Statistisches Data Mining (StDM)
Woche 12

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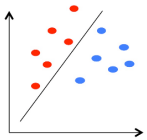
No laptops, no phones, no problems

Multitasking senkt Lerneffizienz:

- **Keine Laptops im Theorie-Unterricht Deckel zu oder fast zu (Sleep modus)**

Overview of classification (until the end to the semester)

Classifiers



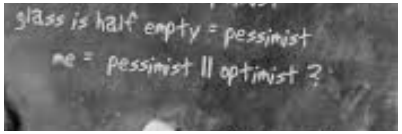
K-Nearest-Neighbors (KNN)
Logistic Regression
Linear discriminant analysis
Support Vector Machine (SVM)
Classification Trees
Neural networks NN
Deep Neural Networks (e.g. CNN, RNN)
...

Evaluation

Cross validation
Performance measures
ROC Analysis / Lift Charts

Theoretical Guidance / General Ideas

Bayes Classifier
Bias Variance Trade off (Overfitting)

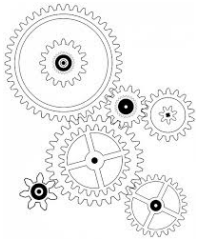


Combining classifiers

Bagging
Random Forest
Boosting

Feature Engineering

Feature Extraction
Feature Selection

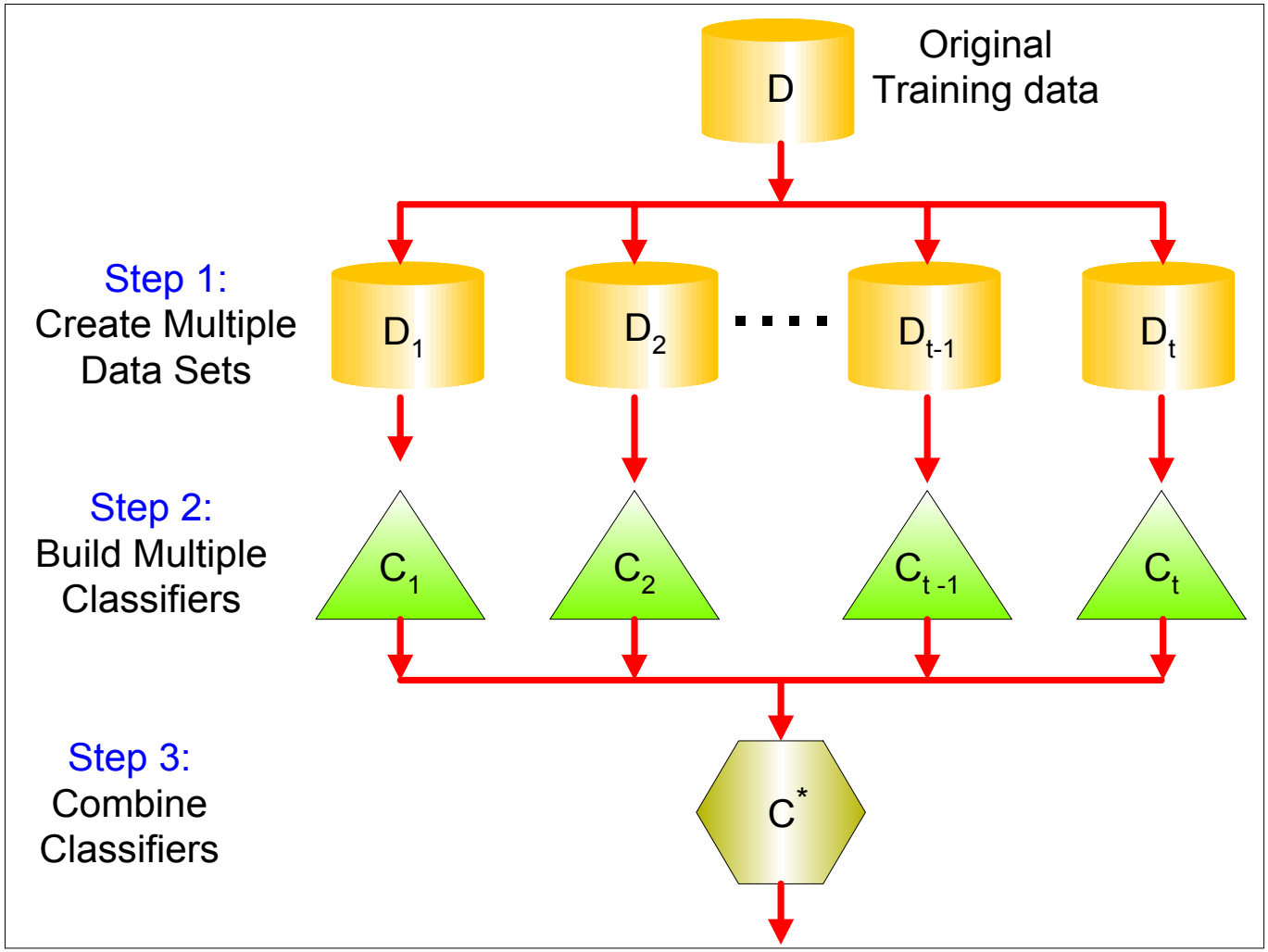


Overview of Ensemble Methods

- Many instances of the same classifier
  - Bagging (bootstrapping & aggregating)
    - Create “new” data using bootstrap
    - Train classifiers on new data
    - Average over all predictions (e.g. take majority vote)
  - Bagged Trees
    - Use bagging with decision trees
  - Random Forest
    - Bagged trees with special trick
  - Boosting
    - An iterative procedure to adaptively change distribution of training data by focusing more on previously misclassified records.
- Combining classifiers
  - Weighted averaging over predictions
  - Stacking classifiers
    - Use output of classifiers as input for a new classifier

Bagging / Random Forest
Chapter 8.2 in ILSR

Bagging: Bootstrap Aggregating



Source: Tan, Steinbach, Kumar

Why does it work?

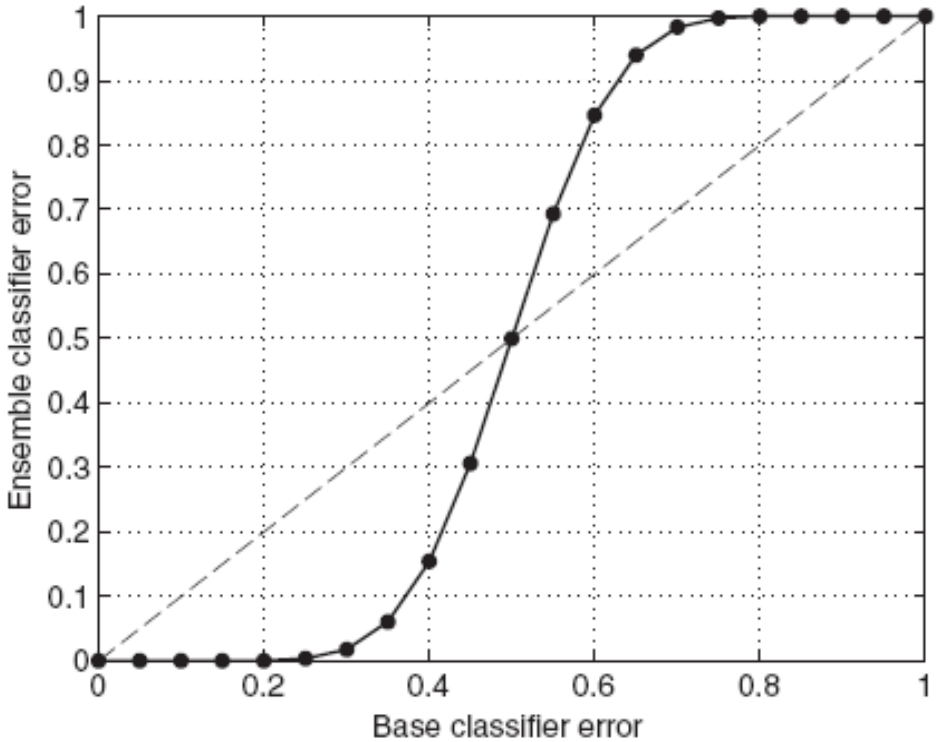
- Suppose there are 25 base classifiers
- Each classifier has error rate, ε = 0.35
- Assume classifiers are independent (that's the hardest assumption)
- Take **majority vote**
- Majority voter is wrong if 13 or more are wrong
- Number of wrong predictors X ~ Bin(size=25, p_0=0.35)

```
> 1 - pbinom(12, size=25, prob = 0.35)
[1] 0.06044491
```

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

Why does it work?

