Regression and Classification with R [1]

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R and Data Mining Course

Canberra, Australia

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[1] Chapters 4 & 5, in *R and Data Mining: Examples and Case Studies*. http://www.rdatamining.com/docs/RDataMining-book.pdf

Outline

Regression and Classification with R [2]

- Basics of regression and classification
- Building a linear regression model to predict CPI data
- Building a generalized linear model (GLM)
- Building decision trees with package *party* and *rpart*
- Training a random forest model with package *randomForest*

[2] Chapter 4: Decision Trees and Random Forest & Chapter 5: Regression, in book *R and Data Mining: Examples and Case Studies*. http://www.rdatamining.com/docs/RDataMining.pdf

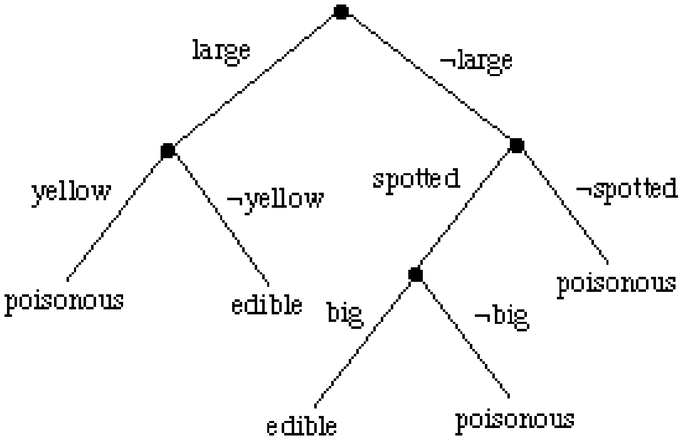
Regression and Classification

- Regression: to predict a continuous value, such as the volume of rain
- Classification: to predict a categorical class label, such as weather: rainy, sunnny, cloudy or snowy

Regression

- Regression is to build a function of *independent variables* (also known as *predictors*) to predict a *dependent variable* (also called *response*).
- For example, banks assess the risk of home-loan applicants based on their age, income, expenses, occupation, number of dependents, total credit limit, etc.
- Linear regression models
- Generalized linear models (GLM)

An Example of Decision Tree



Edible Mushroom decision tree[3]

[3] `http://users.cs.cf.ac.uk/Dave.Marshall/AI2/node147.html`

Random Forest

- Ensemble learning with many decision trees
- Each tree is trained with a random sample of the training dataset and on a randomly chosen subspace.
- The final prediction result is derived from the predictions of all individual trees, with mean (for regression) or majority voting (for classification).
- Better performance and less likely to overfit than a single decision tree, but with less interpretability

Regression Evaluation

- MAE: Mean Absolute Error

$$\mathrm{MAE} = \frac{1}{n} \sum_{i=1}^{n} |\hat{y}_i - y_i| \tag{1}$$

- MSE: Mean Squared Error

$$\mathrm{MSE} = \frac{1}{n} \sum_{i=1}^{n} (\hat{y}_i - y_i)^2 \tag{2}$$

- RMSE: Root Mean Squared Error

$$\mathrm{RMSE} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (\hat{y}_i - y_i)^2} \tag{3}$$

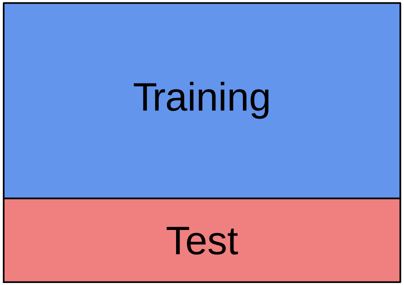
where y_i is actual value and $\hat{y}_i$ is predicted value.

