Supervised Learning: Classification

Tree-based methods and Support Vector Machines

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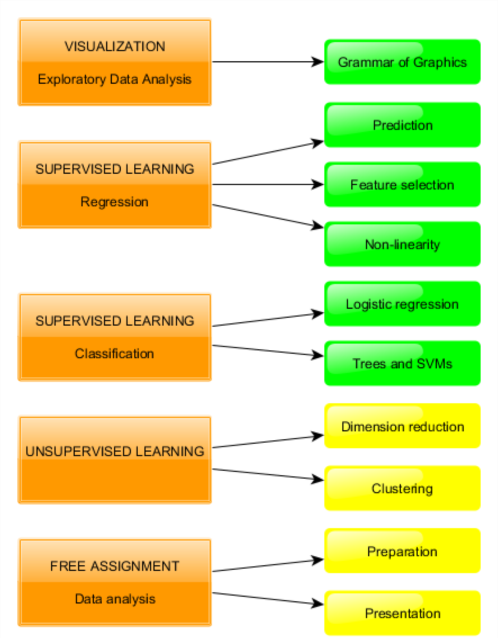
Program


VISUALIZATION
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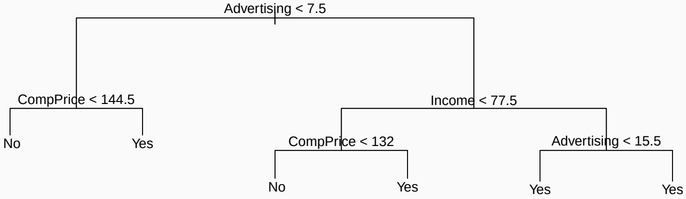
Content

1. Classification trees
2. Pruning
3. Bagging, random forests
4. Boosting
5. Support Vector Machines

Classification trees

1. Recursive binary splitting algorithm
2. Splits on basis of node *purity*
   - Gini index
   - deviance



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

Package `tree`

Growing and plotting trees with function `tree()`

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

plot(train_tree)
text(train_tree)
```

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

Methods to reduce variance:

1. Pruning
   - cross-validation with regularization

2. Bagging
   - bootstrapping

3. Random forests
   - bagging with random set of predictor at each split

4. Boosting
   - weighted combination of weak classifiers

Pruning

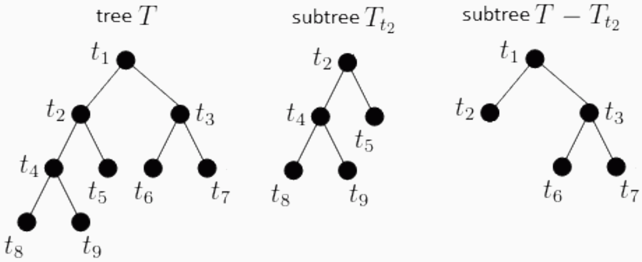
Cost-complexity pruning (package ‘tree)

1. Cross-validate the tree
2. Shows deviance/misclassification as function of nodes
3. Obtain predictions test set

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

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

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

- `cv.tree()` deviance/misclassification as function number of nodes
- `best` in `prune.tree()` is optimal number of nodes in `cv.tree()`
- default `type` yields predicted probabilities

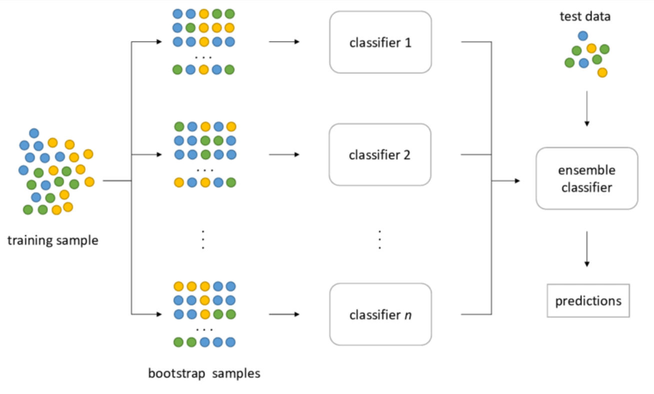
Pruning example



Bagging, random forests

Algorithm

1. Fit classification trees to B bootstrap samples
2. Average the predictions
3. OOB as estimate validation error



Bagging vs random forests

Bagging

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

Random forests

- considers 1/3 of predictors at each step
- all predictors get a fair chance
- decorrelated trees
- lower variance

Out-of-bag error rate

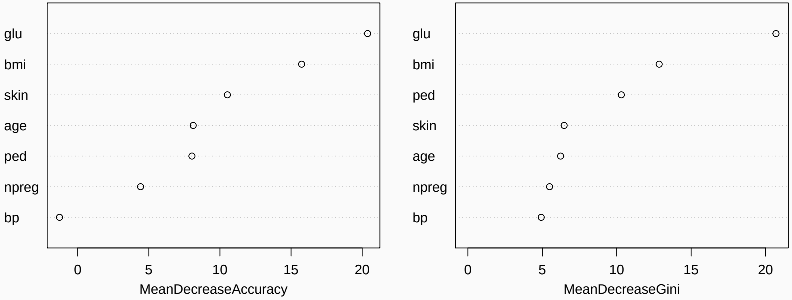
On average 1/3 of observations not in bootstrap (out of bag)

- 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

Training and prediction with bagging/random forest

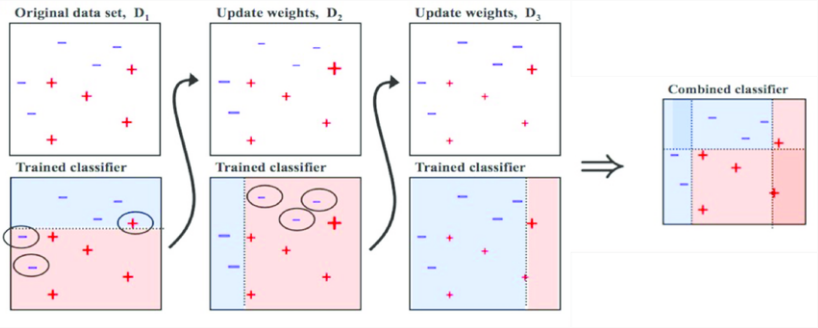
```
fit <- randomForest(formula, data,
                    ntree      = 500,
                    mtry       = <number predictors at each split>,
                    importance = TRUE)