- 25 Base Classifiers



Ensembles are only better than one classifier, if each classifier is better than random guessing!

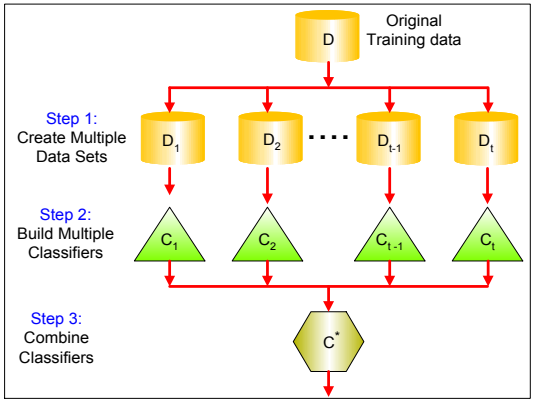
Reminder Trees

```
library(rpart)
fit <- rpart(Kyphosis ~ ., data = kyphosis)
plot(fit)
text(fit, use.n = TRUE)

pred = predict(fit, data=kyphosis)
> head(pred,4) #Probabilities
     absent   present
1 0.4210526 0.5789474
2 0.8571429 0.1428571
3 0.4210526 0.5789474
4 0.4210526 0.5789474
```

Bagging trees

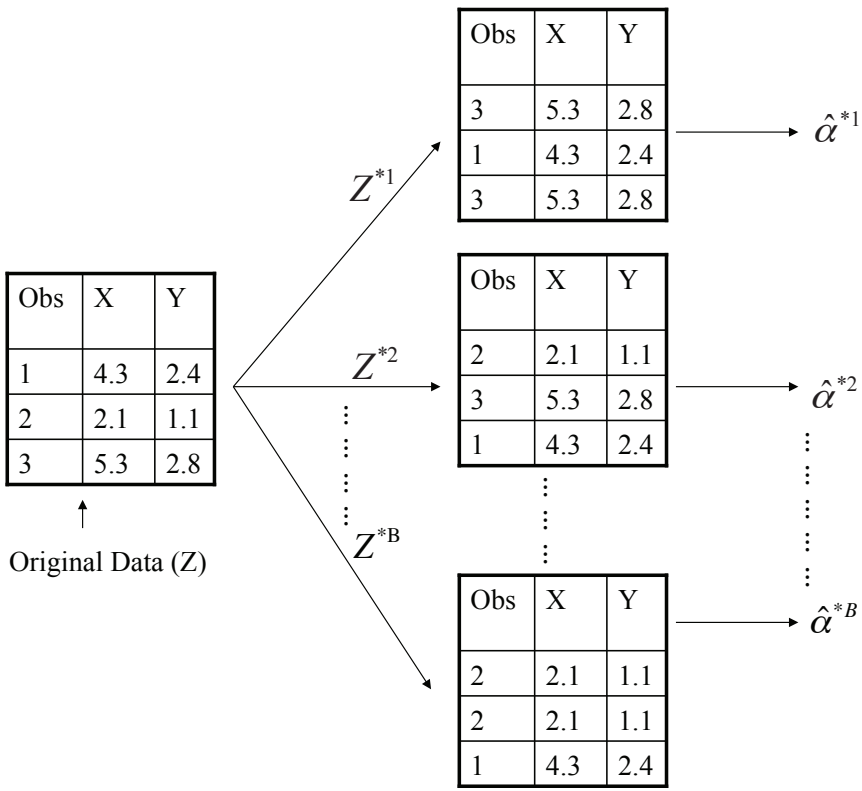
- Decision trees suffer from <u>high variance</u>!
  - If we randomly split the training data into 2 parts, and fit decision trees on both parts, the results could be quite different
  - Averaging reduces Variance
    - Independent ➔ var ~ σ^2 / n (not true strictly)

- Bagging for trees
  - Take bootstrap B samples from training set
  - For each bootstrap sample train a decision tree
  - For the test set take the majority vote of all trained classifiers (or average)



Reminder: Bootstrapping

- Resampling of the observed dataset (and of equal size to the observed dataset), each of which is obtained by **random sampling with replacement** from the original dataset

