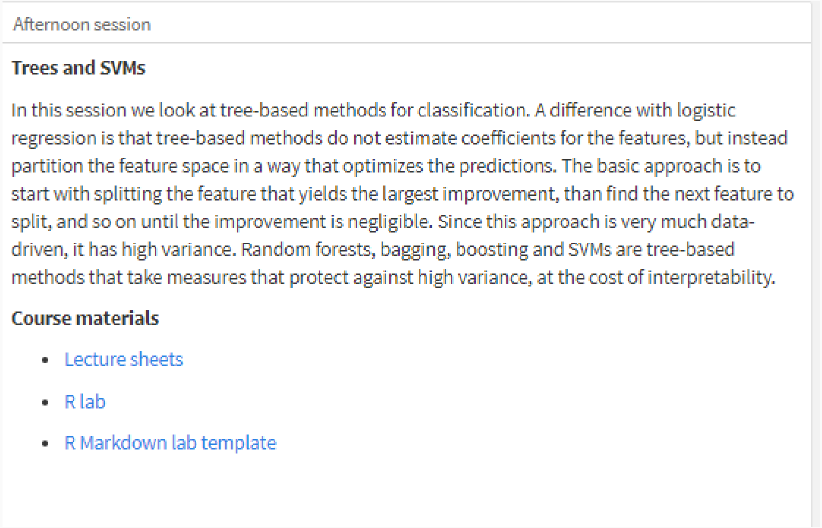
Supervised Learning: Classification

Tree-based methods and Support Vector Machines

Maarten Cruyff

Program



Afternoon session

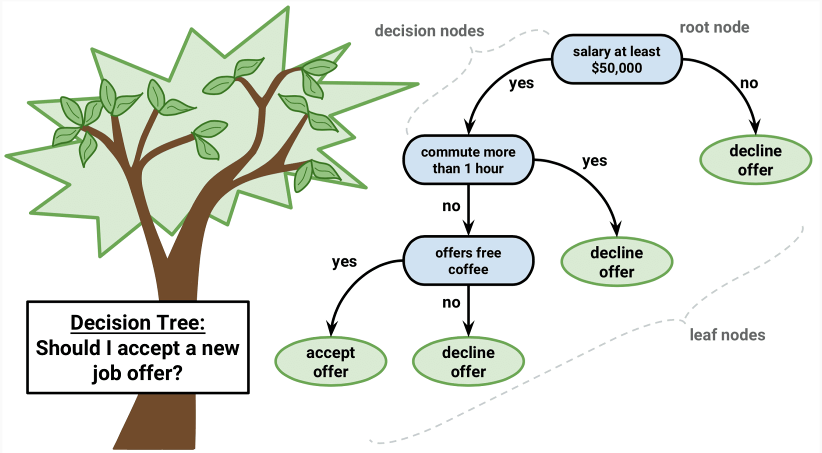
Trees and SVMs

In this session we look at tree-based methods for classification. A difference with logistic regression is that tree-based methods do not estimate coefficients for the features, but instead partition the feature space in a way that optimizes the predictions. The basic approach is to start with splitting the feature that yields the largest improvement, than find the next feature to split, and so on until the improvement is negligible. Since this approach is very much data-driven, it has high variance. Random forests, bagging, boosting and SVMs are tree-based methods that take measures that protect against high variance, at the cost of interpretability.