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` necessary for `varImpPlot()`
- default type yields predicted class

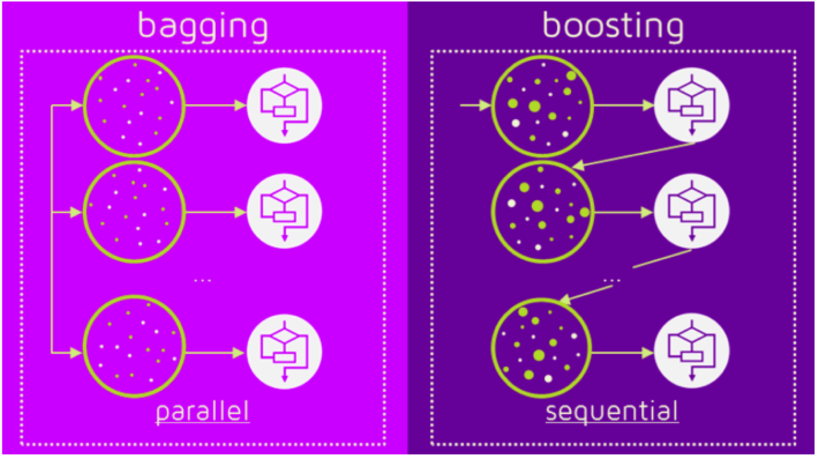
Boosting

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 tuning parameter (overfitting when too large)
- predictions include classes, probabilities and misclassification error

