

# Exploratory Data Mining via Search Strategies Lab #1

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The first lab will go over the basics of programming in R along with covering Smoothing and Stepwise Regression

To get started, I recommend downloading Rstudio as an interface to R. Benefits include:

- ▶ Easier to download packages
- ▶ Easier to view plots
- ▶ Can load datasets without code

# Loading Datasets

Many datasets that we will be using come with installed packages

```
library(MASS) # for boston data  
data(Boston)
```

Now the Boston dataset is in your workplace

```
head(Boston[,1:7],6)
```

```
##      crim zn indus chas   nox   rm  age  
## 1 0.00632 18  2.31    0 0.538 6.575 65.2  
## 2 0.02731  0  7.07    0 0.469 6.421 78.9  
## 3 0.02729  0  7.07    0 0.469 7.185 61.1  
## 4 0.03237  0  2.18    0 0.458 6.998 45.8  
## 5 0.06905  0  2.18    0 0.458 7.147 54.2  
## 6 0.02985  0  2.18    0 0.458 6.430 58.7
```

# Load your own datasets

Data saved as .dat or .txt

```
data = read.table(file.choose(), sep=" ", header=F, na.strings="NA")
```

.csv

```
data = read.csv(file.choose(), header=T, na.strings=".")
```

.sav for SPSS files

```
library(foreign)
data = read.spss(file.choose(), to.data.frame=TRUE)
```

.sas7bdat for SAS data files – note doesn't work very well, best to convert first

```
library(sas7bdat)
data = read.sas7bdat(file.choose())
# note many options
```

# Subsetting datasets

Let's say I have a dataset read in fine. How about subsetting columns and rows: \* specific columns – two ways

```
library(MASS)
data(Boston)
## I want specific columns

Boston.sub <- Boston[,c(1,2,8,9)]
## or
Boston.sub <- Boston[,c("crim","zn","dis","rad")]
```

Have to use c() to combine non-continuous elements in R !!!!! VERY IMPORTANT !!!!!

How about rows – Same process but better shortcuts

```
comps <- complete.cases(Boston)
Boston.comp <- Boston[comps,]

subs <- Boston$zn == 0
Boston.sub <- Boston[subs,]
dim(Boston.sub)
```

```
## [1] 372 14
```

Notice: left of comma = row indicator; right = column indicator

# Dataset Types

For manipulating datasets, almost always best to make sure in data.frame

```
library(MASS)
data(Boston)
```

```
Boston.df <- data.frame(Boston)
```

Can tell type by running str()

Some R packages require X and Y variables to be in separate matrices

```
library(MASS)
data(Boston)

Y <- as.numeric(Boston$medv)
X <- data.matrix(Boston[, -14])

out <- lm.fit(X,Y)
```

This is very specific to data mining packages

# Missing Data

Can be summed up in two words: Not Fun

R requires all missingness to be coded as NA, therefore it is best to deal with when reading in data:

```
data = read.csv(file.choose(),header=T,na.strings=".")
```

This takes all missing values coded with a period in the original dataset and converts them to NA for R

Once you have a dataset in R and missingness coded as NA:

```
# have to use is.na a lot  
is.na(c(1,2,NA,6))
```

```
## [1] FALSE FALSE TRUE FALSE
```

Returns a logical indicator. Can save this to subset dataset based on number of missings

## Missing Data Continued

```
library(psych)
data(bfi)
dim(bfi)
```

```
## [1] 2800  28
```

Now, subsetting based on number of missing values per person

```
ids <- rowSums(is.na(bfi)) < 3
bfi.sub <- bfi[ids,]
dim(bfi.sub)
```

```
## [1] 2779  28
```