Course materials

- Lecture sheets
- R lab
- R Markdown lab template

Classification trees



Content

Classification trees

1. Recursive binary splitting algorithm
2. Splits features on basis of node *purity*

- Gini index
- deviance

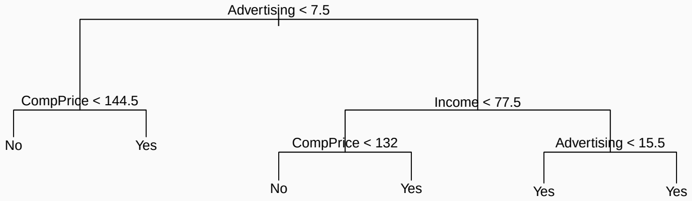


Figure 1: Sale of car seats (Yes/No)

Recusrsive binary splitting

Algorithm

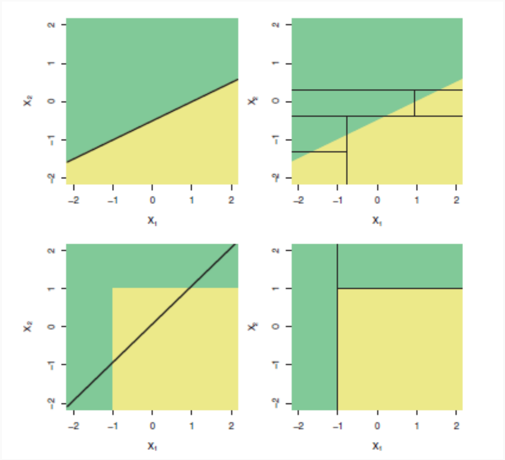
1. Divide feature space in non-overlapping, rectangular regions
2. Choose splits that minimize *node impurity* (homogeneity of nodes)
3. Assign region to class with highest mode
4. Stop when node purity no longer increases

Algorithm is top-down and greedy, so

- high variance

Classification with trees or regression?

Depends on nature of relationship between classes and features



Package tree

Growing and plotting trees with function tree()

```r
fit_tree <- tree(formula, data, split = c("deviance", "gini"))

plot(fit_tree)
text(fit_tree)
```

- minimization of deviance or gini impurity
- text() for adding labels to nodes

Methods to reduce variance:

1. Pruning
   - cut branches with cross-validation and regularization
2. Bagging
   - average predictions of bootstrapped trees
3. Random forests
   - average predictions of decorrelated bootstrapped trees
4. Boosting
   - weighted combination of weak classifiers (small trees)

Pruning

Cost-complexity pruning (package `tree`)

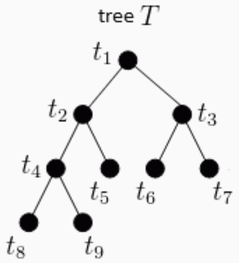
1. Cross-validate tree to find optimal number of nodes
   - based on either deviance or misclassification error rate

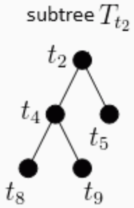
2. Prune the tree with optimal number of nodes
   - number of nodes with smallest deviance/misclassification error rate

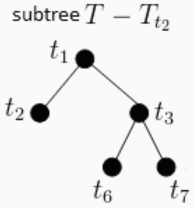
3. Get predictions of pruned tree on test set
   - `predict.tree` returns either probabilities or classifications

```r
cv.tree(fit_tree, method = c("deviance", "misclass"))

pruned_tree <- prune.tree(fit_tree, best = <number>)

predict(pruned_tree, newdata, type = "class")
```

Pruning example



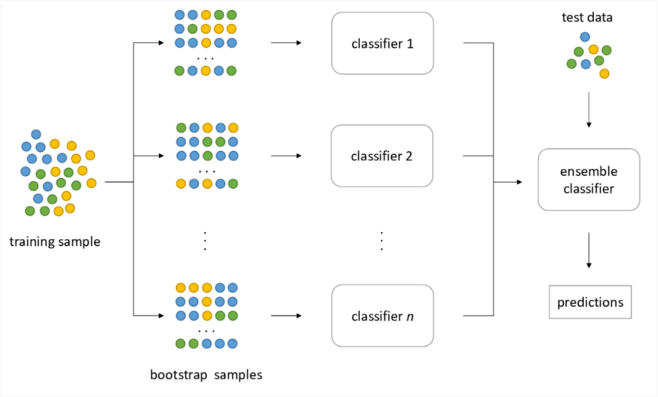




Bagging, random forests

Algorithm

1. Fit classification trees to B bootstrap samples
2. Average the predictions
3. Out-Of-Bag (OOB) as estimate validation error



