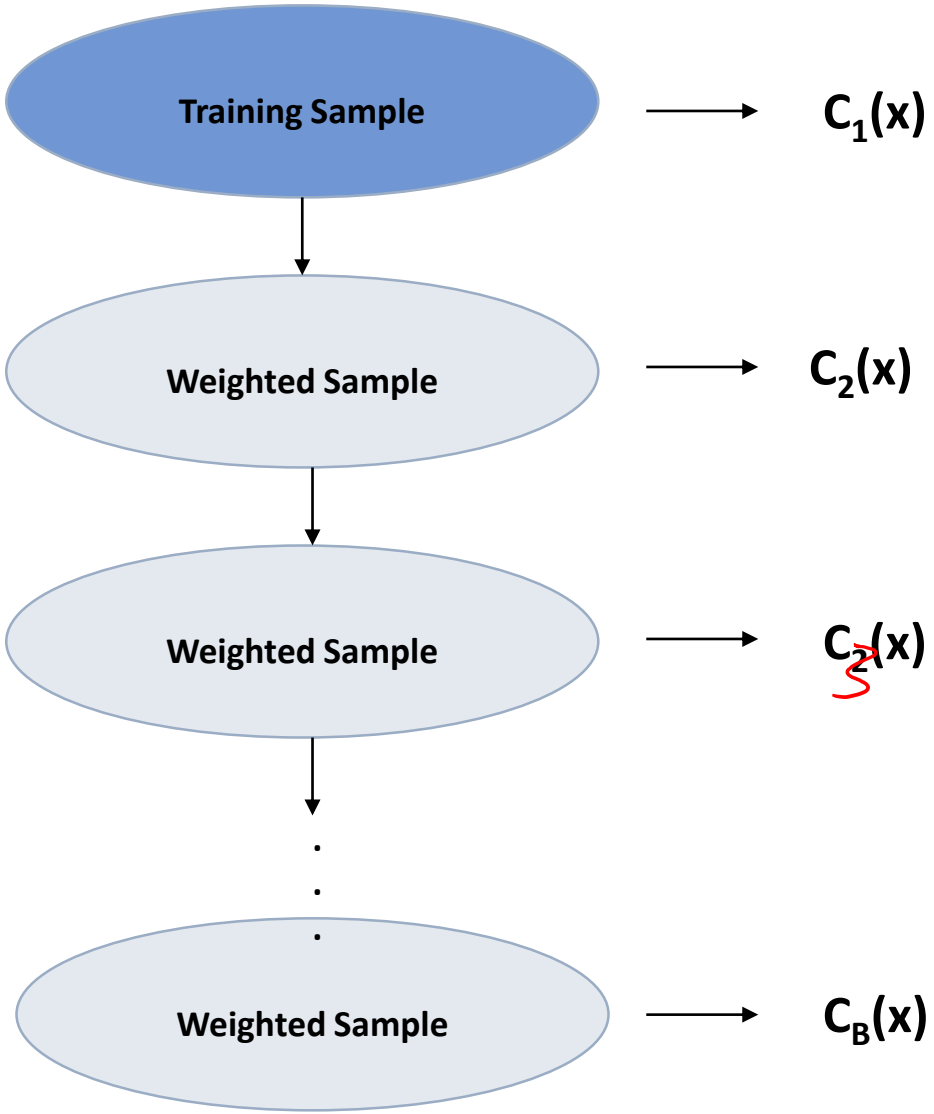
$$H(x) = \text{sign}\left(h_1(x) + \alpha_2 h_2(x) + \alpha_3 h_3(x) + \ldots\right)$$

AdaBoost: Decision Stumps



Example: Classes +1 , -1





Final hypothesis

$$C(x) = sign\left[\sum_{m=1}^{B} \alpha_m C_m(x)\right]$$

Algorithm AdaBoost.M1 - Adaptive Boosting

1. Initialize example weights $w_i = \frac{1}{N} \quad (i = 1, \ldots N)$
2. for m = 1 to B // B ... number of iterations
   a) learn a classifier C_m using the current example weights
   b) compute a weighted error estimate

$$err_m = \frac{\sum w_i \text{ of all incorrectly classifed } e_i}{\sum_{i=1}^{N} w_i}$$

   c) compute a classifier weight $\alpha_m = \frac{1}{2}\ln(\frac{1-err_m}{err_m})$
   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