Overfitting

- A model is over complex and performs very well on training data but poorly on unseen data.
- To evaluate models with out-of-sample test data, i.e., data that are not included in training data

Training and Test

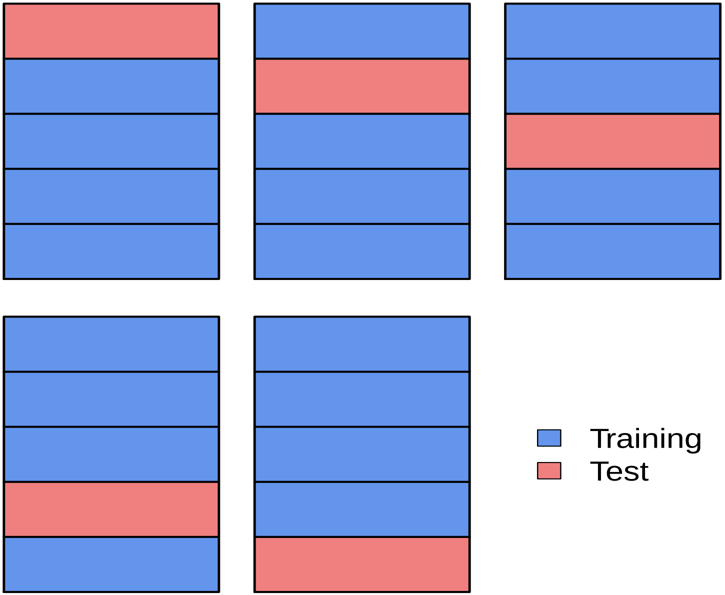
- Randomly split into training and test sets
- 80/20, 70/30, 60/40 ...



k-Fold Cross Validation

- Split data into *k* subsets of equal size
- Reserve one set for test and use the rest for training
- Average performance of all above

An Example: 5-Fold Cross Validation



🟦 Training
🟥 Test

Outline

Linear Regression

- Linear regression is to predict response with a linear function of predictors as follows:

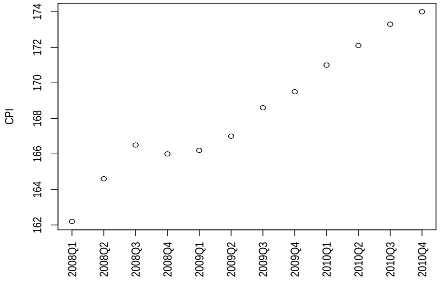
$$y = c_0 + c_1 x_1 + c_2 x_2 + \cdots + c_k x_k,$$

  where $x_1, x_2, \cdots, x_k$ are predictors, y is the response to predict, and $c_0, c_1, \cdots, c_k$ are cofficients to learn.
- Linear regression in R: `lm()`
- The Australian Consumer Price Index (CPI) data: quarterly CPIs from 2008 to 2010 [4]

[4] From Australian Bureau of Statistics, `http://www.abs.gov.au`.

The CPI Data

```r
year <- rep(2008:2010, each = 4)
quarter <- rep(1:4, 3)
cpi <- c(162.2, 164.6, 166.5, 166.0,
         166.2, 167.0, 168.6, 169.5,
         171.0, 172.1, 173.3, 174.0)
plot(cpi, xaxt="n", ylab="CPI", xlab="")
# draw x-axis, where "las=3" makes text vertical
axis(1, labels=paste(year,quarter,sep="Q"), at=1:12, las=3)
```



Linear Regression

```
## correlation between CPI and year / quarter
cor(year,cpi)
## [1] 0.9096316

cor(quarter,cpi)
## [1] 0.3738028

## build a linear regression model with function lm()
fit <- lm(cpi ~ year + quarter)
fit
##
## Call:
## lm(formula = cpi ~ year + quarter)
##
## Coefficients:
## (Intercept)         year      quarter
##   -7644.488        3.888        1.167
```

With the above linear model, CPI is calculated as

$$\text{cpi} = c_0 + c_1 * \text{year} + c_2 * \text{quarter},$$

where c_0, c_1 and c_2 are coefficients from model `fit`.

What will the CPI be in 2011?

```
cpi2011 <- fit$coefficients[[1]] +
           fit$coefficients[[2]] * 2011 +
           fit$coefficients[[3]] * (1:4)
cpi2011
## [1] 174.4417 175.6083 176.7750 177.9417
```

With the above linear model, CPI is calculated as

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cpi2011
## [1] 174.4417 175.6083 176.7750 177.9417
```

An easier way is to use function `predict()`.

More details of the model can be obtained with the code below.