Boosting with package caret

Determine nIter with cross validation (caret)

```
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

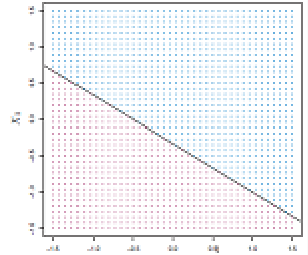
Classifiers using support vectors

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

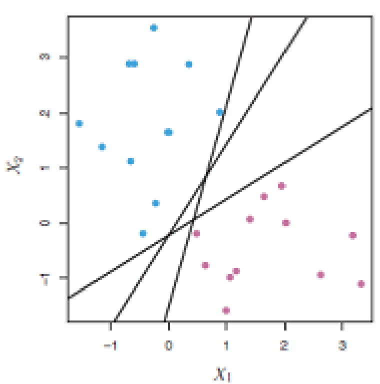
- in two dimensions hyperplane is simply a line



Separating hyperplane

Perfectly separates the two classes of the outcome variable

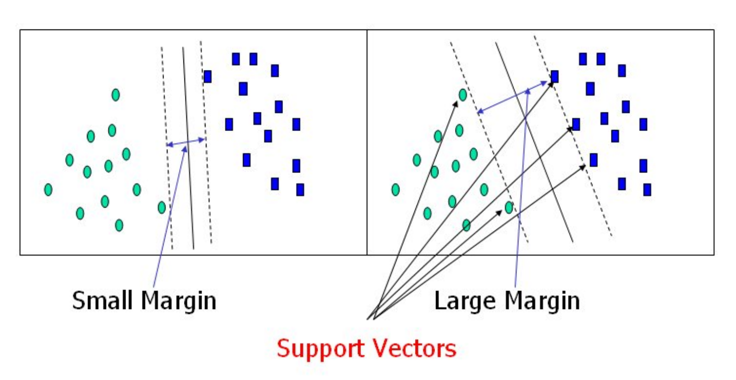
- hyperplane not uniquely identified
- high variance



Maximal Margin Classifier

Identifies hyperplane by specification of a maximal marging

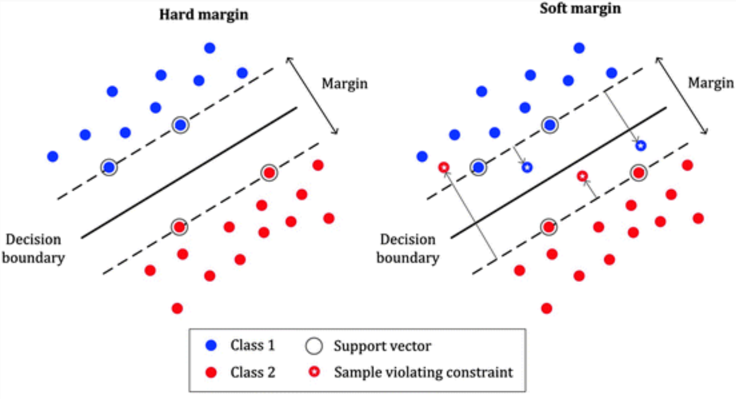
- points on margin are support vectors
- only works idf cases are *separable*



Support Vector Classifier (SVC)

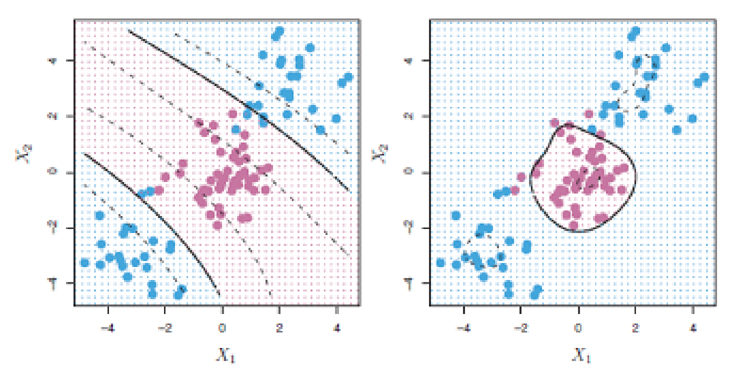
Allows for violations of the margin (soft margin)

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



Support Vector Machines (SVM)

Allows for nonlinear hyperplanes, e.g. polynomial and radial



SVM with pacakge e1071

Training and prediction

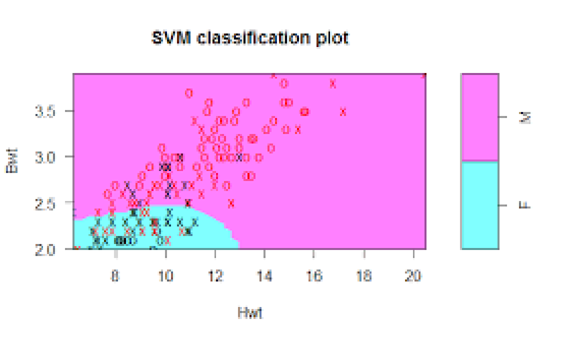
```
svm_train <- tune(svm, formula, data,
                  degree = 3, #default
                  coef0  = 0, #default
                  cost   = 1, #default
                  kernel = c("linear", "polynomial", "radial"),
                  ranges = list(cost = <sequence>), etc.)

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(...$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