Boosting – Algorithm AdaBoost.M1

…

3. for each test example
   a) try all classifiers C_m
   b) predict the class that receives the highest sum of weights α_m

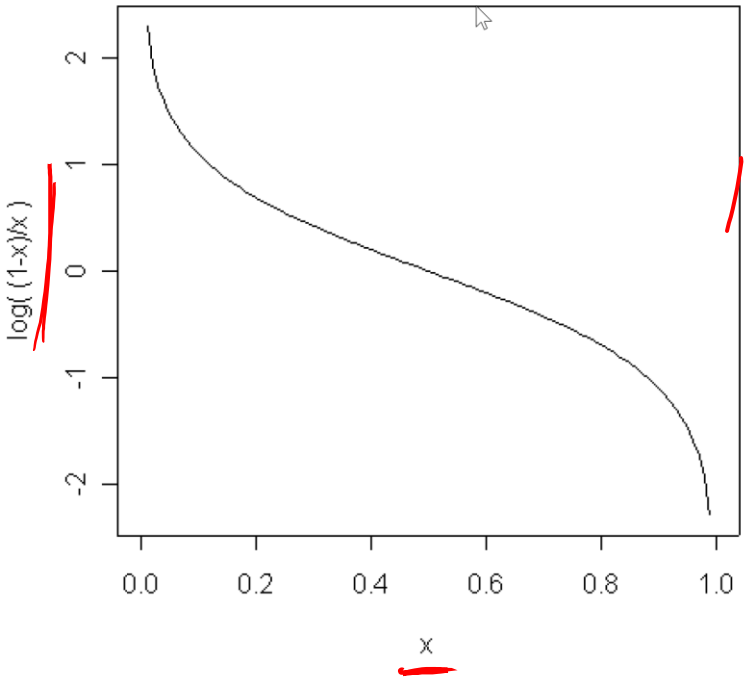
Illustration of the Weights

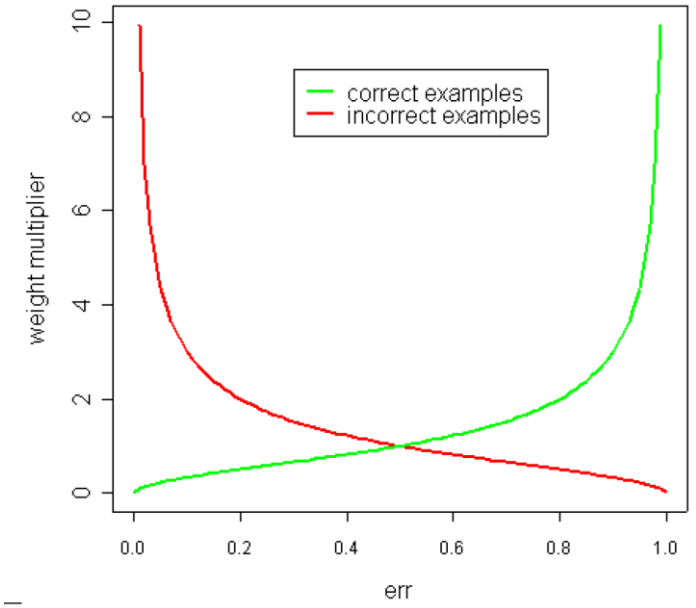