# Variable Types

This is really important as it will change the type of estimator used e.g. logistic vs. linear regression

```
bfi.sub <- bfi[,1:5]
library(rpart)
out1 <- rpart(A1 ~ ., bfi.sub)
out1
```

```
## n=2784 (16 observations deleted due to missingness)
##
## node), split, n, deviance, yval
##      * denotes terminal node
##
## 1) root 2784 5515.1380 2.413434
##    2) A2>=4.5 1907 3382.5430 2.126377
##      4) A2>=5.5 874 1618.1660 1.925629 *
##      5) A2< 5.5 1033 1699.3550 2.296225 *
##    3) A2< 4.5 877 1633.7580 3.037628
##      6) A2>=3.5 554 879.9495 2.819495 *
##      7) A2< 3.5 323 682.2353 3.411765 *
```

## Variable Types Continued

```
out2 <- rpart(as.factor(A1) ~ ., bfi.sub)
out2
```

```
## n=2784 (16 observations deleted due to missingness)
##
## node), split, n, loss, yval, (yprob)
##      * denotes terminal node
##
## 1) root 2784 1862 1 (0.33 0.29 0.14 0.12 0.08 0.029)
##    2) A2>=5.5 874  386 1 (0.56 0.22 0.072 0.064 0.055 0.03) *
##    3) A2< 5.5 1910 1285 2 (0.23 0.33 0.18 0.15 0.092 0.029) *
```

Changing the variable type, from integer to factor also changes the cost function. This results in very different equations and also very different results.

Most important is the variable type of the Y variable. Also can change it in the actual function by setting “family =”

Also can change variable type in dataset and the data mining function will recognize this. However, I almost always just include it in the actual script to make sure it changes to the correct estimator.

# How to get help

```
library(caret)  
?train
```

However, I usually just google the R package and look at the manual

Once you have run a script and have it save as an object, you can

```
library(MASS)  
data(Boston)  
out <- lm(medv ~ ., data=Boston)  
str(out)
```

Using `str()` will list all of the attributes of the “out” object. This is important to use if `print()` or `summary()` don't give you the information you want. Most applicable if you need nitty gritty details

# Parallelization

The caret package makes it easy to parallelize different methods. Its built in to their control function <http://topepo.github.io/caret/parallel.html>

```
library(MASS);library(caret)
data(Boston)
library(doParallel)
cl <- makeCluster(detectCores())
registerDoParallel(cl)

out <- train(medv ~ ., data=Boston,method="rf")
```

A lot of the methods we will be talking about are very parallelizable and will vastly decrease the amount of time it takes to run

# Most Important Details for Learning R

1. Read in data
2. How to subset dataset
3. Missing data handling
4. Variable types
5. Understand where the results go and how to access them
6. The intricacies to each package
7. How to parallelize analyses

This is obviously not enough time to cover R as a programming language but our goal is to give you a working knowledge and learn enough as we proceed that you can implement all of the models we talk about.

Questions?

# Regression

## Linear Regression

```
data.1 = read.table("C:/Users/RJacobucci/Documents/GitHub/search16_labs/apexpos  
names(data.1) = c('id', 'apexpos', 'fsiq7')  
head(data.1)
```

```
##   id apexpos fsiq7  
## 1  1      2.2   121  
## 2  2      5.5    98  
## 3  3      5.2    93  
## 4  4      3.6    98  
## 5  5      7.2    89  
## 6  6      7.3   115
```

```
# Sort Data  
data.2 <- data.1[order(data.1$apexpos),]  
  
attach(data.2)  
  
## Plotting empirical data ##  
  
plot(apexpos, fsiq7, ylab = 'Full Scale IQ', xlab = 'PHE Exposure')
```

# Linear Regression Continued

```
lm.1 = lm(fsiq7 ~ apexpos)
```

```
summary(lm.1)
```

```
##
```

```
## Call:
```

```
## lm(formula = fsiq7 ~ apexpos)
```

```
##
```

```
## Residuals:
```

```
##      Min       1Q   Median       3Q      Max
```

```
## -33.108  -8.790  -0.232   8.004  39.749
```

```
##
```

```
## Coefficients:
```

```
##              Estimate Std. Error t value Pr(>|t|)
```

```
## (Intercept) 107.4337      1.4289   75.19  <2e-16 ***
```

```
## apexpos      -2.9068      0.1079  -26.93  <2e-16 ***
```

```
## ---
```

```
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
##
```

```
## Residual standard error: 13.25 on 312 degrees of freedom
```

```
## Multiple R-squared:  0.6992, Adjusted R-squared:  0.6982
```

```
## F-statistic: 725.1 on 1 and 312 DF,  p-value: < 2.2e-16
```