```
attributes(fit)
## $names
##  [1] "coefficients"  "residuals"     "effects"
##  [4] "rank"          "fitted.values" "assign"
##  [7] "qr"            "df.residual"   "xlevels"
## [10] "call"          "terms"         "model"
##
## $class
## [1] "lm"

fit$coefficients
##  (Intercept)        year     quarter
## -7644.487500    3.887500    1.166667
```

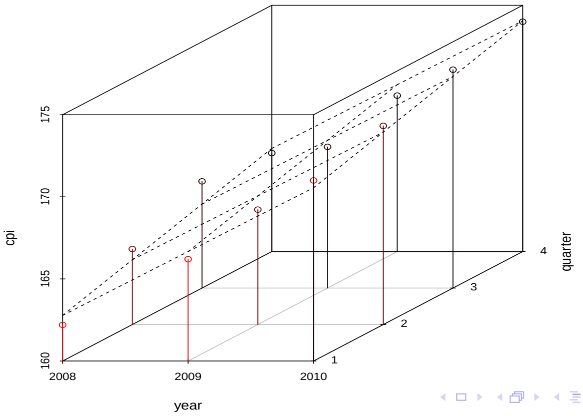
Function residuals(): differences btw observed & fitted valu

```
# differences between observed values and fitted values
residuals(fit)
##           1           2           3           4           5
## -0.57916667  0.65416667  1.38750000 -0.27916667 -0.46666667
##           6           7           8           9          10
## -0.83333333 -0.40000000 -0.66666667  0.44583333  0.37916667
##          11          12
##  0.41250000 -0.05416667

summary(fit)
##
## Call:
## lm(formula = cpi ~ year + quarter)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -0.8333 -0.4948 -0.1667  0.4208  1.3875
##
## Coefficients:
##               Estimate Std. Error t value Pr(>|t|)
## (Intercept) -7644.4875   518.6543 -14.739 1.31e-07 ***
## year            3.8875     0.2582  15.058 1.09e-07 ***
## quarter         1.1667     0.1885   6.188 0.000161 ***
```

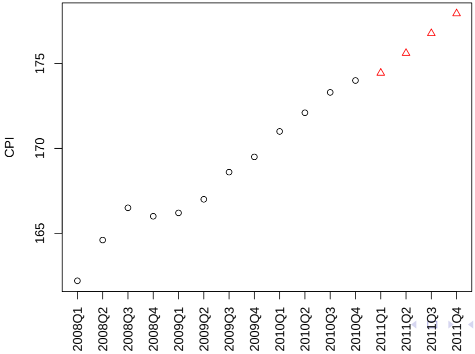
3D Plot of the Fitted Model

```r
library(scatterplot3d)
s3d <- scatterplot3d(year, quarter, cpi, highlight.3d=T, type="h",
          lab=c(2,3)) # lab: number of tickmarks on x-/y-axes
s3d$plane3d(fit) # draws the fitted plane
```



Prediction of CPIs in 2011

```r
data2011 <- data.frame(year=2011, quarter=1:4)
cpi2011 <- predict(fit, newdata=data2011)
style <- c(rep(1,12), rep(2,4))
plot(c(cpi, cpi2011), xaxt="n", ylab="CPI", xlab="",
     pch=style, col=style)
txt <- c(paste(year,quarter,sep="Q"),
         "2011Q1", "2011Q2", "2011Q3", "2011Q4")
axis(1, at=1:16, las=3, labels=txt)
```



Outline

Generalized Linear Model (GLM)

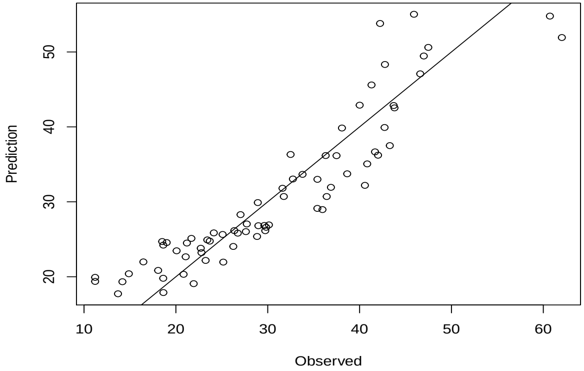
- Generalizes linear regression by allowing the linear model to be related to the response variable via a link function and allowing the magnitude of the variance of each measurement to be a function of its predicted value
- Unifies various other statistical models, including linear regression, logistic regression and Poisson regression
- Function glm(): fits generalized linear models, specified by giving a symbolic description of the linear predictor and a description of the error distribution

Build a Generalized Linear Model