Classifier Weights α_m

differences near 0 or 1 are emphasized

Example Weights

multiplier for correct and incorrect examples, depending on error





Boosting – Error rate example

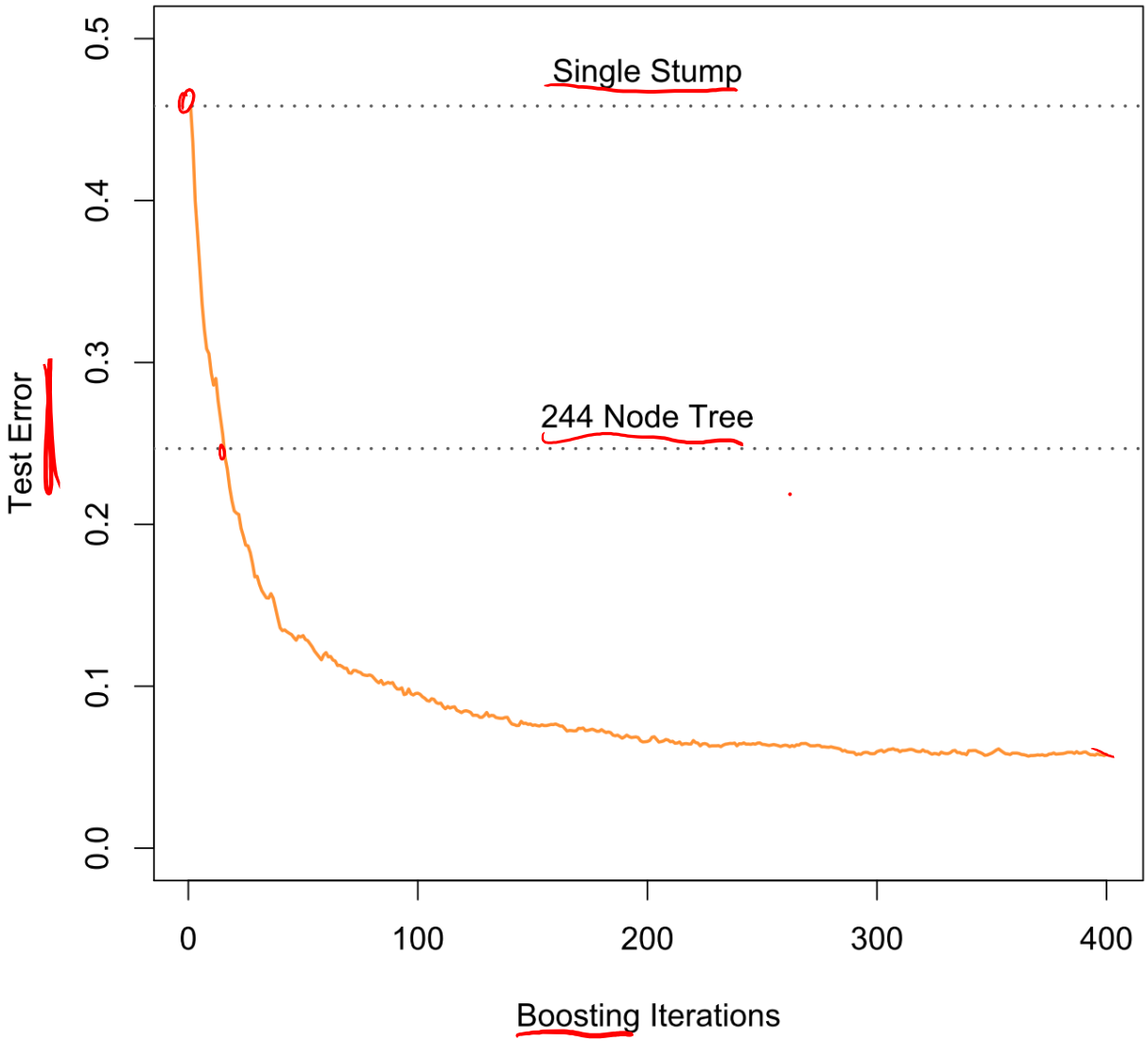
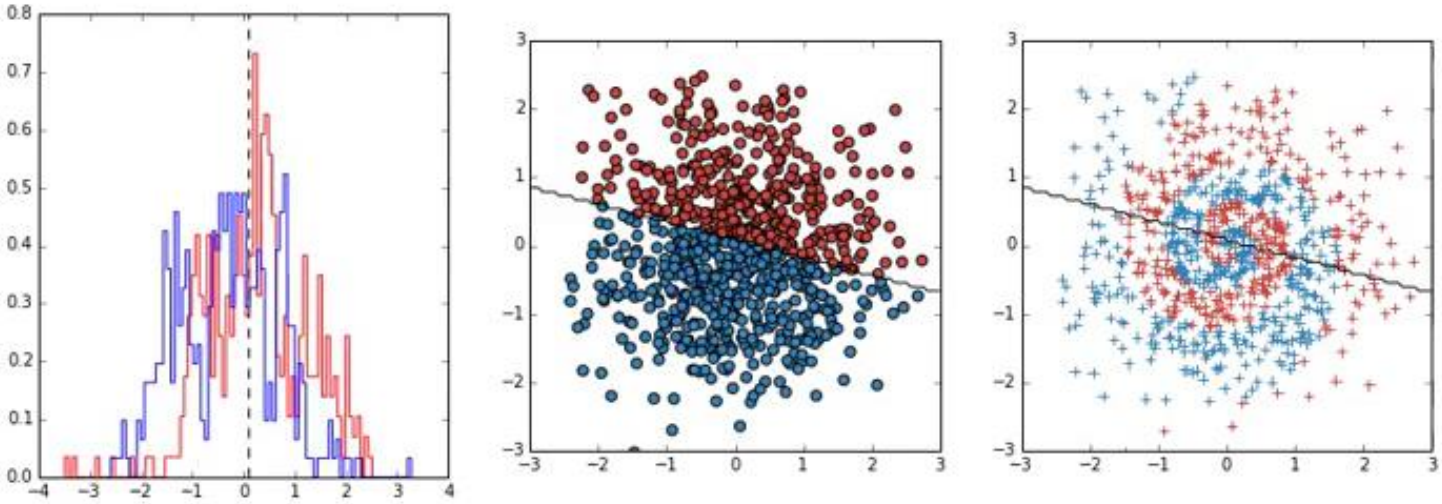


