Lecture 7: Classification

October 24, 2017

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Classification

- Classification is a supervised methood which deals with prediction outcomes or response variables that are qualitative, or categorical.
- The task is to classify or assign each observation to a category or a class.
- Examples of classification problems include:
 - predicting what medical condition or disease a patient has base on their symptoms,
 - determining cell types based on their gene expression profiles (single cell RNA-seq data).
 - detecting fraudulent transactions based on the transaction history

Logistic Regression

Logistic Regression

- Logistic regression is actually used for **classification**, and not regression tasks, $Y \in \{0, 1\}$.
- The name regression comes from the fact that the method fits a linear function to a continuous quantity, the log odds of the response.

$$p = P[Y = 1 \mid X]$$

$$\log\left(\frac{p}{1-p}\right) = X\beta = \beta_0 + \beta_1^T x$$

• The method performs binary classification (k = 2), but can be generalized to handle k > 2 classes (multinomial logistic regression).

$$g(p) = \log\left(\frac{p}{1-p}\right), \qquad \text{(logit a link function)}$$

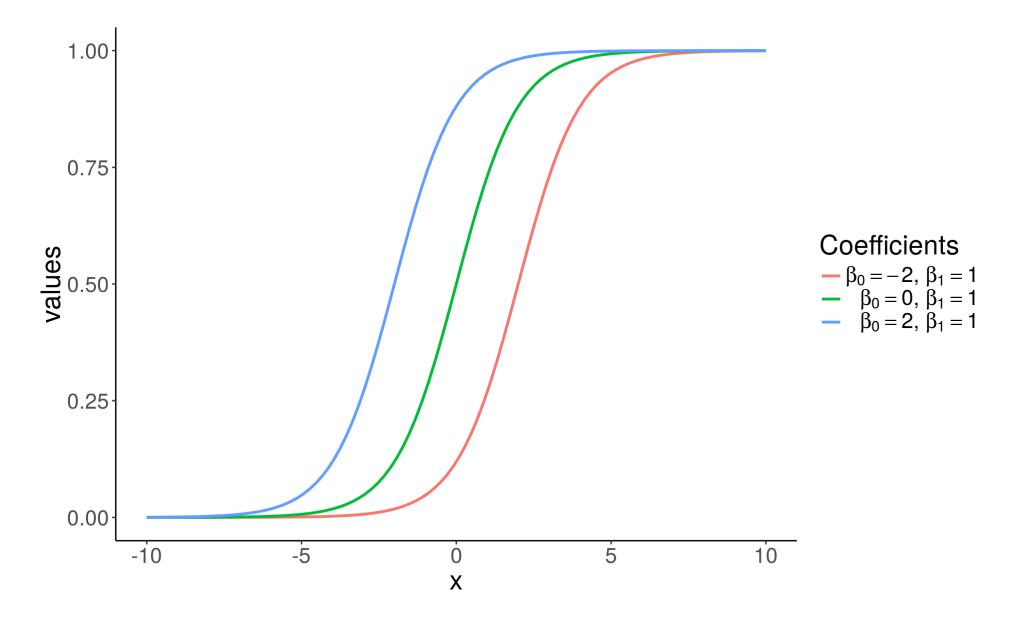
$$g^{-1}(\eta) = \frac{1}{1+e^{-\eta}}, \qquad \text{(logistic function)}$$

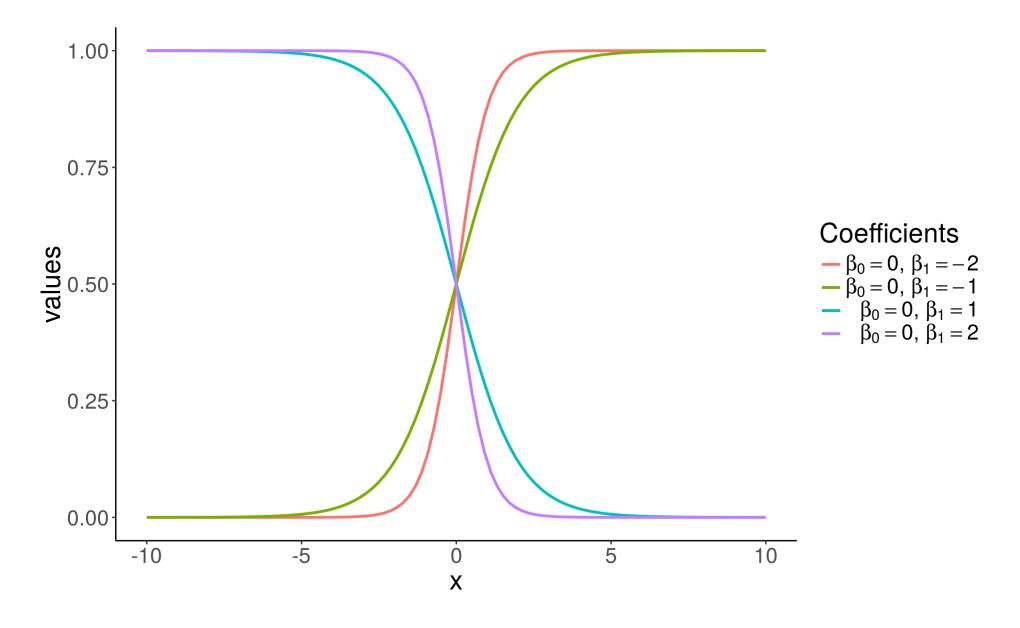
$$\eta = X\beta, \qquad \text{(linear predictor)}$$

$$E[Y] = P[Y = 1 \mid X = x] \qquad \text{(probability of outcome)}$$

$$= p = g^{-1}(\eta)$$

$$= \frac{1}{1+e^{-X\beta}}$$





Grad School Admissions

Suppose we would like to predict students' admission to graduate school based their GRE, GPA, and the rank of their undergraduate institution.

```
admissions <- read.csv("https://stats.idre.ucla.edu/stat/data/binary.csv" )
admissions <- tbl_df(admissions)
admissions</pre>
```

```
## # A tibble: 400 x 4
     admit
             gre
                   gpa rank
     <int> <int> <dbl> <int>
             380 3.61
             660 3.67
            800 4.00
         1 640
                 3.19
           520
                 2.93
         1 760
                 3.00
##
           560
                 2.98
                 3.08
             400
             540
                 3.39
             700
                 3.92
## # ... with 390 more rows
```

summary(admissions) ## admit rank gpa gre Min. :220.0 Min. :2.260 Min. :0.0000 Min. :1.000 1st Qu.:0.0000 1st Qu.:520.0 1st Qu.:3.130 1st Qu.:2.000 Median :2.000 ## Median :0.0000 Median :3.395 Median :580.0 ## Mean :0.3175 Mean :587.7 Mean :3.390 Mean :2.485 3rd Qu.:3.670 3rd Qu.:3.000 ## 3rd Qu.:1.0000 3rd Qu.:660.0 ## Max. :1.0000 :800.0 Max. :4.000 :4.000 Max. Max. sapply(admissions, sd) ## admit rank gre gpa 0.3805668 0.4660867 115.5165364 0.9444602