```
data("bodyfat", package="TH.data")
myFormula <- DEXfat ~ age + waistcirc + hipcirc + elbowbreadth +
                      kneebreadth
bodyfat.glm <- glm(myFormula, family=gaussian("log"), data=bodyfat)
summary(bodyfat.glm)
##
## Call:
## glm(formula = myFormula, family = gaussian("log"), data = b...
##
## Deviance Residuals:
##      Min        1Q    Median        3Q       Max
## -11.5688   -3.0065    0.1266    2.8310   10.0966
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  0.734293   0.308949   2.377  0.02042 *
## age          0.002129   0.001446   1.473  0.14560
## waistcirc    0.010489   0.002479   4.231 7.44e-05 ***
## hipcirc      0.009702   0.003231   3.003  0.00379 **
## elbowbreadth 0.002355   0.045686   0.052  0.95905
## kneebreadth  0.063188   0.028193   2.241  0.02843 *
## ---
```

Prediction with Generalized Linear Regression Model

```
pred <- predict(bodyfat.glm, type="response")
plot(bodyfat$DEXfat, pred, xlab="Observed", ylab="Prediction")
abline(a=0, b=1)
```



Outline

The iris Data

```
str(iris)
## 'data.frame': 150 obs. of  5 variables:
##  $ Sepal.Length: num  5.1 4.9 4.7 4.6 5 5.4 4.6 5 4.4 4.9 ...
##  $ Sepal.Width : num  3.5 3 3.2 3.1 3.6 3.9 3.4 3.4 2.9 3.1...
##  $ Petal.Length: num  1.4 1.4 1.3 1.5 1.4 1.7 1.4 1.5 1.4 1...
##  $ Petal.Width : num  0.2 0.2 0.2 0.2 0.2 0.4 0.3 0.2 0.2 0...
##  $ Species     : Factor w/ 3 levels "setosa","versicolor",....

# split data into two subsets: training (70%) and test (30%);
# set a fixed random seed  to make results reproducible
set.seed(1234)
ind <- sample(2, nrow(iris), replace=TRUE, prob=c(0.7, 0.3))
train.data <- iris[ind==1,]
test.data <- iris[ind==2,]
```

Build a ctree

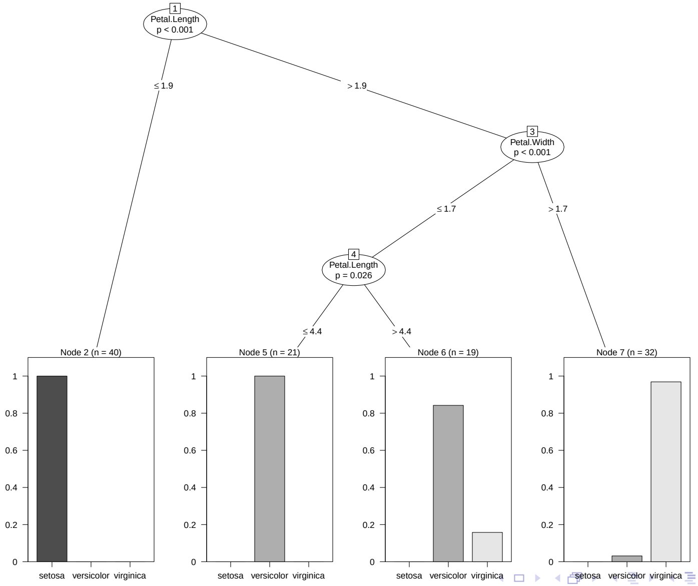
- Control the training of decision trees: MinSplit, MinBusket, MaxSurrogate and MaxDepth
- Target variable: Species
- Independent variables: all other variables