FIGURE 10.2. Simulated data (10.2): test error rate for boosting with stumps, as a function of the number of iterations. Also shown are the test error rate for a single stump, and a 244-node classification tree.

Hastie, T., Tibshirani, R., & Friedman, J. H. (2017). The elements of statistical learning: Data mining, inference, and prediction (12th ed). Springer series in statistics. New York: Springer.



Source: https://www.youtube.com/watch?v=2bECSz1R5EQ

Boosting – Error rate example

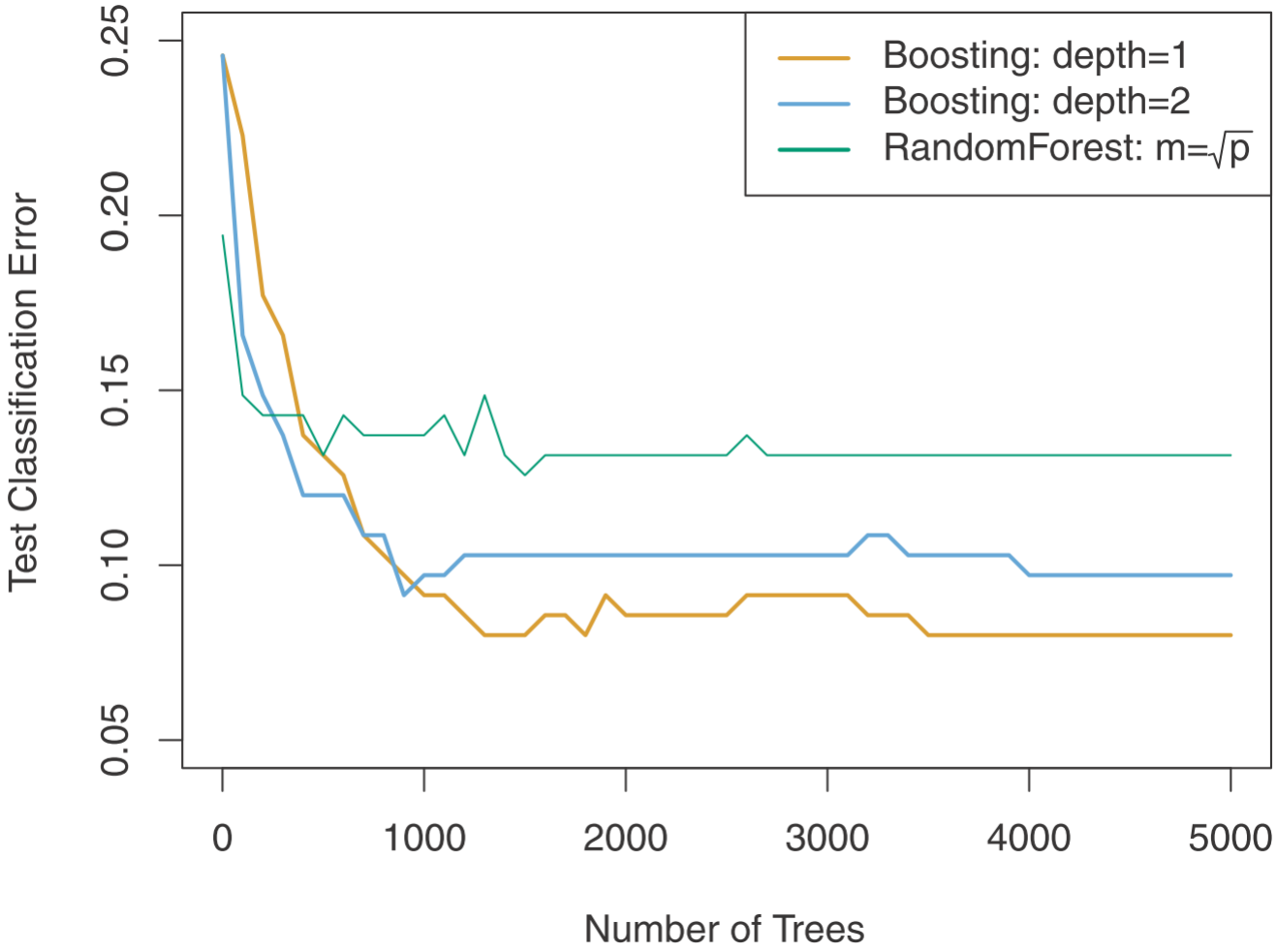