Check that there are observations included in each subgroup, and whether the data is balanced:

```
with(admissions, table(admit, rank))
##    rank
## admit 1 2 3 4
##    0 28 97 93 55
##    1 33 54 28 12
```

Logistic Regression in R

- In R logistic regression can be done using a function glm().
- glm stands for Generalized Linear Model.
- The function can fit many other regression models. Use ?glm to learn more.
- For cases with k>2 classes, multinom() function from nnet package can be used. To see how go over this example.

Note that currently the column 'admit' and 'rank' in admissions are integers.

```
sapply(admissions, class)

## admit gre gpa rank
## "integer" "integer" "integer"
```

We convert the two columns to factors.

```
admissions <- mutate(admissions,
   admit = factor(admit, levels = c(0, 1), labels = c("rejected", "admitted")),
   rank = factor(rank, levels = 1:4)
)
admissions</pre>
```

```
## # A tibble: 400 x 4
  admit
               gre gpa
                          rank
## <fctr> <int> <dbl> <fctr>
               380 3.61
## 1 rejected
## 2 admitted
               660 3.67
## 3 admitted
               800 4.00
               640 3.19
## 4 admitted
## 5 rejected
               520 2.93
## 6 admitted
             760 3.00
## 7 admitted
               560 2.98
## 8 rejected
             400 3.08
## 9 admitted
             540 3.39
             700 3.92
## 10 rejected
## # ... with 390 more rows
```

Split data

Divide data into train and test set so that we can evaluate the model accuracy I on. Here we use 70%-30% split.

```
set.seed(123456)
train.idx <- sample(nrow(admissions), 0.7*nrow(admissions))
train <- admissions[train.idx, ]
test <- admissions[-train.idx, ]</pre>
```

Fitting a logistic regression model

- The first argument, formula = admit ~ gre + gpa + rank, specifies the linear predictor part, $\eta = X\beta$.
- You need to set the family to family = "binomial" equivalent to choosing a logistic regression, i.e. using a logit link function $g(\cdot)$ in a GLM model.

summary(fit.logit)

```
##
## Call:
## glm(formula = admit ~ gre + gpa + rank, family = "binomial",
##
       data = train)
##
## Deviance Residuals:
                  1Q Median
       Min
                                     3Q
                                             Max
## -1.4811 -0.8899 -0.6611 1.1862
                                          2.0721
##
## Coefficients:
                 Estimate Std. Error z value Pr(>|z|)
##
## (Intercept) -3.626928 1.333747
                                       -2.719 0.00654
       0.003061 0.001311 2.335 0.01953 *
## gre
## gpa 0.500902 0.386621 1.296 0.19512
## rank2 -0.502376 0.378062 -1.329 0.18391
## rank3 -0.980873 0.407041 -2.410 0.01596 *
                -1.237913 0.493217
                                       -2.510 0.01208 *
## rank4
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
       Null deviance: 350.14 on 279 degrees of freedom
## Residual deviance: 324.87 on 274 degrees of freedom
## AIC: 336.87
##
## Number of Fisher Scoring iterations: 4
```

Logistic regression coefficients for continuous predictors (covariates) give the fold change in the odds of the outcome corresponding to a unit increase in the predictor.

$$\beta_{cont} = \log \left(\frac{P[Y = 1 \mid X_{cont} = x + 1]}{P[Y = 1 \mid X_{cont} = x]} \right)$$

Categorical features (factors) are first converted to indicator variables and the model fits separate coefficients for each level of the factor. Coefficients corresponding to a specific indicator variable give the increase/decrease in the odds of the outcome in case the observation is recorded with that level.

$$\beta_{facL} = \log \left(\frac{P[Y=1 \mid X_{fac} = L]}{P[Y=1 \mid X_{fac} \neq L]} \right)$$

- For every unit increase in gre, the log odds of admitted (versus rejected) increases by ≈ 0.0030612 .
- For every unit increase in gpa, the log odds increases by \approx 0.5009016.
- There are three coefficients for the rank variable, e.g. a student attending a college with rank 2, one with rank 1 (base level), has the log admission odds decreased by \approx -0.5023758.

You can get the confidence intervals for the coefficients with the confint() fuinction

The 95% CI are away from zero which indicates significance.

Rank variable effect is given with three different coefficients.

We can sse wald.test() function from the aod package to test the overall end of 'rank'.

```
# install.packages(aod)
library(aod)
wald.test(b = coef(fit.logit), Sigma = vcov(fit.logit), Terms = 4:6)

## Wald test:
## ------
##
## Chi-squared test:
## X2 = 8.8, df = 3, P(> X2) = 0.033
```

- b supplies the coefficients,
- Sigma supplies the variance covariance matrix of the error terms,
- Terms indices of the coefficients to be tested; here 4, 5, and 6, corresponding to 'rank'.

The p-value indicates that the overall effect of rank is statistically significant.

Predictions

Predictions can be computed using predict() function, with the argument type = "response". Otherwise, the default will compute predictions on the scale of the linear predictors.

Test Set Predictions

Exercise

- Go to the "Lec7_Exercises.Rmd" file, which can be downloaded from the class website under the Lecture tab.
- Complete Exercise 1.