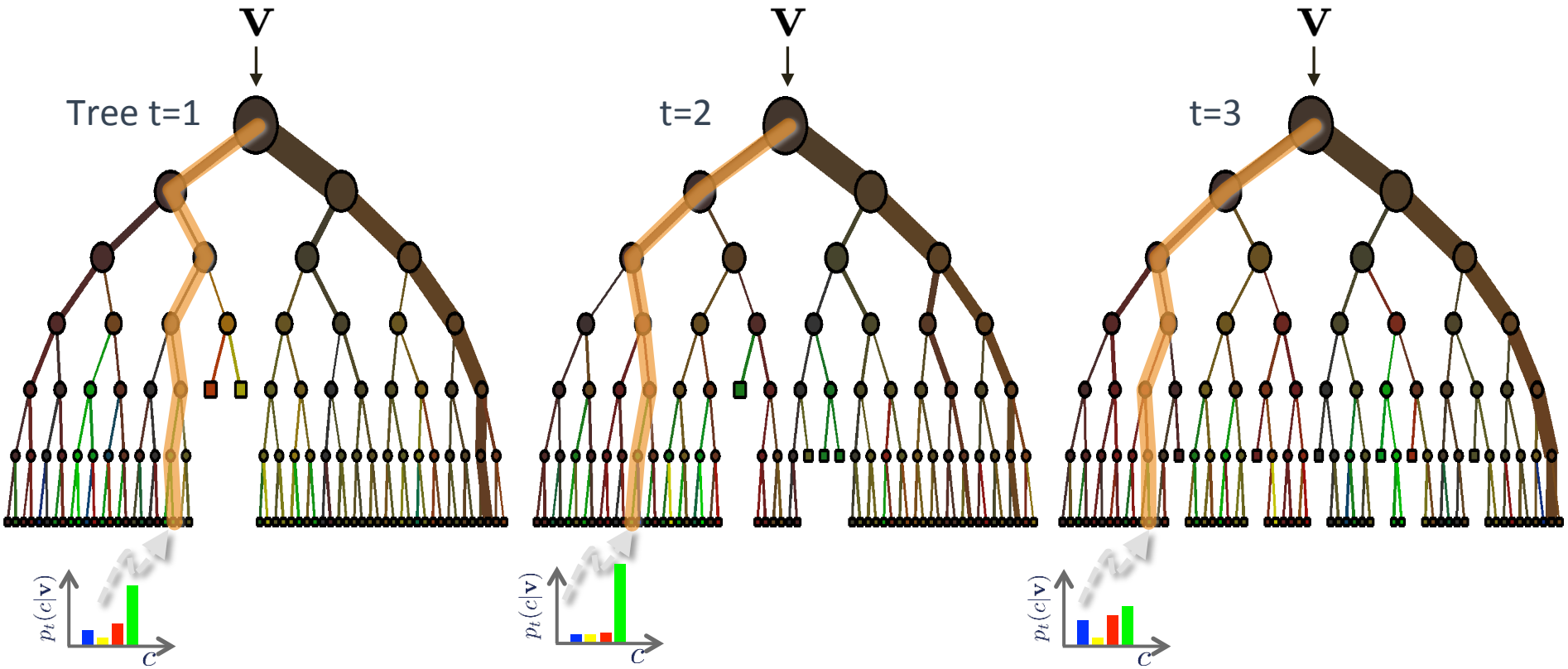


Slide taken from Al Sharif: http://www.alsharif.info/#!iom530/c21o7

Lösung der Aufgabe: Bagging von Hand

```
library(rpart)
library(MASS) # For the data set

Boston$crim = Boston$crim > median(Boston$crim)

# Split in Training and Testset
idt = sample(nrow(Boston), size = floor(nrow(Boston)*3/4))
data.train = Boston[idt, ]
data.test = Boston[- idt, ]

# Single Tree
d = rpart( as.factor(crim) ~ ., data = data.train)
sum(predict(fit, data.test, type='class') == Boston$crim[-idt]) / nrow(data.test) #0.88

n.trees = 100
preds = rep(0, nrow(data.test))
for (j in 1:n.trees ){
  # Doing the bootstrap
  index.train = sample( nrow(data.train), size = nrow(data.train), replace = TRUE )
  # Fitting to the training data
  fit = rpart( as.factor(crim) ~ ., data = data.train[index.train,])
  # Predict the test set
  tree.fit.test = predict(fit, data.test, type='class')
  preds = preds + ifelse(tree.fit.test == TRUE, 1, -1) #Trick with +-1
}

sum(Boston$crim[-idt] == (preds > 0)) / nrow(data.test) #0.96
```

How to classify a new observation?

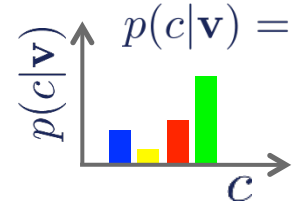


Two ways to derive the ensemble result:

1) Each tree has a “winner-class”
Take the class which was most often the winner

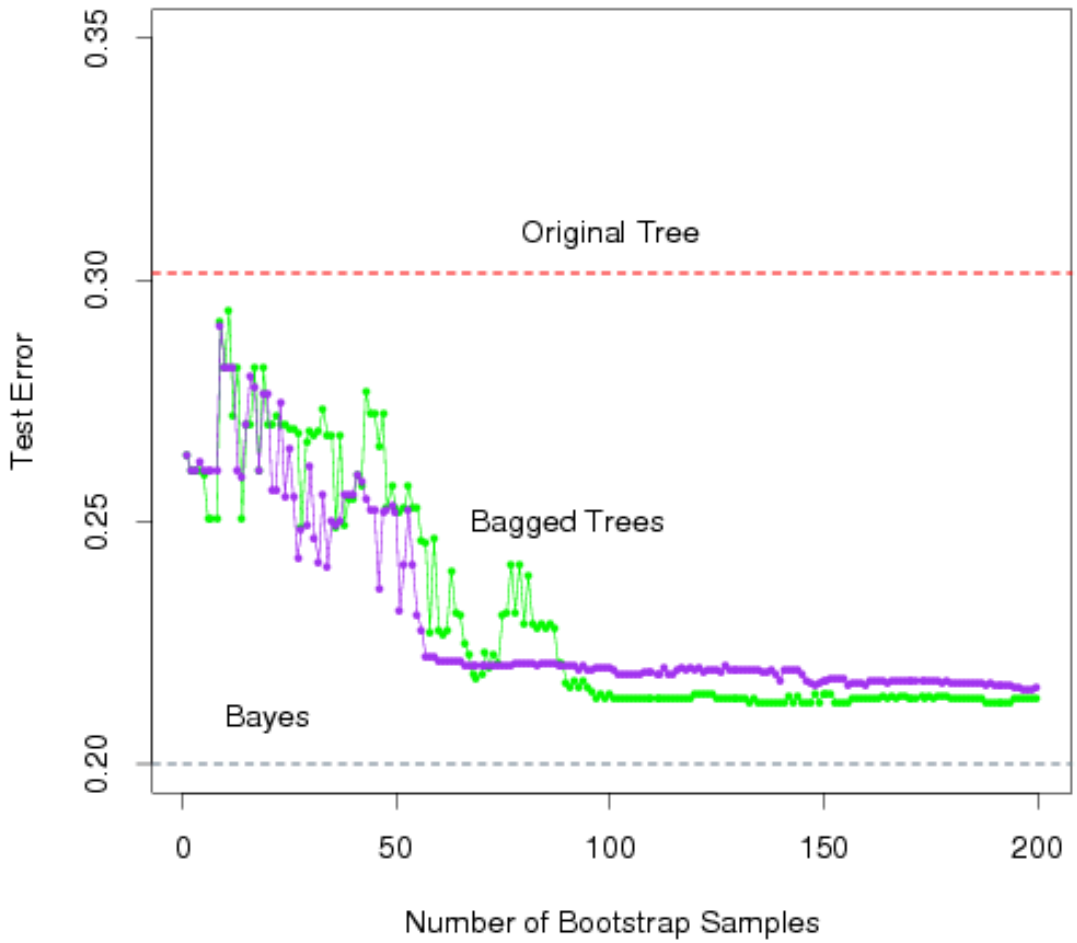
2) average probabilities:

$$p(c|\mathbf{v}) = \frac{1}{T}\sum_{t}^{T} p_t(c|\mathbf{v})$$



A Comparison of Error Rates

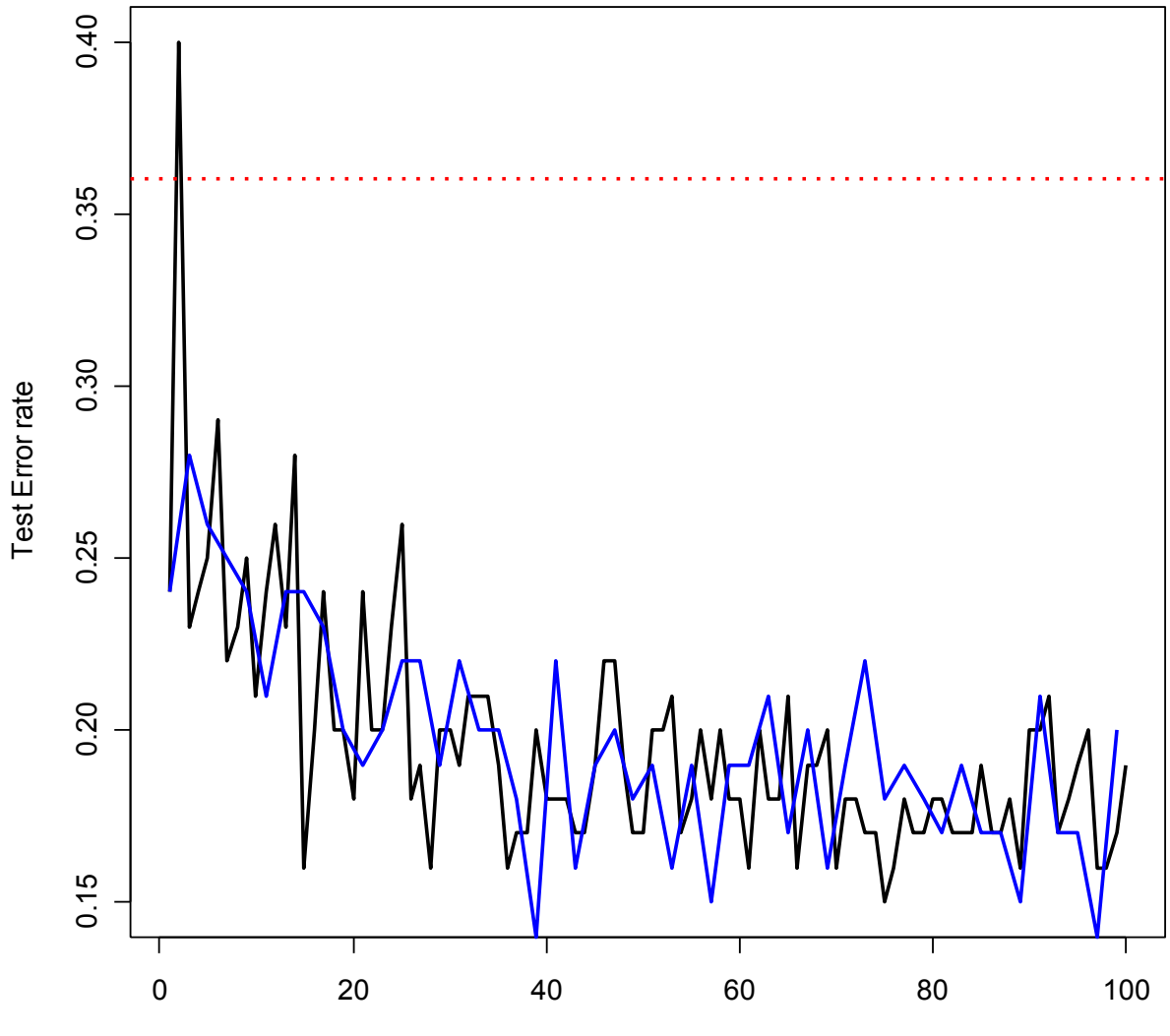
- Here the green line represents a simple majority vote approach
- The purple line corresponds to averaging the probability estimates.
- Both do far better than a single tree (dashed red) and get close to the Bayes error rate (dashed grey).