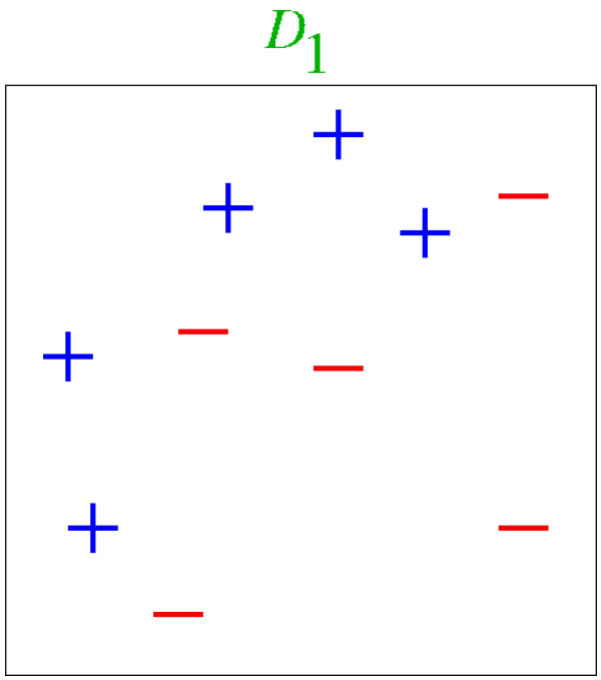


FIGURE 8.11. Results from performing boosting and random forests on the 15-class gene expression data set in order to predict cancer versus normal. The test error is displayed as a function of the number of trees. For the two boosted models, $\lambda = 0.01$. Depth-1 trees slightly outperform depth-2 trees, and both out-perform the random forest, although the standard errors are around 0.02, making none of these differences significant. The test error rate for a single tree is 24 %.