Bagging vs random forests

Bagging

- considers all predictors at each split
- best predictors turn up in each tree
- highly correlated trees
- high variance

Random forests

- considers random sample of predictors at each step
- all predictors get a fair chance
- decorrelated trees
- lower variance

Out-of-bag error rate

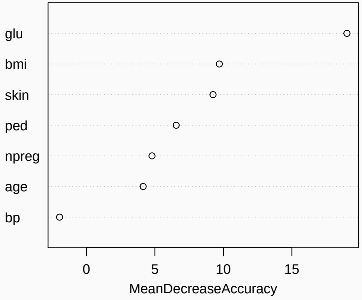
On average 1/3 of observations not in bootstrap (Out-Of-Bag)

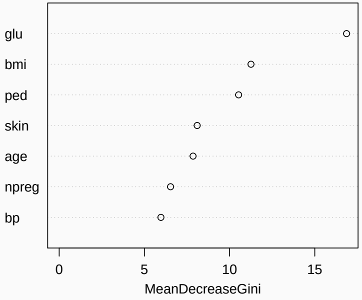
- OOB cases used to compute validation error
- no need for cross validation
- computationally very efficient

Variable importance

When averaging trees the tree structure is lost

- how to interpret solution then?
- effect predictors averaged over trees
- visualize with *variable importance* plots





Package randomForest

Functions for bagging/random forest

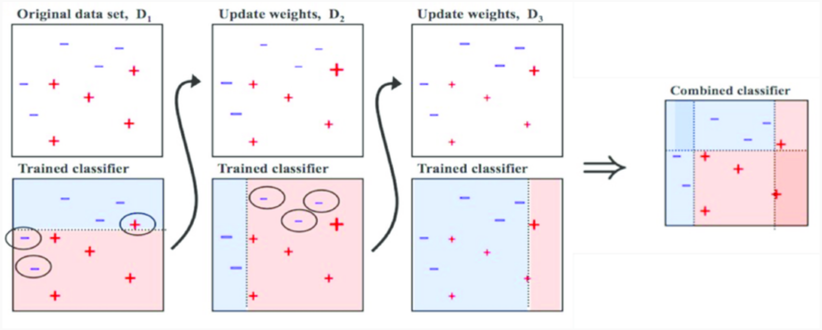
```r
fit <- randomForest(formula, data,
                    ntree    = 500,
                    mtry     = <number predictors at each split>,
                    importance = TRUE)

varImpPlot(fit)

predict(fit, newdata, type = "prob")
```

- `mtry`: default random forest (bagging total number predictors)
- `ntree` is tuning parameter (overfitting when too large)
- `importance = TRUE` for `varImpPlot()`
- default `type` yields predicted class

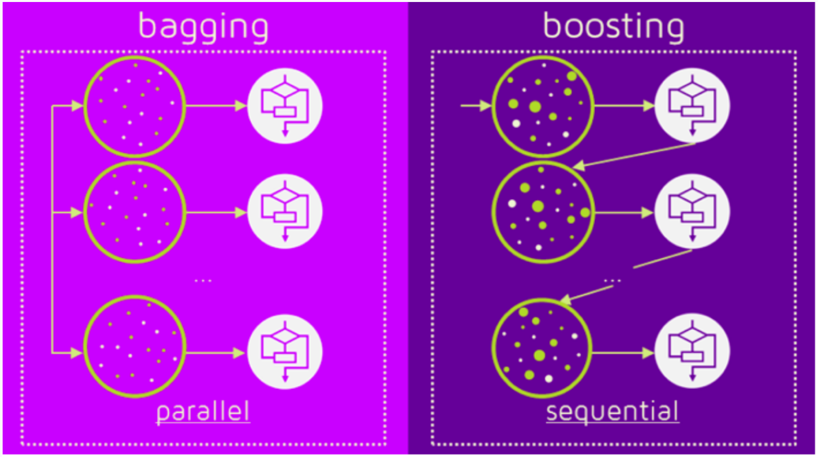
Boosting

Algorithm

1. Apply a weak classifier (e.g. stump) to training data
2. Increase weights for incorrect classifications, and repeat
3. Classifier is linear combination of weak classifiers