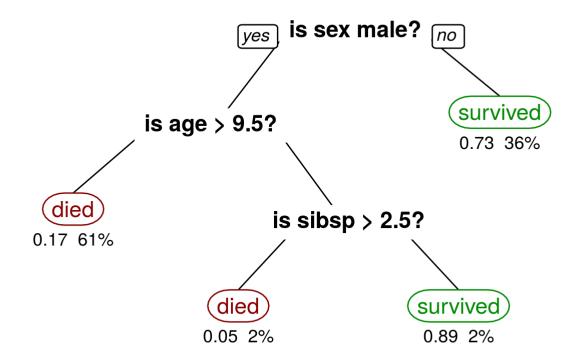
Random Forest

Random Forest

- Random Forest is an ensemble learning method based on classification and regression trees, CART, proposed by Breinman in 2001.
- RF can be used to perform **both classification and regression**.
- RF models are robust as they combine predictions calculated from a large number of decision trees (a forest).
- Details on RF can be found in Chapter 8 of ISL and Chapter 15 ESL; also a good write-up can also be found here

Decision trees

- Cool visualization explaining what decision trees are: link
- Decision tree on classification of Titanic Survivors:



Tree bagging Algorithm

Suppse we have an input data matrix, $X \in \mathbb{R}^{N \times p}$ and a response vector, $Y \in \mathbb{F}$

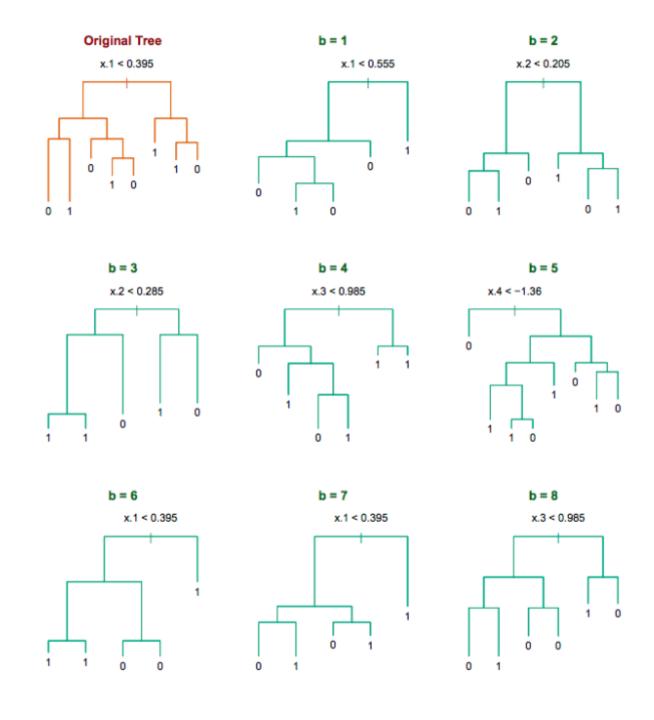
For
$$b = 1, 2, ..., B$$
:

- 1. Generate a random subset of the data (X_b, Y_b) contatining n < N observations sampled with replacement.
- 2. Train a decision tree T_b on (X_b, Y_b)
- 3. Predict the outcome for N-n unseen (complement) samples (X_b',Y_b')

Afterwards, combine predictions from all decision trees and compute the averapredicted outcome.

Averaging over a collection of decision trees makes the predictions more stal

Decision trees for bootrap samples



Source: Chapter 8 ESL

Random Forest Characteristics

- Random forests differ in only one way from tree bagging: it uses a modified tree learning algorithm sometimes called feature bagging.
- At each candidate split in the learning process, **only a random subset of the features is included in a pool** from which the variables can be selected for splitting the branch.
- Introducing randomness into the candidate splitting variables, reduces correlation between the generated trees.

Random Forest: Ensemble of Trees Tree Tree Random Forest [Ref] Rattle R Data Mining Tool

Source: link

Wine Quality

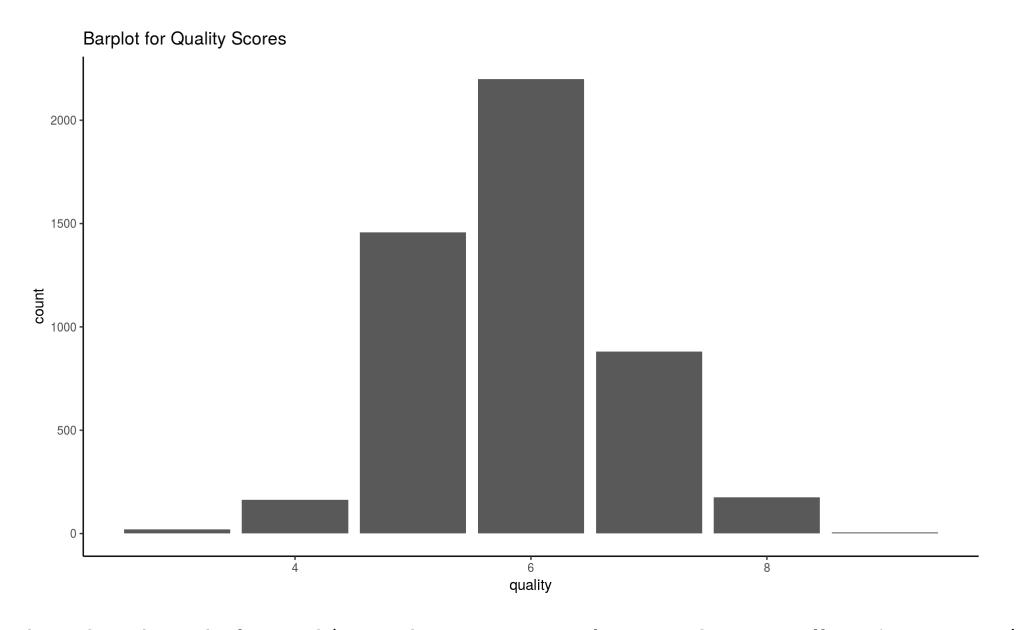
UCI ML Repo includes two datasets on red and white variants of the Portugues "Vinho Verde" wine. The datasets contain information on physicochemical and sensory characteristics of the wine quality score.