```
library(party)
# myFormula <- Species ~ . # predict Species with all other variables
myFormula <- Species ~ Sepal.Length + Sepal.Width +
             Petal.Length + Petal.Width
iris.ctree <- ctree(myFormula, data=train.data)
# check the prediction
table(predict(iris.ctree), train.data$Species)
##
##               setosa versicolor virginica
##    setosa         40          0         0
##    versicolor      0         37         3
##    virginica       0          1        31
```

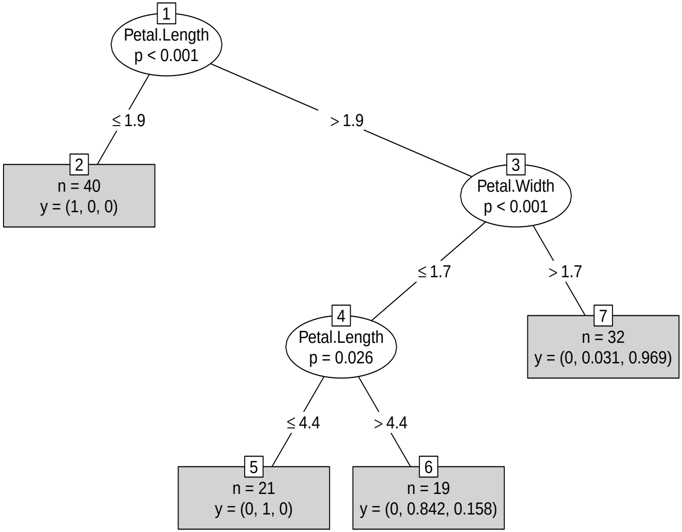
Print ctree

```
print(iris.ctree)
##
##   Conditional inference tree with 4 terminal nodes
##
## Response:  Species
## Inputs:  Sepal.Length, Sepal.Width, Petal.Length, Petal.Width
## Number of observations:  112
##
## 1) Petal.Length <= 1.9; criterion = 1, statistic = 104.643
##   2)*  weights = 40
## 1) Petal.Length > 1.9
##   3) Petal.Width <= 1.7; criterion = 1, statistic = 48.939
##     4) Petal.Length <= 4.4; criterion = 0.974, statistic = ...
##       5)*  weights = 21
##     4) Petal.Length > 4.4
##       6)*  weights = 19
##   3) Petal.Width > 1.7
##     7)*  weights = 32
```

```
plot(iris.ctree)
```



```
plot(iris.ctree, type="simple")
```



Test

```
# predict on test data
testPred <- predict(iris.ctree, newdata = test.data)
table(testPred, test.data$Species)
##
## testPred     setosa versicolor virginica
##   setosa         10          0         0
##   versicolor      0         12         2
##   virginica       0          0        14
```

Outline

The bodyfat Dataset

```
data("bodyfat", package = "TH.data")
dim(bodyfat)
## [1] 71 10

# str(bodyfat)
head(bodyfat, 5)
##    age DEXfat waistcirc hipcirc elbowbreadth kneebreadth
## 47  57  41.68     100.0   112.0          7.1         9.4
## 48  65  43.29      99.5   116.5          6.5         8.9
## 49  59  35.41      96.0   108.5          6.2         8.9
## 50  58  22.79      72.0    96.5          6.1         9.2
## 51  60  36.42      89.5   100.5          7.1        10.0
##    anthro3a anthro3b anthro3c anthro4
## 47     4.42     4.95     4.50    6.13
## 48     4.63     5.01     4.48    6.37
## 49     4.12     4.74     4.60    5.82
## 50     4.03     4.48     3.91    5.66
## 51     4.24     4.68     4.15    5.91
```

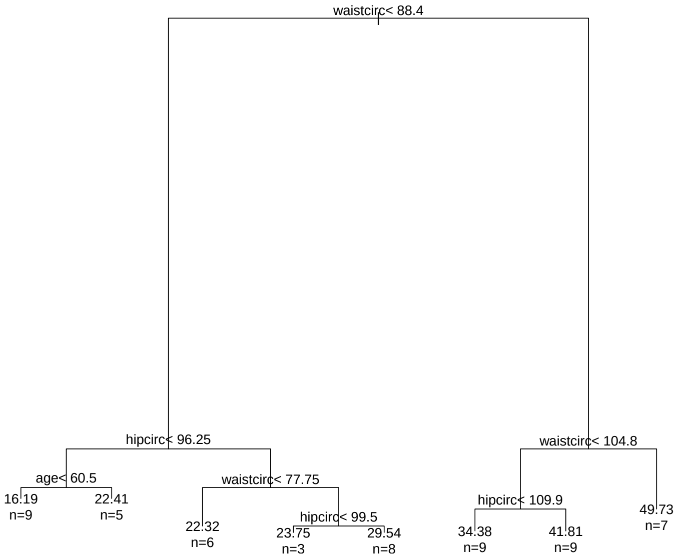
Train a Decision Tree with Package rpart