Slide taken from Al Sharif: http://www.alsharif.info/#!iom530/c21o7

Example 2: Car Seat Data

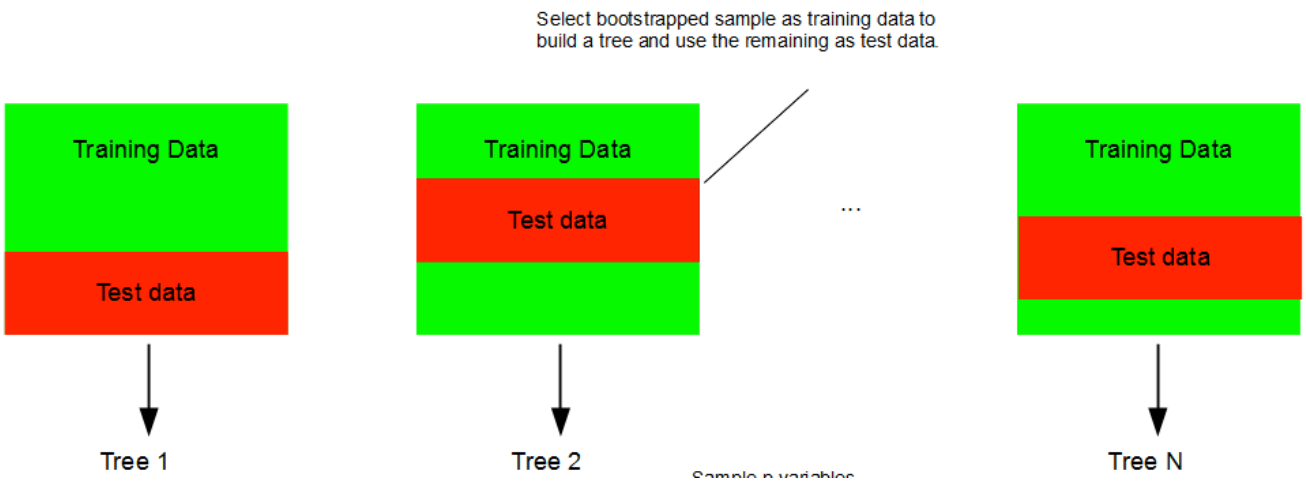
- The red line represents the test error rate using a single tree.
- The black line corresponds to the bagging error rate using majority vote while the blue line averages the probabilities.



Slide taken from Al Sharif: http://www.alsharif.info/#!iom530/c2167

Out-of-Bag Estimation: "Cross-validation on the fly"

- Since bootstrapping involves random selection of subsets of observations to build a training data set, then the remaining non-selected part could be the testing data.
- On average, each bagged tree makes use of around 2/3 of the observations, so we end up having 1/3 of the observations used for testing



Slide taken from Al Sharif: http://www.alsharif.info/#!iom530/c21o7

The importance of independence

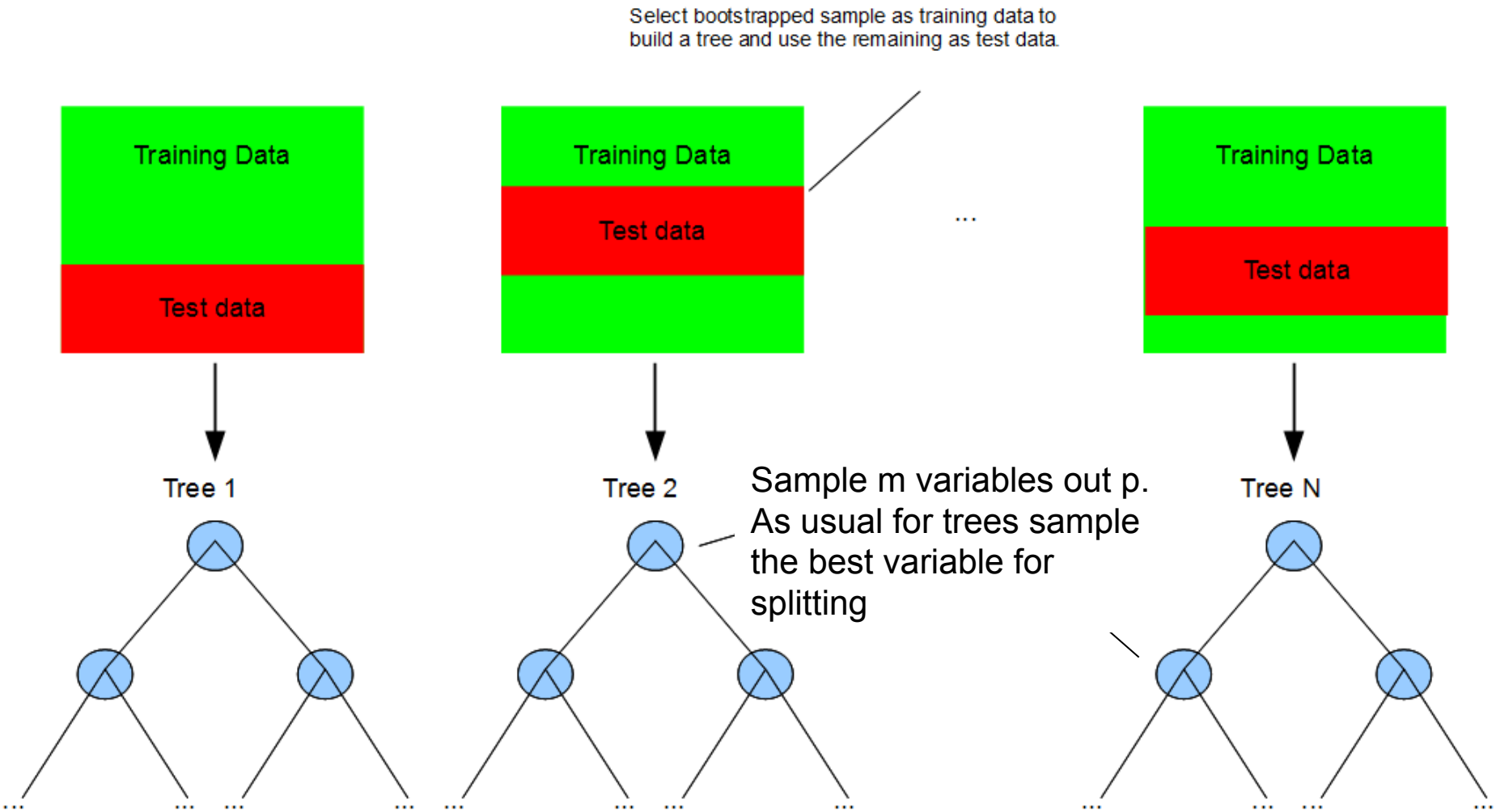
- It's a quite strong assumption, that all classifiers are independent.
- Since the same features are used in each bag, the resulting classifiers are quite dependent.
  - **We don't really get new classifiers or trees**
  - The bagging has high bias but low variance.
- **De-correlate by any means! ➔ Random Forest**

Random Forest

Random Forests

- It is a very efficient statistical learning method
- It builds on the idea of bagging, but it provides an improvement because it de-correlates the trees
- How does it work?
  - Build a number of decision trees on bootstrapped training sample, but when building these trees, each time a split in a tree is considered, **a random sample of *m* predictors** is chosen as split candidates from the full set of *p* predictors (Usually $m \approx \sqrt{p}$)

Random Forest: Learning algorithm



Why are we considering a random sample of m predictors instead of all p predictors for splitting?