We will use the white wines dataset to classify wines according to their quality classes.

```
url <- 'https://archive.ics.uci.edu/ml/machine-learning-databases/wine-quality/w</pre>
wines <- tbl_df(read.csv(url, sep = ";"))
print(wines, n = 6)
## # A tibble: 4,898 x 12
     fixed.acidity volatile.acidity citric.acid residual.sugar chlorides
##
             <db1>
                               <db1>
                                           <dbl>
                                                           <db1>
                                                                     <dbl>
## 1
               7.0
                                0.27
                                            0.36
                                                            20.7
                                                                     0.045
               6.3
                                0.30
                                            0.34
                                                                     0.049
## 3
                                0.28
                                                             6.9
                                            0.40
                                                                     0.050
                                0.23
                                            0.32
                                                             8.5
                                                                     0.058
                                            0.32
                                0.23
                                                             8.5
                                                                     0.058
                                0.28
                                            0.40
                                                             6.9
                                                                     0.050
## # ... with 4,892 more rows, and 7 more variables:
       free.sulfur.dioxide <dbl>, total.sulfur.dioxide <dbl>, density <dbl>,
       pH <dbl>, sulphates <dbl>, alcohol <dbl>, quality <int>
```

Class Frequency

```
ggplot(wines, aes(x = quality)) +
  geom_bar() + theme_classic() +
  ggtitle("Barplot for Quality Scores")
```



The classes are ordered and not balanced (munch more normal wines than excellent/poor ones).

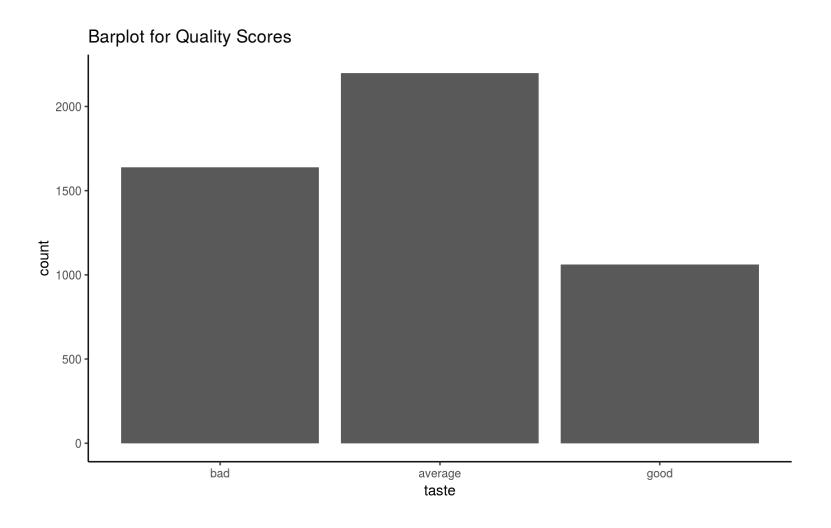
To make things easier, we will wines into "good", "average" and "bad" categorie. The new classes will be more balanced, and it will be easier to fit the model.

```
## # A tibble: 4,898 x 13
      fixed.acidity volatile.acidity citric.acid residual.sugar chlorides
##
              <db1>
                                                                    <dbl>
##
                               <dbl>
                                           <dbl>
                                                          <dbl>
                                0.27
                                            0.36
                                                           20.7
                                                                    0.045
## 1
                7.0
## 2
                6.3
                                0.30
                                           0.34
                                                                    0.049
## 3
## 4
## 5
                8.1
                                                            6.9
                                0.28
                                           0.40
                                                                    0.050
                                0.23
                                           0.32
                                                                    0.058
                7.2
                                                           8.5
                                0.23
                                           0.32
                                                                    0.058
## 6
                8.1
                                0.28
                                     0.40
                                                           6.9
                                                                    0.050
## 7
                6.2
                                0.32
                                                           7.0
                                           0.16
                                                                    0.045
## 8
                7.0
                                0.27
                                           0.36
                                                           20.7
                                                                    0.045
                                0.30
                6.3
                                            0.34
                                                            1.6
                                                                    0.049
                                0.22
## 10
                                            0.43
                                                            1.5
                                                                    0.044
## # ... with 4,888 more rows, and 8 more variables:
       free.sulfur.dioxide <dbl>, total.sulfur.dioxide <dbl>, density <dbl>,
       pH <dbl>, sulphates <dbl>, alcohol <dbl>, quality <int>, taste <fctr>
```

table(wines\$quality)

```
##
## 3 4 5 6 7 8 9
## 20 163 1457 2198 880 175 5
```

```
ggplot(wines, aes(x = taste)) +
  geom_bar() + theme_classic() +
  ggtitle("Barplot for Quality Scores")
```



Splitting data

We include 60% of the data in a train set and the remaining into a test set.

Random Forest in R

In R there is a convenient function randomForest from randomForest pack

```
# install.packages("randomForest")
library(randomForest)
## randomForest 4.6-12
## Type rfNews() to see new features/changes/bug fixes.
##
## Attaching package: 'randomForest'
## The following object is masked from 'package:dplyr':
##
       combine
##
## The following object is masked from 'package:ggplot2':
##
       margin
##
rf.wines <- randomForest(taste ~ . - quality, data = train,
                         mtry = 6, ntree = 600, importance = TRUE)
```

 Note that in the formula 'taste ~ . - quality' means we include all features EXCEPT for 'quality' (the response variable).

- mt ry the number of variables randomly sampled as candidates at each split. Defaults: for classification \sqrt{p} and for regression p/3, where p is number of all variables in the model.
- ntree the number of trees in the forest.
- importance whether importance of predictors be computed.

Observe, that RF is good at distinguishing "bad" wines from good" wines, but struggles when it comes to "average" wines.

```
rf.wines
##
## Call:
  randomForest(formula = taste \sim . - quality, data = train, mtry = 6,
                                                                              ntre
                  Type of random forest: classification
##
                        Number of trees: 600
##
## No. of variables tried at each split: 6
##
           OOB estimate of error rate: 30.12%
## Confusion matrix:
           bad average good class.error
## bad
           677
                   278 18
                              0.3042138
## average 228
                   971 117 0.2621581
## good
                   224 405
                              0.3759630
```

Model Accuracy

- You should always evaluate your model's performance on a test set, which was set aside and not observed by the method at all.
- In case of RF, performance on train and test set should be similar; this is because the method averages predictions computed by individual trees for observations unseen by the tree.
- Inspect the confusion matrix to asses the model accuracy.

https://stats.stackexchange.com/questions/197827/how-to-interpret-mean-decrease-in-accuracy-and-mean-decrease-gini-in-random-fore