Boosting vs bagging/random forest



Boosting with package `fastAdaboost`

Boosting a single model

- `nIter` is number of weak classifiers

```
ada <- adaboost(formula, data, nIter)

predict(ada, newdata)
```

- `nIter` is number of weak classifiers (overfitting when too large)
- predictions include classes, probabilities and misclassification error

Boosting with package `caret`

Determine `nIter` with cross validation

- use the method `adaboost` in the function `train()`
- specify a sequence of values for `nIter`

```r
ada <- train(formula,
             data,
             method    = "adaboost",
             trControl = trainControl(method = "cv", number = 5),
             tuneGrid  = expand.grid(method = "Adaboost.M1",
                                     nIter  = <test sequence>))

predict(ada, newdata, type = "prob")
```

- "Adaboost.M1" restricts search to one of two methods
- default `type` yields predicted class

Support Vector Machines (SVM)

SVM for binary classification

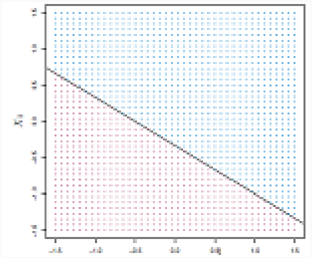
Classifiers using support vectors

1. *maximal margin classifier*
   - classes perfectly separable by hyperplane
2. *support vector classifier*
   - allows for non-separable cases
3. *support vector machine*
   - allows for non-linear boundaries

Hyperplane

Divides the feature space in two

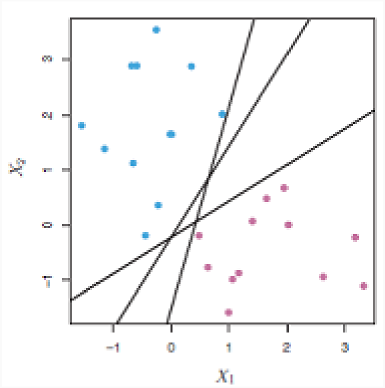
- in two dimensions hyperplane is simply a line



Separating hyperplane

Perfectly separates the two classes of the outcome variable

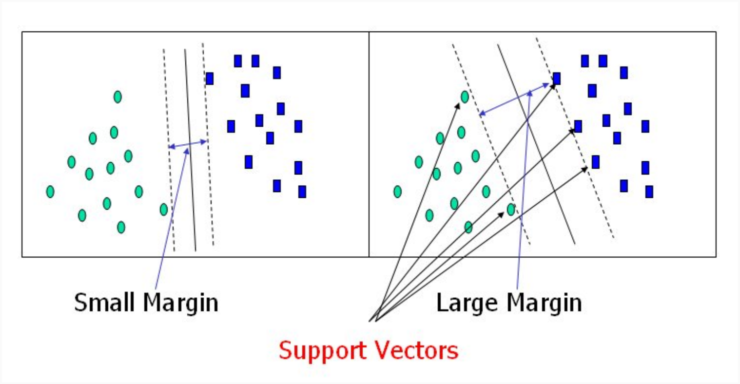
- hyperplane not uniquely identified
- high variance