```r
# split into training and test subsets
set.seed(1234)
ind <- sample(2, nrow(bodyfat), replace=TRUE, prob=c(0.7, 0.3))
bodyfat.train <- bodyfat[ind==1,]
bodyfat.test <- bodyfat[ind==2,]
# train a decision tree
library(rpart)
myFormula <- DEXfat ~ age + waistcirc + hipcirc + elbowbreadth +
                      kneebreadth
bodyfat.rpart <- rpart(myFormula, data = bodyfat.train,
                       control = rpart.control(minsplit = 10))
# print(bodyfat.rpart£cptable)
print(bodyfat.rpart)
plot(bodyfat.rpart)
text(bodyfat.rpart, use.n=T)
```

The rpart Tree

```
## n= 56
##
## node), split, n, deviance, yval
##       * denotes terminal node
##
##  1) root 56 7265.0290000 30.94589
##    2) waistcirc< 88.4 31  960.5381000 22.55645
##      4) hipcirc< 96.25 14  222.2648000 18.41143
##        8) age< 60.5 9   66.8809600 16.19222 *
##        9) age>=60.5 5   31.2769200 22.40600 *
##      5) hipcirc>=96.25 17  299.6470000 25.97000
##       10) waistcirc< 77.75 6   30.7345500 22.32500 *
##       11) waistcirc>=77.75 11  145.7148000 27.95818
##         22) hipcirc< 99.5 3    0.2568667 23.74667 *
##         23) hipcirc>=99.5 8   72.2933500 29.53750 *
##    3) waistcirc>=88.4 25 1417.1140000 41.34880
##      6) waistcirc< 104.75 18  330.5792000 38.09111
##       12) hipcirc< 109.9 9   68.9996200 34.37556 *
##       13) hipcirc>=109.9 9   13.0832000 41.80667 *
##      7) waistcirc>=104.75 7  404.3004000 49.72571 *
```

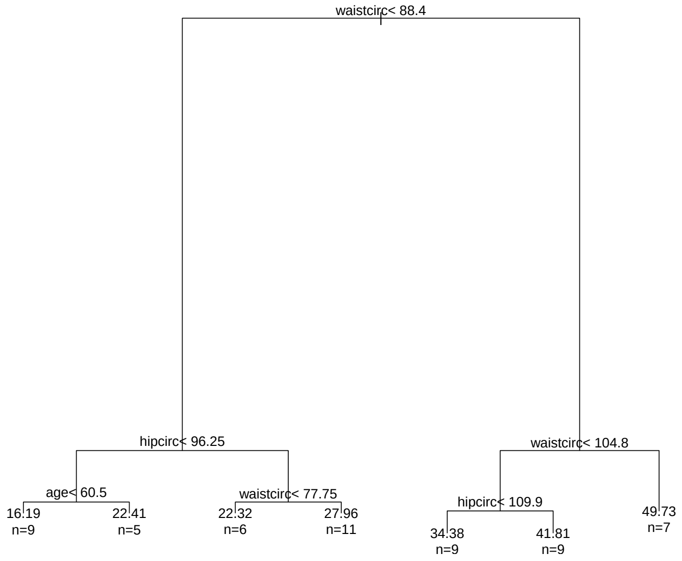
The rpart Tree



Select the Best Tree

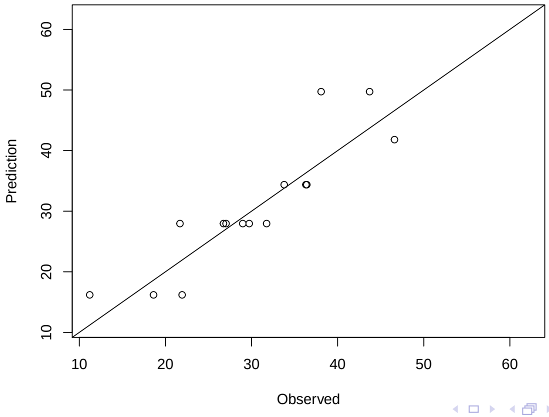
```r
# select the tree with the minimum prediction error
opt <- which.min(bodyfat.rpart$cptable[,"xerror"])
cp <- bodyfat.rpart$cptable[opt, "CP"]
# prune tree
bodyfat.prune <- prune(bodyfat.rpart, cp = cp)
# plot tree
plot(bodyfat.prune)
text(bodyfat.prune, use.n=T)
```

Selected Tree



Model Evaluation