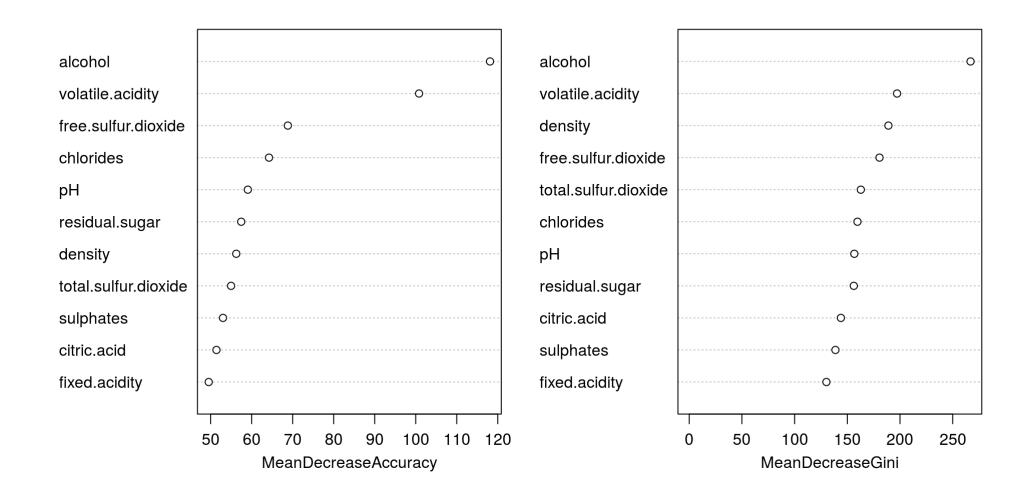
```
## Look at variable importance:
importance(rf.wines)
```

```
##
                                               good MeanDecreaseAccuracy
                                   average
                         31.61926 25.98041 36.16006
## fixed.acidity
                                                                 49.52878
## volatile.acidity
                         65.62247 53.90561 78.14410
                                                                100.81170
## citric.acid
                         29.32895 30.59606 42.66566
                                                                 51.41656
## residual.sugar
                         34.76200 36.22169 34.11017
                                                                 57.45461
## chlorides
                         38.82683 24.70974 59.44965
                                                                 64.23190
## free.sulfur.dioxide
                         51.67186 35.52296 44.81158
                                                                 68.81886
## total.sulfur.dioxide 29.64474 25.20661 44.60063
                                                                 54.97681
## density
                         32.81271 26.11959 44.55753
                                                                 56.24973
## pH
                         37.88014 26.46448 46.75563
                                                                 59.06318
## sulphates
                         28.53080 28.27934 42.38525
                                                                 53.00674
## alcohol
                         88.94843 39.38382 96.90979
                                                                118.11452
##
                        MeanDecreaseGini
## fixed.acidity
                                 130 1805
## volatile acidity
                                 197.2117
## citric.acid
                                 143 9020
## residual.sugar
                                 156.1524
## chlorides
                                 159.6429
## free.sulfur.dioxide
                                 180.5619
## total.sulfur.dioxide
                                 162.8233
## density
                                 188.9939
## pH
                                 156.6557
## sulphates
                                 138.7374
## alcohol
                                 266.9109
```

What seems to be the conclusion? What are the characteristics that are prediction of the wine quality score?

varImpPlot(rf.wines)

rf.wines



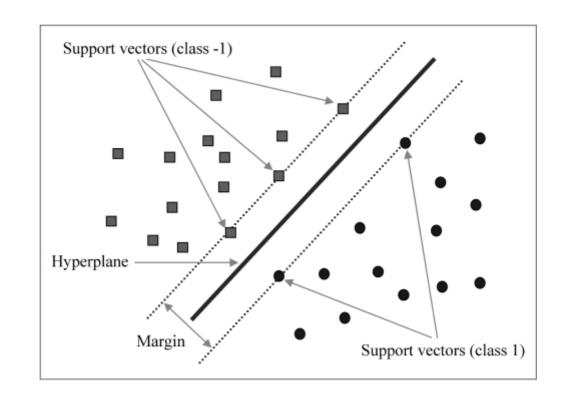
Exercise

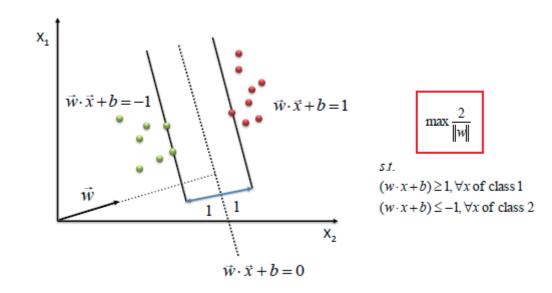
- Go to the "Lec7_Exercises.Rmd" file, which can be downloaded from the class website under the Lecture tab.
- Complete Exercise 2.

Support Vector Machines

Suport Vector Machines (SVM)

- Method invented by Vladimir N. Vapnik and Alexey Ya. Chervonenkis in 1963.
- The idea is to find the best hyperplane sepparating observations from 2 different classes, where the best means the one that represents the largest separation or margin.
- The Andrew Ng's CS229 lecture and notes are good resources to learn about principles of SVMs.
- More details can also be found in Chapter 9 ISL and Chapter 12 ESL





SVM Problem

$$\max_{w,b} \frac{2}{\|w\|}$$

 $s. t. \ \forall i: \ y_i(w \cdot x_i + b) \ge 1$

which can be converted to:

$$\min_{w,b} \frac{1}{2} ||w||^2
s. t. \forall i: y_i(w \cdot x_i + b) \ge 1$$

SVM Problem

Sometimes the data is not linearly separable, and regularization/soft-margin w better:

$$\min_{w,b} \frac{1}{2} ||w||^2 + C \sum_{i=1}^{n} \xi_i$$
s. t. $\forall i : y_i(w \cdot x_i + b) \ge 1 - \xi_i$

$$\xi_i \ge 0$$

Lagrangian:

$$\mathcal{L}(w, b, \xi, \alpha, r) = \frac{1}{2} w^T w + C \sum_{i=1}^n \xi_i - \sum_{i=1}^n r_i \xi_i$$