- Suppose that we have a very strong predictor in the data set along with a number of other moderately strong predictor, then in the collection of bagged trees, most or all of them will use the very strong predictor for the first split!

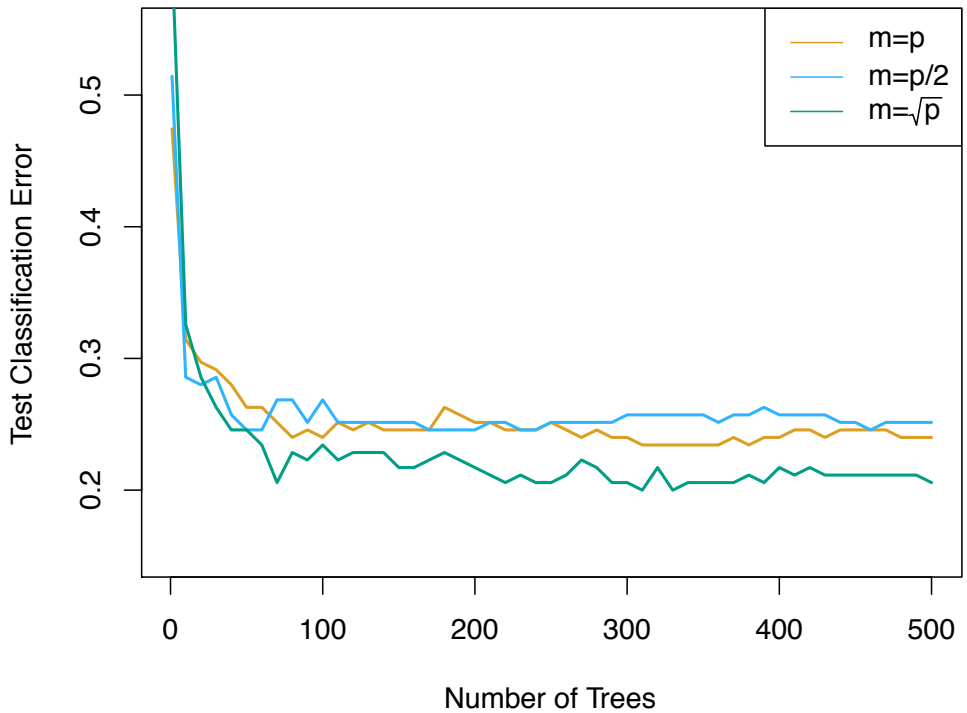
- All bagged trees will look similar. Hence all the predictions from the bagged trees will be highly correlated

- Averaging many highly correlated quantities does not lead to a large variance reduction, and thus random forests “de-correlates” the bagged trees leading to more reduction in variance

- This makes the individual trees weaker but enhances the overall performance

Random Forest with different values of "m"

- Notice when random forests are built using m = p, then this amounts simply to bagging.



Random Forest in R (basic)

```
fit = randomForest(as.factor(crim) ~ ., data=data.train)
predict(fit, data.test)

####
# Parameters
randomForest(as.factor(crim) ~ ., data=data.train,
ntree=100, mtry = 42)

#ntree number of trees grown
#mtry number of features used in each split. If set to p
```

➔Bagged Trees

Variable Importance Measure

- Bagging typically improves the accuracy over prediction using a single tree, but it is now hard to interpret the model!
- We have hundreds of trees, and it is no longer clear which variables are most important to the procedure
- Thus bagging improves prediction accuracy at the expense of interpretability
- But, we can still get an overall summary of the importance of each predictor using Relative Influence Plots

Slide taken from Al Sharif: http://www.alsharif.info/#!iom530/c21o7

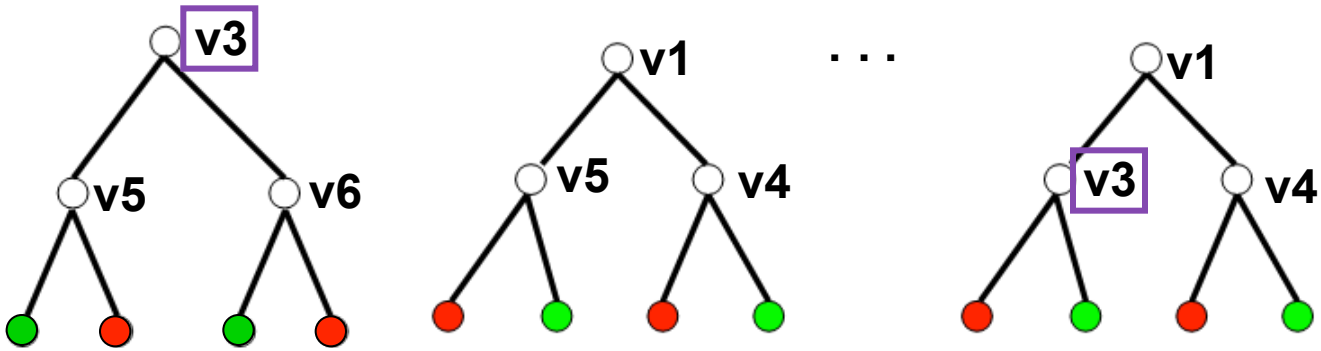
Variable Importance 1: performance-loss by permutation

Determine importance-2 for v4:

1) obtain standard oob-performance
2) values of v4 are randomly permuted in oob samples and oob-performance is again computed. If variable is not important nothing happends. Hence:
3) Use decrease of performace as important measure of v4

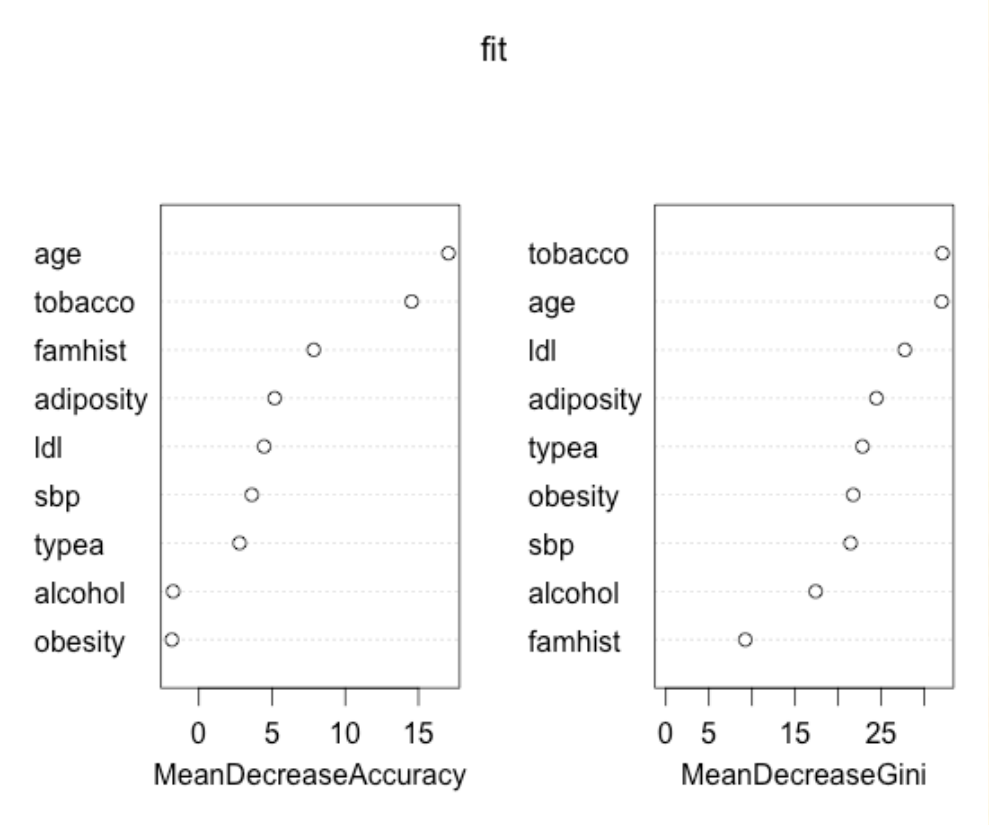
v1	v2	v3	v4	v5	v6	v7
0	1	1	2	0	1	0
0	2	2	1	2	0	1
1	0	0	1	1	2	0
1	0	0	1	1	0	2
0	2	1	0	2	0	1