```
DEXfat_pred <- predict(bodyfat.prune, newdata=bodyfat.test)
xlim <- range(bodyfat$DEXfat)
plot(DEXfat_pred ~ DEXfat, data=bodyfat.test, xlab="Observed",
     ylab="Prediction", ylim=xlim, xlim=xlim)
abline(a=0, b=1)
```



Outline

R Packages for Random Forest

- Package *randomForest*
  - very fast
  - cannot handle data with missing values
  - a limit of 32 to the maximum number of levels of each categorical attribute
  - extensions: *extendedForest*, *gradientForest*
- Package *party*: `cforest()`
  - not limited to the above maximum levels
  - slow
  - needs more memory

Train a Random Forest

```
# split into two subsets: training (70%) and test (30%)
ind <- sample(2, nrow(iris), replace=TRUE, prob=c(0.7, 0.3))
train.data <- iris[ind==1,]
test.data <- iris[ind==2,]
# use all other variables to predict Species
library(randomForest)
rf <- randomForest(Species ~ ., data=train.data, ntree=100,
                   proximity=T)
```

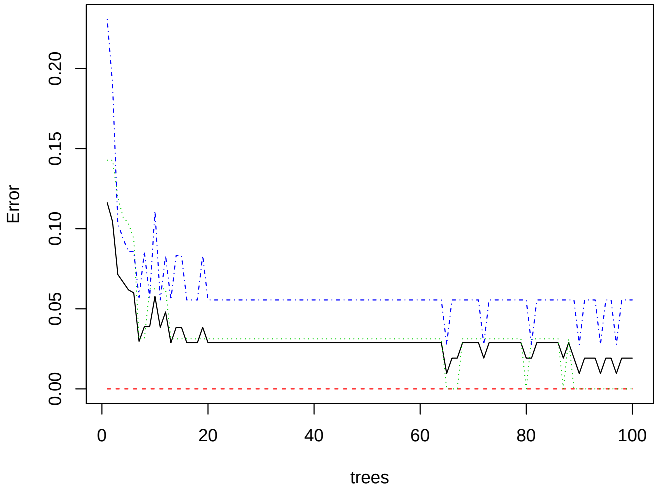
```
table(predict(rf), train.data$Species)
##
##                 setosa versicolor virginica
##   setosa            36          0         0
##   versicolor         0         32         2
##   virginica          0          0        34

print(rf)
##
## Call:
##  randomForest(formula = Species ~ ., data = train.data, ntr...
##                Type of random forest: classification
##                      Number of trees: 100
## No. of variables tried at each split: 2
##
##         OOB estimate of  error rate: 1.92%
## Confusion matrix:
##             setosa versicolor virginica class.error
## setosa          36          0         0  0.00000000
## versicolor       0         32         0  0.00000000
## virginica        0          2        34  0.05555556