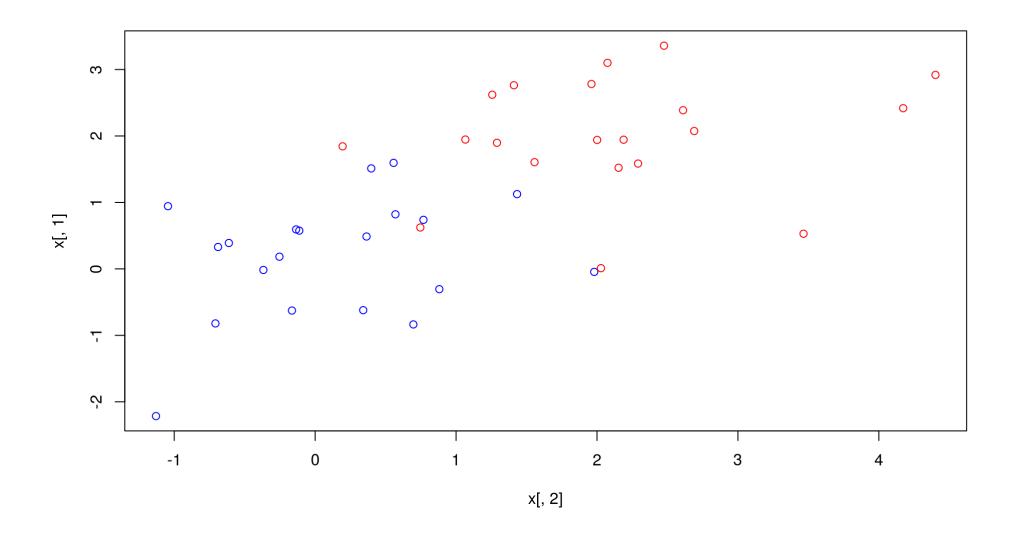
$$-\sum_{i=1}^{\infty} \alpha_i \left[y_i(w \cdot x_i + b) - 1 + \xi_i \right]$$

SVM Example

We will do a simple example from the ISL computing SVM on a simulated data:

```
set.seed(1)
x <- matrix(rnorm(40*2), ncol=2)
y <- c(rep(-1,20), rep(1,20))
x[y == 1, ] <- x[y == 1, ] + 2
dat <- data.frame(x = x, y=as.factor(y))
head(dat)</pre>
```

plot(x[, 2], x[, 1], col=(3-y))



SVM in R

You can use the e1071 package to perform svm in R.

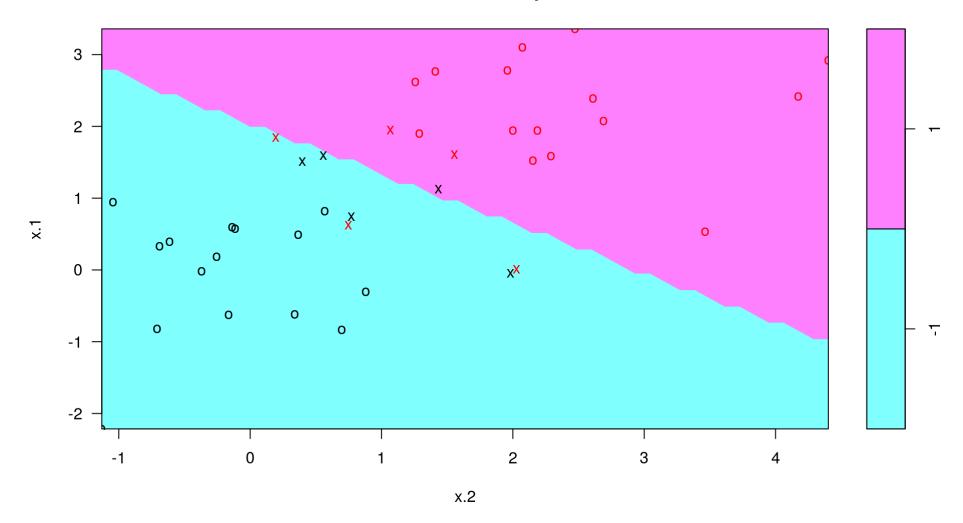
```
library(e1071)
# Set scale to be FALSE otherwise by default x is scaled to zero mean and unit va
svmfit <- svm(y ~ ., data=dat, kernel="linear", cost = 10, scale=FALSE)</pre>
summary(svmfit)
##
## Call:
## svm(formula = y \sim ., data = dat, kernel = "linear", cost = 10,
       scale = FALSE
##
##
## Parameters:
## SVM-Type: C-classification
## SVM-Kernel: linear
##
          cost: 10
         gamma: 0.5
##
##
## Number of Support Vectors: 10
##
## (55)
##
## Number of Classes: 2
##
## Levels:
## -1 1
```

svmfit\$index

[1] 4 8 11 15 16 24 27 34 35 37

plot(svmfit, dat)

SVM classification plot

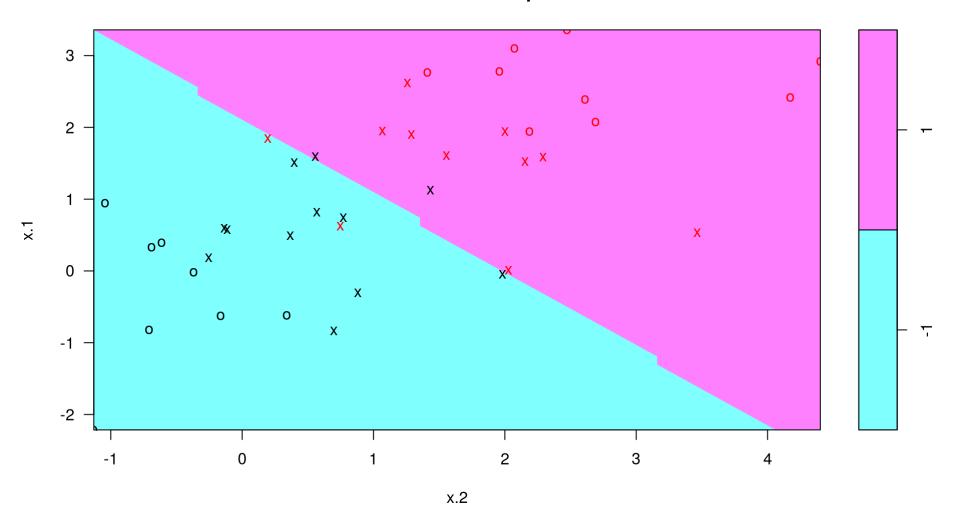


```
svmfit$index
## [1] 2 3 4 7 8 9 10 11 15 16 19 20 24 25 27 28 29 32 34 35 36 37 38
summary(svmfit)
##
## Call:
## svm(formula = y \sim ., data = dat, kernel = "linear", cost = 0.05,
       scale = FALSE
##
##
##
## Parameters:
## SVM-Type: C-classification
## SVM-Kernel: linear
          cost: 0.05
##
         gamma: 0.5
##
##
## Number of Support Vectors: 23
##
## ( 12 11 )
##
##
## Number of Classes: 2
##
## Levels:
## -1 1
```

svmfit <- svm(y~., data=dat, kernel="linear", cost=0.05, scale=FALSE)</pre>

plot(svmfit, dat)