Variable Importance 2: Score improvement at each Split



At each split where the variable, e.g. v3, is used the improvement of the score (Decrease of Giniindex) is measured. The average over all these v3-involving splits in all trees is the importance-1 measure of v3.

varImp



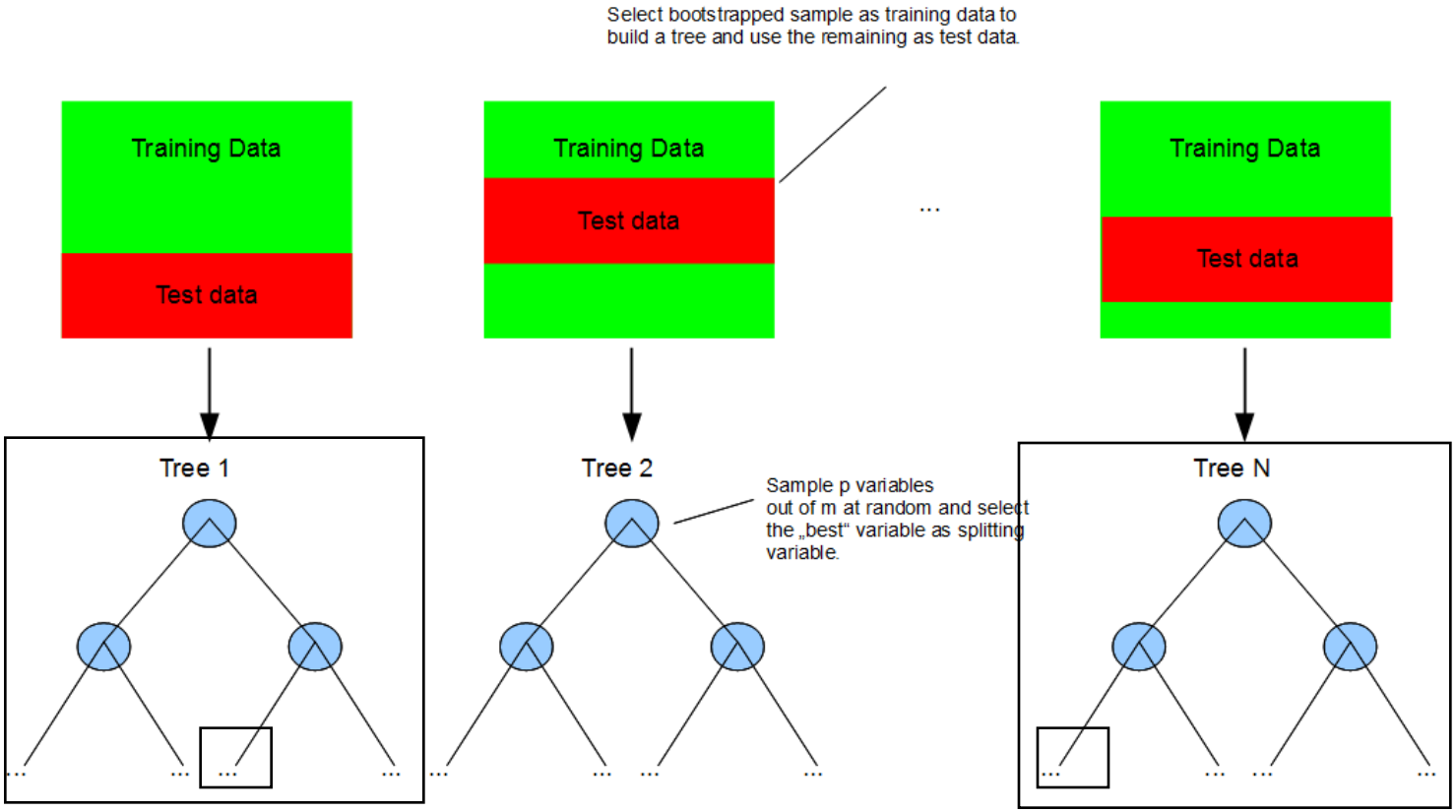

```
library(randomForest)
library(ElemStatLearn)
heart = SAheart
#importance = TRUE sonst keine Accuracy
fit = randomForest(as.factor(chd) ~ ., data =
heart, importance=TRUE)
predict(fit, data=kyphosis, type='prob')
varImpPlot(fit)
```

Interpreting Variable Importance

- RF in standard implementation is biased towards continuous variables
- Problems with correlations:
  - If two variables are highly correlated removing one yield no degeneration in performance
  - Same with Gini index measure
  - Not specific for random forest: correlation often posses problems

Using RF as similarity measure

Proximity: Similarity between two observation according to supervised RF



The test data contains now a pair of observation random forest determines proximity by counting in how many trees both observation end up in the same leaf. Since the RF was built in a supervised modus, the proximity is also influenced by the class label of the observations.

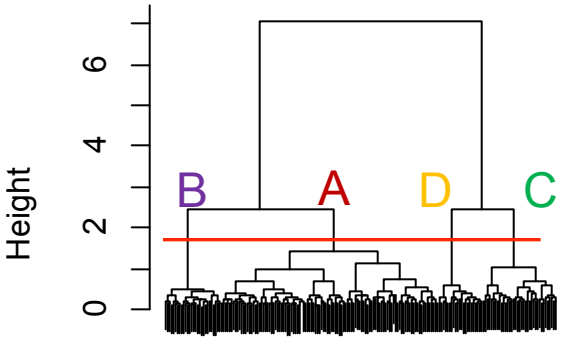
Similarity Measure (details)

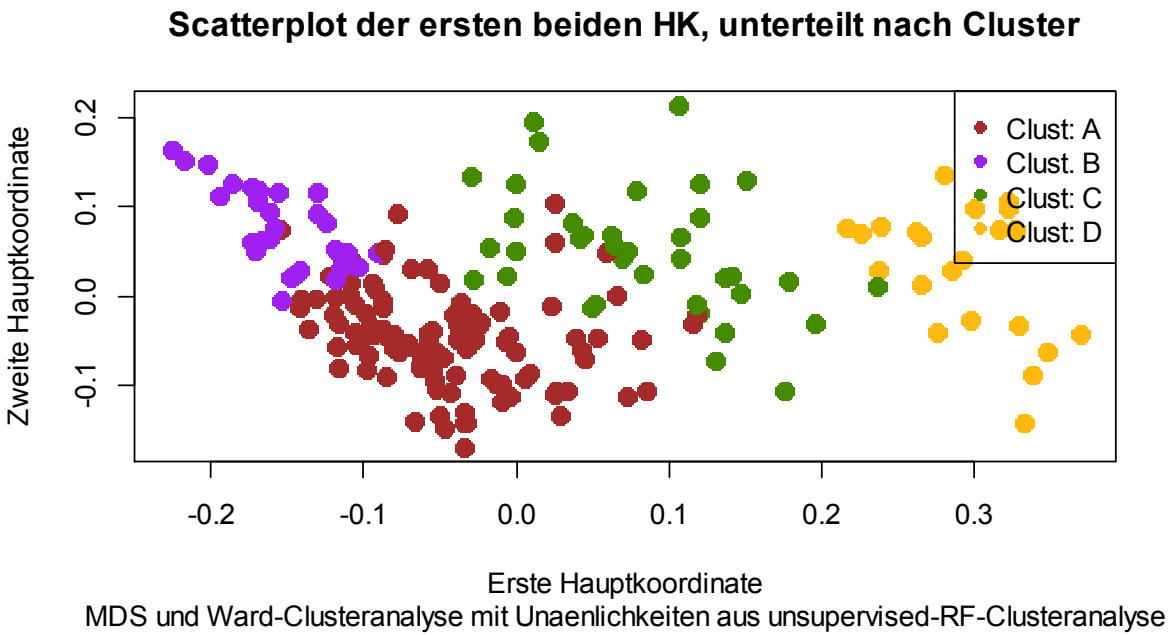
- Only use out of bag estimates
- If case i and case j both land in the same terminal node, increase the similarity between i and j by 1.
- At the end of the run normalize
- Dissimilarity = sqrt(1-Similarity)