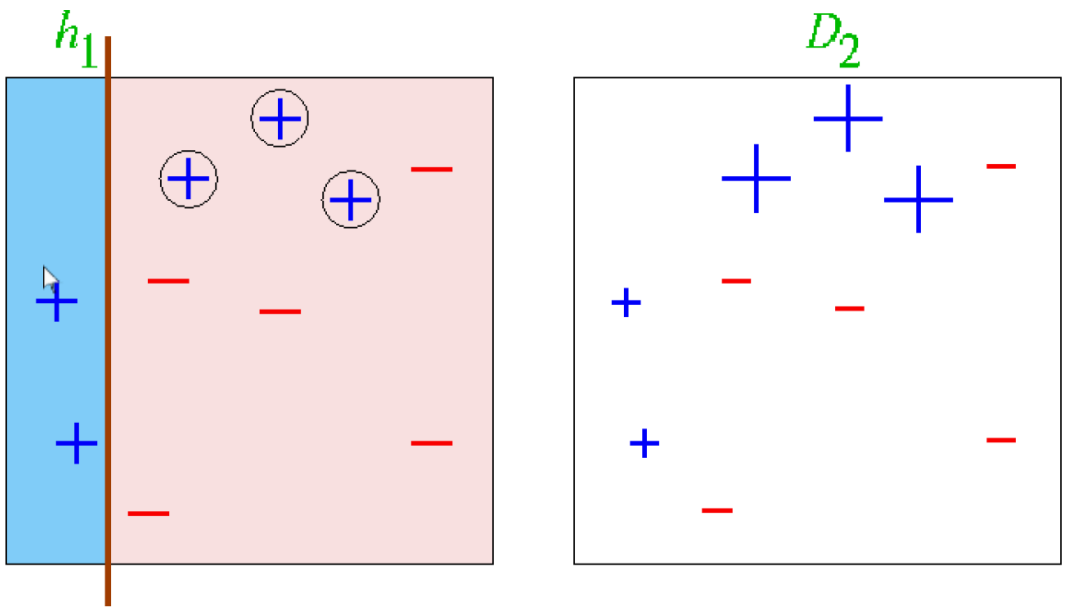
James, G., Witten, D., Hastie, T., & Tibshirani, R. (2014). An introduction to statistical learning: With applications in R (Corrected at 4th print). Springer texts in statistics. New York: Springer.