SVM classification plot

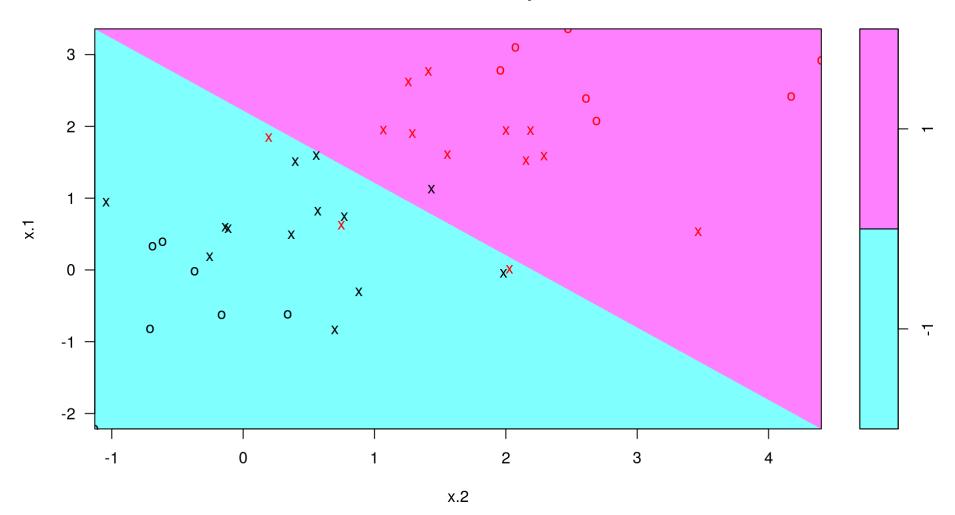


To find a best choice of the tuning parameter "C" use the tune () function

```
set.seed(1)
tune.out < tune(svm,y ~ ., data=dat, kernel="linear", ranges=list(cost=c(0.001, 0.01, 0.05, 0.1, 1,5,10,20)))
summary(tune.out)
##
## Parameter tuning of 'svm':
##
## - sampling method: 10-fold cross validation
##
## - best parameters:
## cost
## 0.05
##
## - best performance: 0.1
##
## - Detailed performance results:
      cost error dispersion
## 1 1e-03 0.625 0.2946278
## 2 1e-02 0.450 0.2581989
## 3 5e-02 0.100 0.1290994
## 4 1e-01 0.125 0.1767767
## 5 1e+00 0.150 0.1748015
## 6 5e+00 0.125 0.1317616
## 7 1e+01 0.125 0.1317616
## 8 2e+01 0.125
                   0.1317616
```

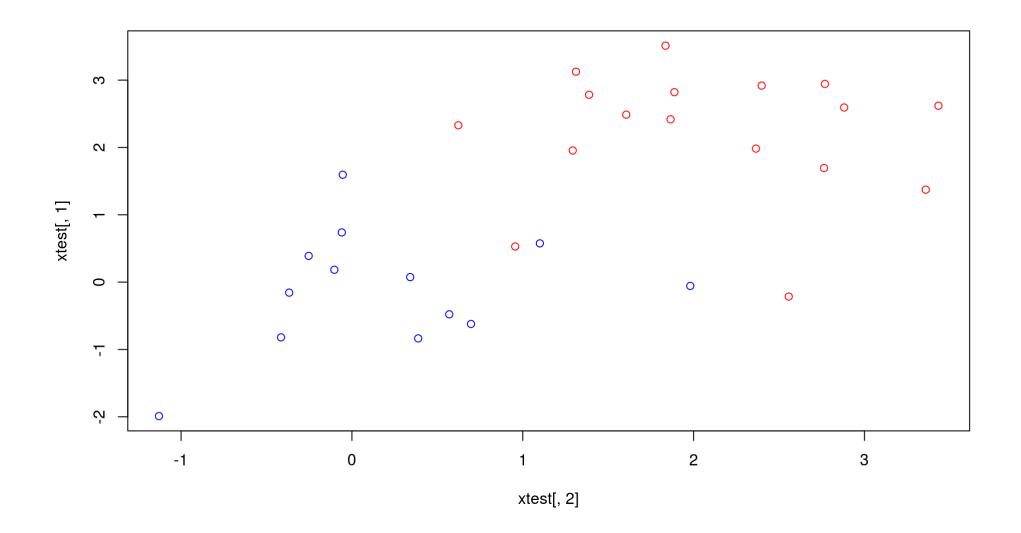
bestmod <- tune.out\$best.model
plot(bestmod, dat)</pre>