Maximal Margin Classifier

Identifies hyperplane by specification of a maximal marging

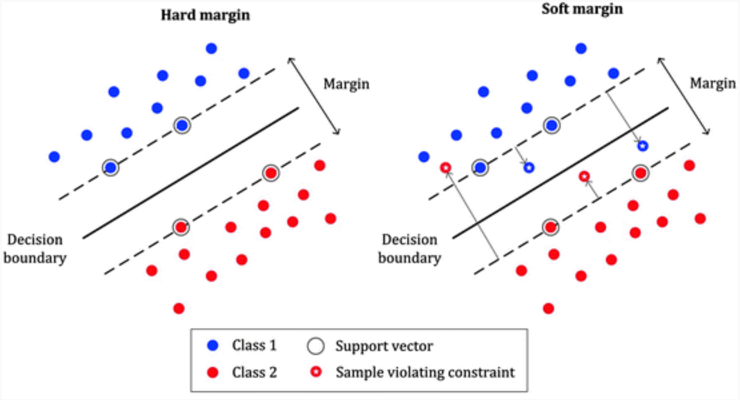
- points on margin are support vectors
- only works if cases are *separable*



Support Vector Classifier (SVC)

Allows for violations of the margin (soft margin)

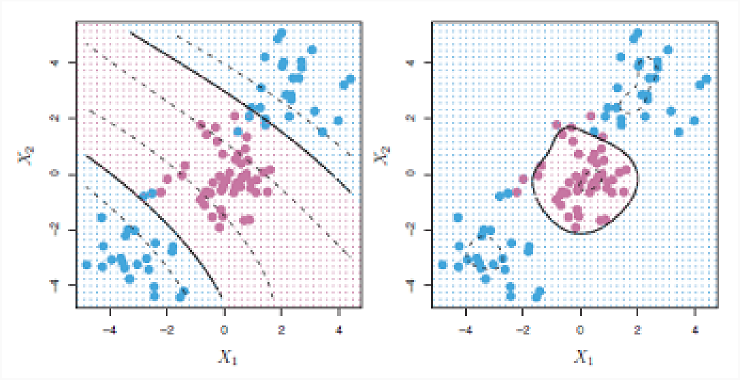
- budget for violations is called *cost* (C)
- cases the wrong side of hyperplane contribute to the cost



Support Vector Machines (SVM)

Kernels allow for nonlinear hyperplanes, e.g.

- polynomial kernel (left)
- radial kernel (right)



SVM with pacakge e1071

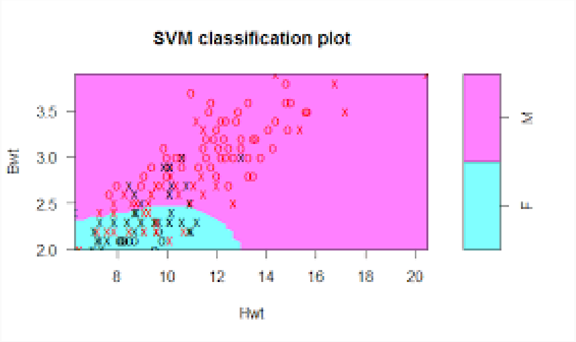
```
svm_train <- tune(svm, formula, data,
                  degree = 3, #default
                  coef0  = 0, #default
                  cost   = 1, #default
                  kernel = c("linear", "polynomial", "radial"),
                  ranges = list(cost = <sequence>), etc.)

svm_train$best.model # performance summary

svm_class <- predict(svm_train, newdata, probability = TRUE)
svm_prob  <- attr(svm_class, "probabilities")
```

- `cost`, `degree` and `coef0` are tuning parameters
- `ranges` works similar as `tuneGrid()`

SVM classification plot

Compression hyperplane two dimensions

```
plot(svm_train$best.model, data, x1 ~ x2)
```



Pro's and con's classifiers

BLR

- robust against outliers but potentially unstable

LDA

- better stability but sensitive to normality violations

Tree-based methods

- top-down and greedy, so bias-variance control needed
- boosting considered as one of the best methods

SVM

- similar to BLR (same loss function), but allow for non-linearity