Toy Example



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

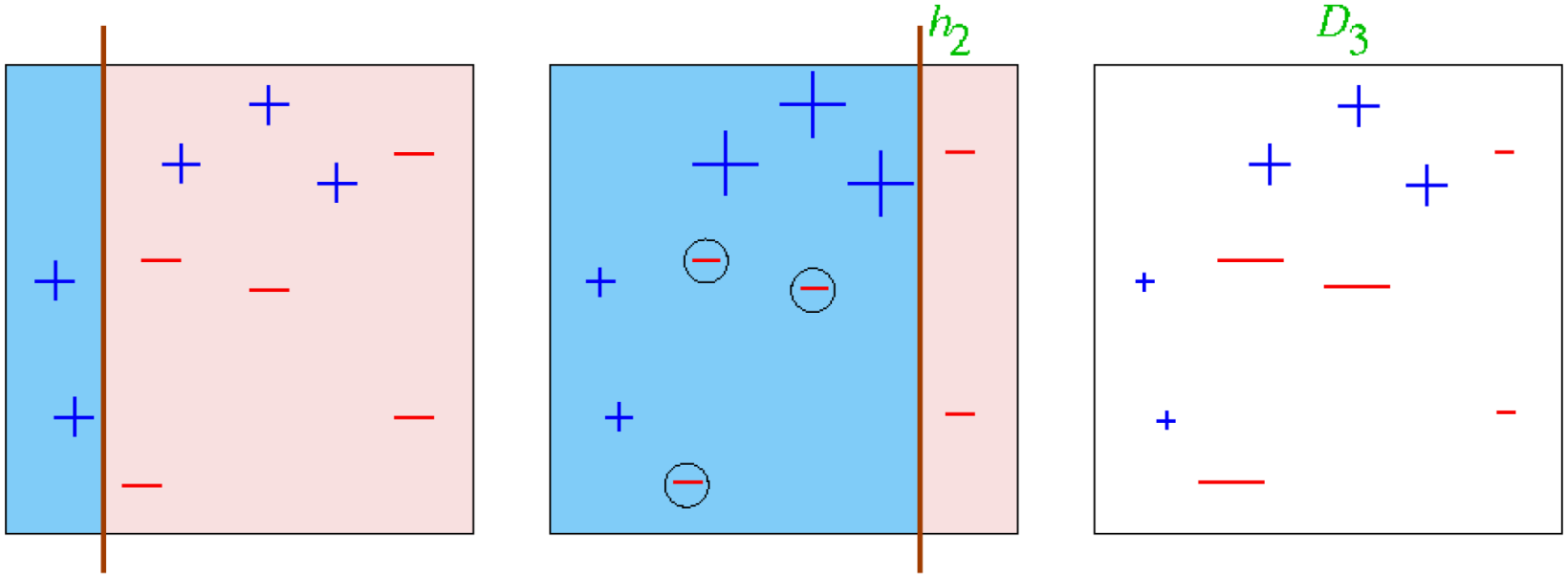
Round 1



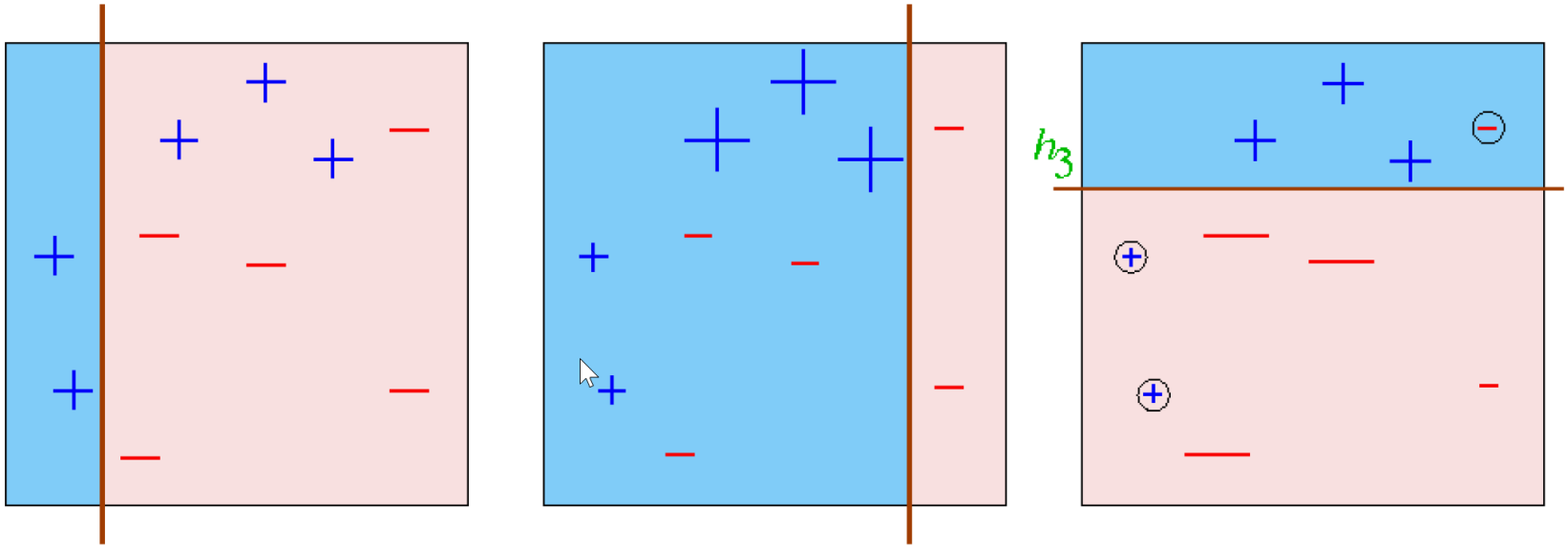
$\varepsilon_1 = 0.30$

$\alpha_1 = 0.42$

Round 2



Round 3

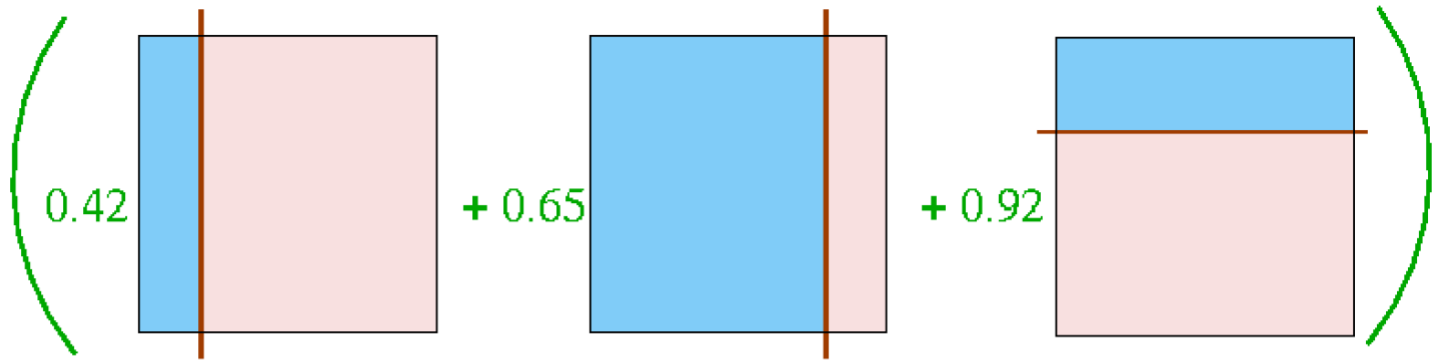


$\varepsilon_3 = 0.14$

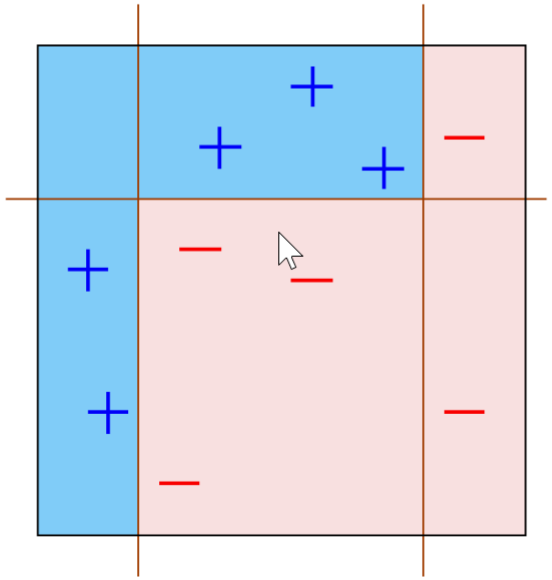
$\alpha_3 = 0.92$

Final Hypothesis

$H_{\text{final}} = \text{sign}\left(0.42 \; + 0.65 \; + 0.92 \right)$



$=$



Boosting

- Each of the trees can be rather small, with just a few terminal nodes.
- They learn slowly.
- In general, statistical learning approaches that learn slowly tend to perform well.
- Unlike bagging and random forests, boosting can overfit if the number of trees is too large, although this overfitting tends to occur slowly if at all. We use cross-validation to select the number of trees.
- In boosting, unlike in bagging, the construction of each tree depends strongly on the trees that have already been grown.

Outline

- Ensemble Methods
- Random Forests
- AdaBoost
- Stacking
- Summary

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

Learn a function that combines the predictions of the individual classifiers

- Train n different classifiers $C_1 ... C_n$ The base classifiers.
- Obtain predictions of the classifiers for the training examples
- Form a new data set (the meta data)
  i. Classes
     the same as the original dataset
  ii. 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!

Example Using a stacked classifier

Attributes			Class
x_{11}	...	x_{1n_a}	t
x_{21}	...	x_{2n_a}	f
...	...	...	...
x_{n_c1}	...	$x_{n_cn_a}$	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

Try each of the classifiers $C_1 ... C_n$

Form a feature vector consisting of their predictions

Submit these feature vectors to the meta classifier M

Outline

- Ensemble Methods
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- Summary

Summary