SVM classification plot



We build a new test dataset from a similar model as we did for the train data.

```
set.seed(1)
xtest <- matrix(rnorm(30*2), ncol=2)
ytest <- sample(c(-1,1), 30, rep=TRUE)
xtest[ytest == 1, ] <- xtest[ytest == 1,] + 2
testdat <- data.frame(x = xtest, y = as.factor(ytest))
plot(xtest[, 2], xtest[, 1], col=(3-ytest))</pre>
```



```
ypred <- predict(bestmod, testdat)
table(predict = ypred, truth = testdat$y)

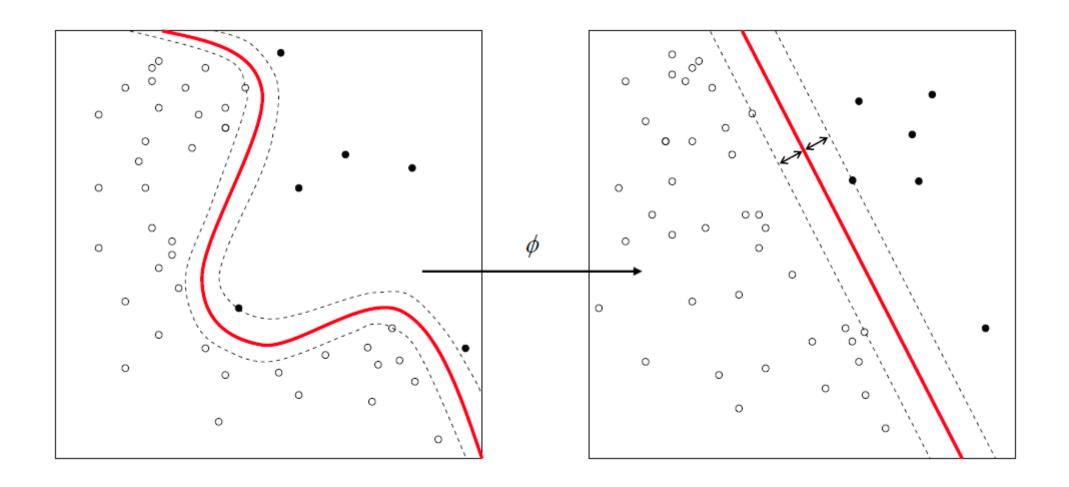
## truth
## predict -1 1
## -1 13 1
## 1 0 16</pre>
```

And for the non-tuned model we have:

```
svmfit <- svm(y~., data=dat, kernel = "linear", cost=10, scale = FALSE)
ypred <- predict(svmfit, testdat)
table(predict = ypred, truth = testdat$y)</pre>
```

```
## truth
## predict -1 1
## -1 13 2
## 1 0 15
```

Kernel SVM

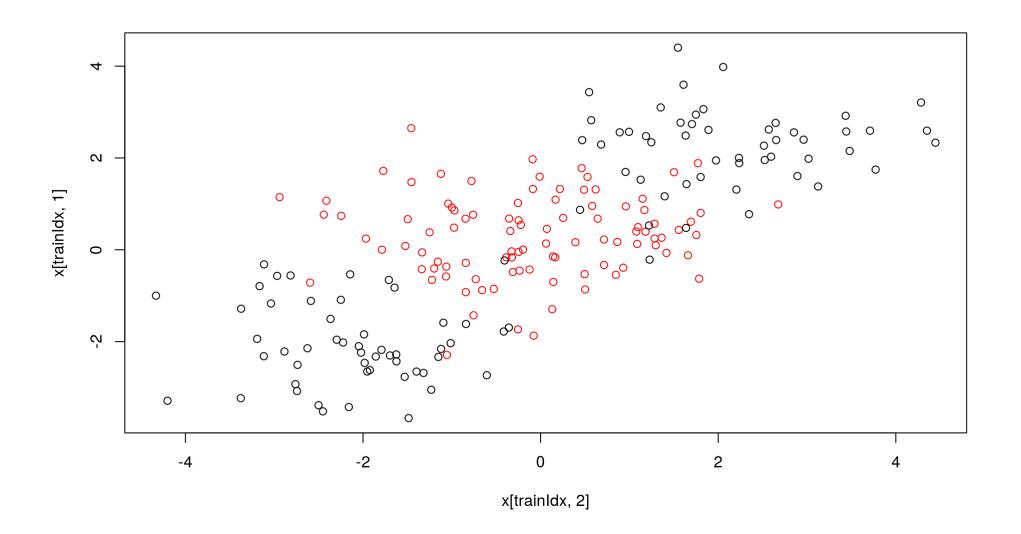


Kernel SVM Example

Now suppose we have non-linearly separable data:

```
set.seed(1)
# Generate 200 points
x <- matrix(rnorm(400*2), ncol=2)
x[1:100,] <- x[1:100,] + 2
x[101:200,] <- x[101:200,] - 2
y <- c(rep(1,200), rep(2,200))
dat <- data.frame(x = x, y = as.factor(y))
# Let a random half be a training set
trainIdx <- sample(400, 200)</pre>
```

plot(x[trainIdx, 2], x[trainIdx, 1], col=y[trainIdx])



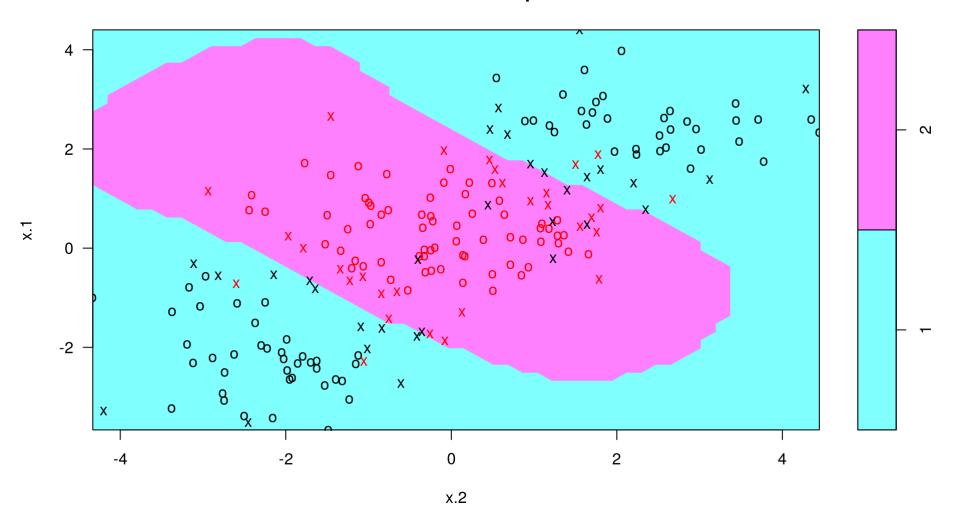
We will use the SVM with a radial kernel. Note that here we can additionally specify the gamma parameter for the radial function:

```
svmfit <- svm(y~., data=dat[trainIdx,], kernel = "radial", gamma=1, cost=1)
table(true = dat[-trainIdx, "y"], pred=predict(svmfit, newdata = dat[-trainIdx, ]

## pred
## true 1 2
## 1 81 16
## 2 11 92</pre>
```

plot(svmfit, dat[trainIdx,])

SVM classification plot



We can tune both gamma and cost parameters:

```
## pred
## true 1 2
## 1 84 13
## 2 12 91
```

plot(tune.out\$best.model, dat[trainIdx,])

SVM classification plot