Unsupervised

- In the unsupervised modus we do not provide a class label to the observations.
- In this modus RF creates new artificial observations by sampling from the marignal distribution of each feature and assigning the class label 0 to these new artificial observations. The original observations get class label 1.

Use proximities from unsupervised-RF for Clustering and MDS





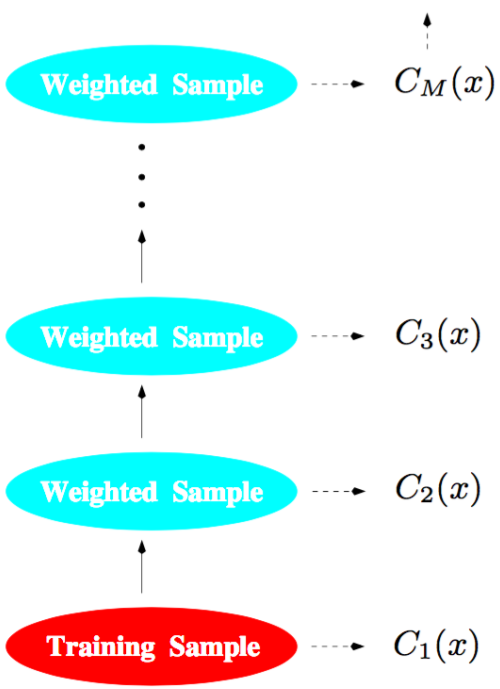
Technical in R:
X is data matrix or data.table **without** the labels
randomForest(X, proximity = TRUE)

Pros and cons of using unsupervised RF for clustering

- Pros
  - Invariant with respect to monotonic transformations
    -> no centering or standardization is required
    -> handles well skewed data
  - Robust against outliers
  - Can identify outlier
  - Can lead to more meaningful clusters (e.g. seen in gene expression data of cancer patients) since RF focuses on variable which are dependent (in gene expression these genes may correspond to disease pathways)
- Cons
  - “Black box”

Boosting

- Consider binary problem with classes coded as +1,-1
- A sequence of classifiers C_m is learnt
- The training data is reweighted (depending on misclassification of example)

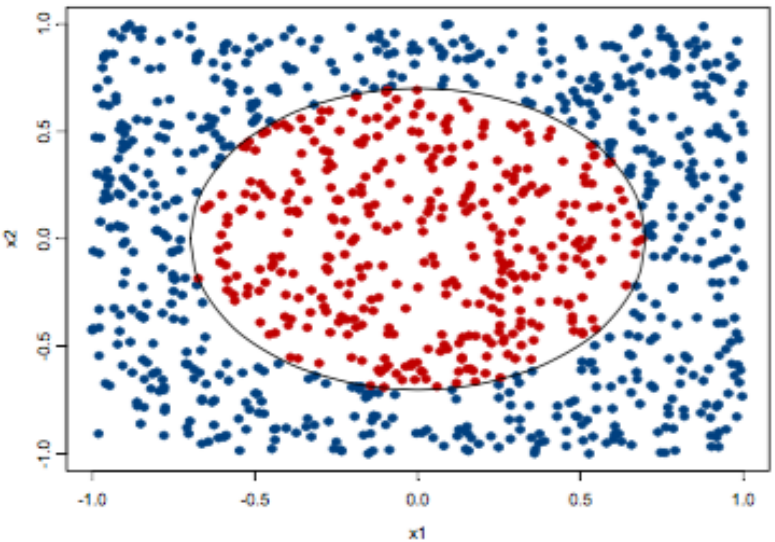


- Average many trees, each grown to re-weighted versions of the training data.
- Final Classifier is weighted average of classifiers:

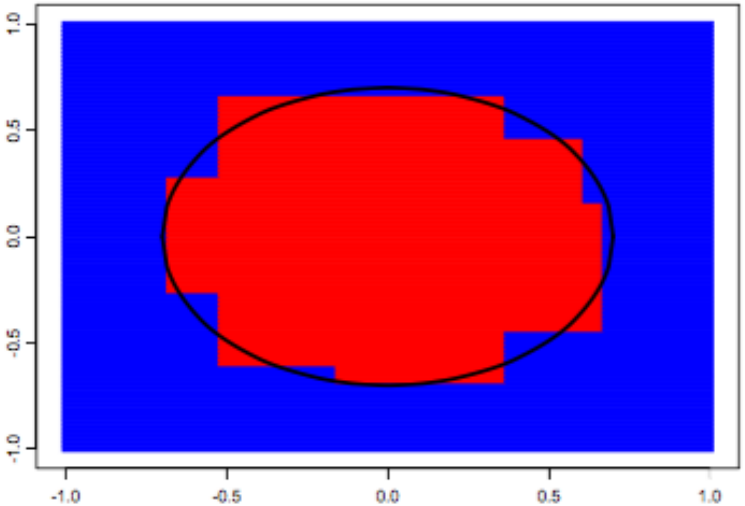
$$C(x) = \text{sign}\left[\sum_{m=1}^{M} \alpha_m C_m(x)\right]$$

Slides: Trevor Hastie

An experiment

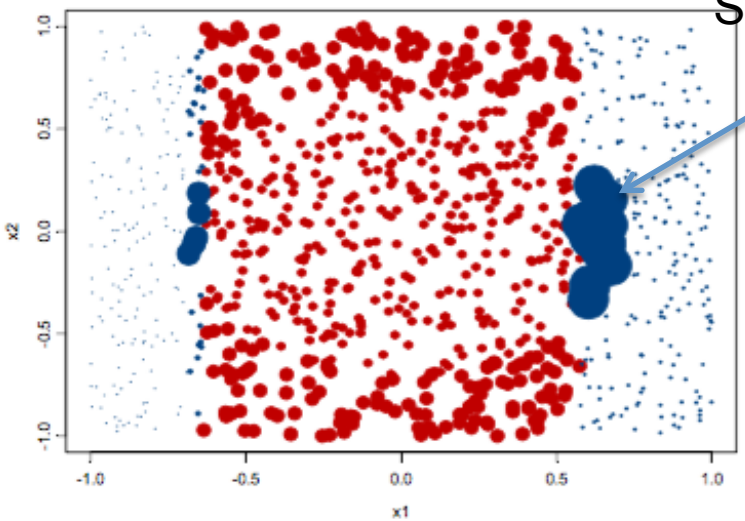


Decission Boundary of a single tree. E.g.