attributes(rf)
```

Error Rate of Random Forest

```
plot(rf, main="")
```

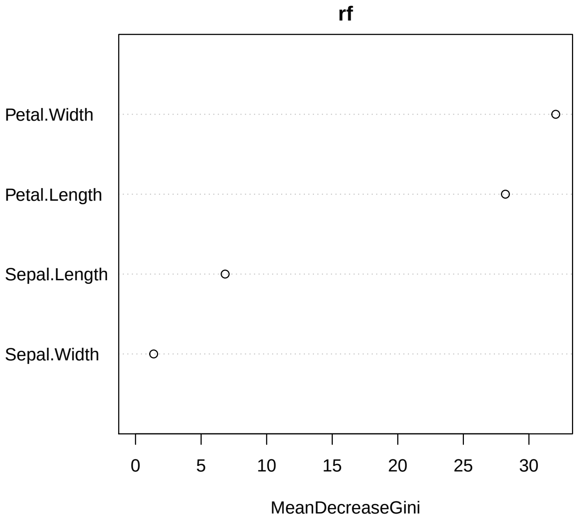


Variable Importance

```
importance(rf)
##              MeanDecreaseGini
## Sepal.Length         6.834364
## Sepal.Width          1.383795
## Petal.Length        28.207859
## Petal.Width         32.043213
```

Variable Importance

```
varImpPlot(rf)
```



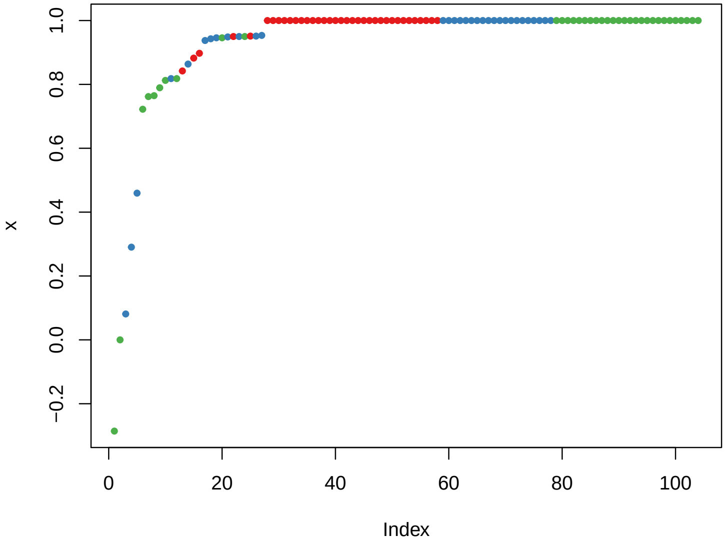
Margin of Predictions

The margin of a data point is as the proportion of votes for the correct class minus maximum proportion of votes for other classes. Positive margin means correct classification.

```
irisPred <- predict(rf, newdata=test.data)
table(irisPred, test.data$Species)
##
## irisPred     setosa versicolor virginica
##   setosa         14          0         0
##   versicolor      0         17         3
##   virginica       0          1        11

plot(margin(rf, test.data$Species))
```

Margin of Predictions



Outline

Online Resources

- Chapter 4: Decision Trees and Random Forest & Chapter 5: Regression, in book *R and Data Mining: Examples and Case Studies*

  `http://www.rdatamining.com/docs/RDataMining-book.pdf`
- R Reference Card for Data Mining

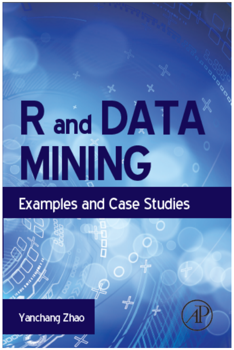
  `http://www.rdatamining.com/docs/RDataMining-reference-card.pdf`
- Free online courses and documents

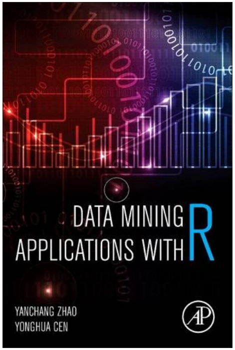
  `http://www.rdatamining.com/resources/`
- RDataMining Group on LinkedIn (26,000+ members)

  `http://group.rdatamining.com`
- Twitter (3,300+ followers)

  @RDataMining

The End





Thanks!

Email: `yanchang(at)RDataMining.com`
Twitter: `@RDataMining`