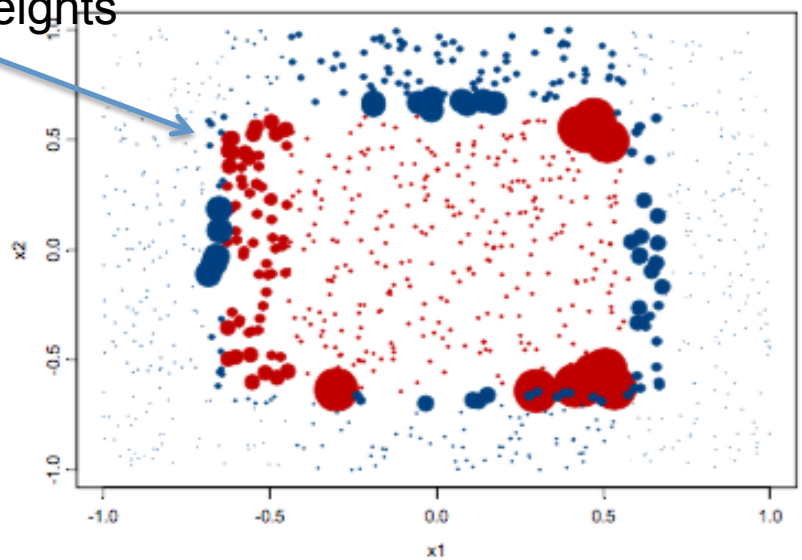
An experiment

Decision Boundary after 1 iteration

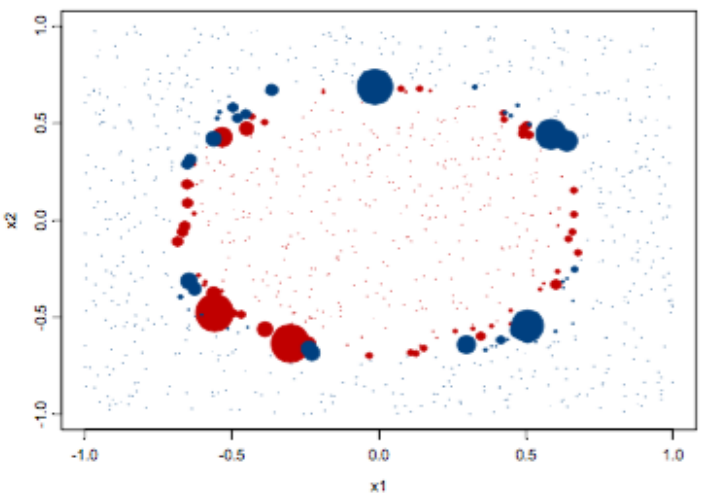


Strong Weights

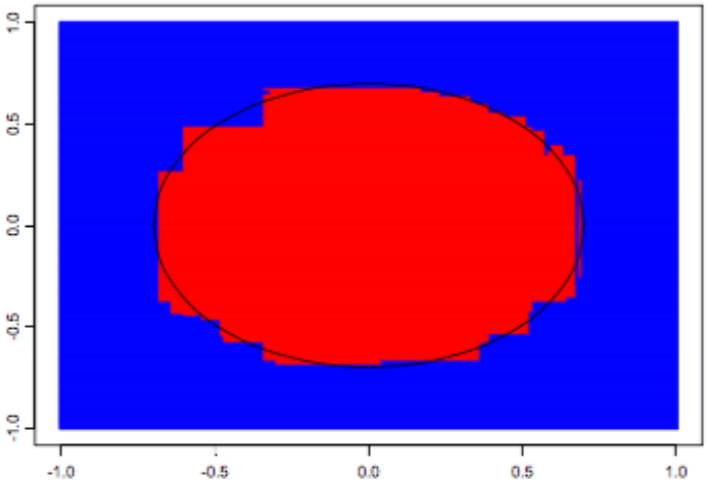
Decision Boundary after 3 iterations



Decision Boundary after 20 iterations



Decision Boundary after 100 iterations



Idea of Ada Boost Algorithm

Basic Idea:

- start with identical weights $w_i = 1/n$, fit a learner $f_1(\cdot)$ and evaluate its insample prediction performance for y_i
- depending on whether or how heavily an observation i was misclassified, increase its weight w_i. Hence the learner is forced to focus on the difficult-to-classify instances.
- the contribution of the learner $f_1(\cdot)$ to the final classifier $F(\cdot)$ is gauged by the averaging weight α_1. It is large if $f_1(\cdot)$ performed well, and small otherwise.

→ Repeat this process M times to obtain the solution $F_M(\cdot)$

Details of Ada Boost Algorithm

Algorithm:

1) Set $y_i \in \{-1,+1\}$ and start with identical weights $w_i = 1/n$

2) Repeat for $m = 1,2,\ldots,M$:

   a) Fit the classifier $f_m(x) \in \{-1,+1\}$ using weights w_i

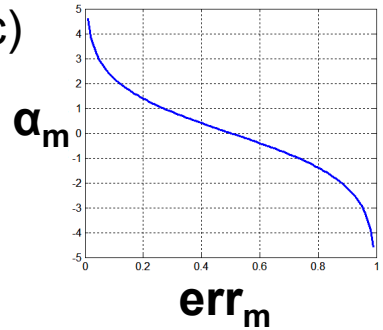
   b) Compute the weighted error $err_m = \sum_i w_i \cdot I[y_i \neq f_m(x_i)]$

   c) Compute the aggregation weight $\alpha_m = \log((1-err_m)/err_m)$

   d) Set $w_i \leftarrow w_i \cdot \exp(\alpha_m \cdot I[y_i \neq f_m(x_i)])$; normalize to $\sum_i w_i = 1$

3) Output $F_M(x) = sign \sum_{m=1}^{M} \alpha_m f_m(x)$

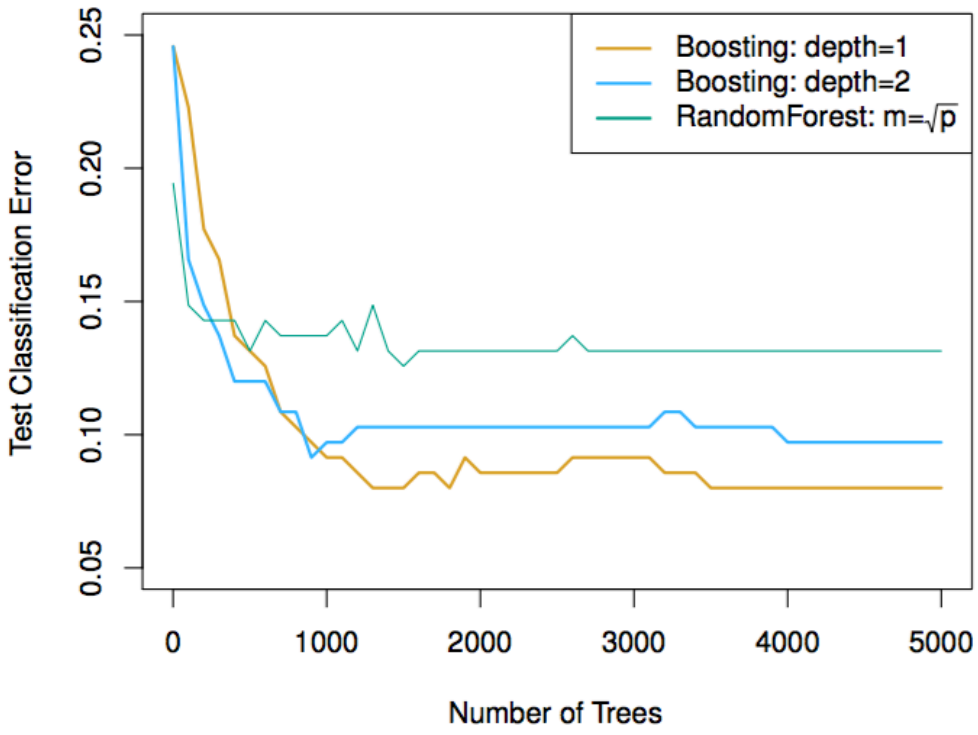
Zu c)



Error small ➔large weight

Error > 0.5 opposite is taken (quite uncommon only for small m)

Performance of Boosting



Boosting most frequently used with trees (not necessary)
Trees are typically only grown to a certain depth (1,2).
If trees of depth 2 would be better than trees of depth 1 (stubs) interactions between features would be important