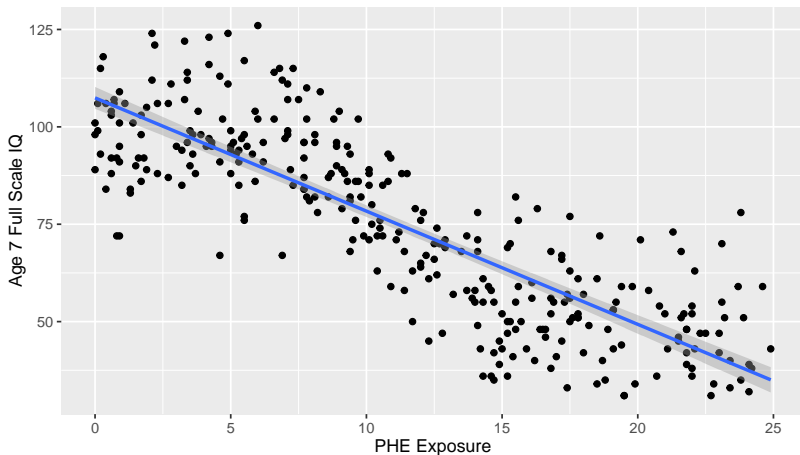
```
#plot(apexpos, fitted(lm.1), ylab = 'Predicted Full Scale IQ', xlab = 'PHE Expos
```

```
#plot(apexpos, fsiq7, ylab = 'Full Scale IQ', xlab = 'PHE Exposure')
```

# Plot Model

```
library(ggplot2)

plot.1 = ggplot(data.1, aes(x=apexpos, y=fsiq7)) + geom_point() +
  stat_smooth(method='lm', formula = y ~ x, size = 1) +
  xlab('PHE Exposure') + ylab('Age 7 Full Scale IQ')
print(plot.1)
```





# Regression Diagnostics on Linear Regression Model

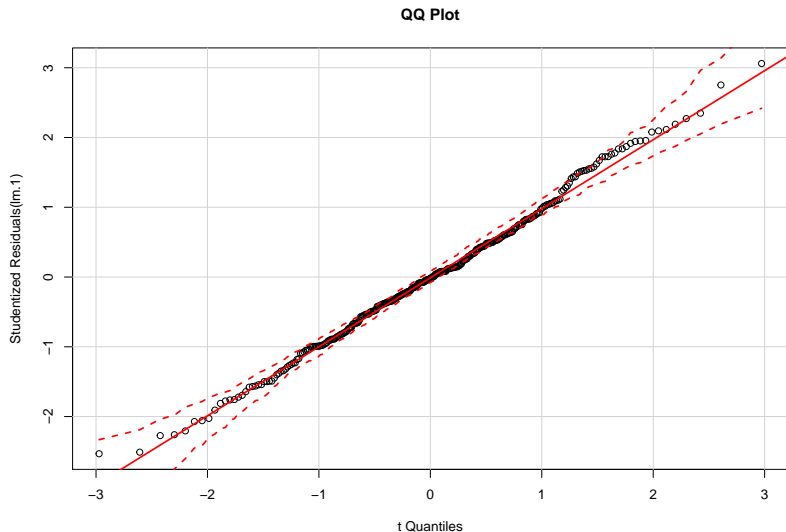
```
library(car)

#Outlier Test
outlierTest(lm.1) # Bonferonni p-value for most extreme obs
```

```
##
## No Studentized residuals with Bonferonni p < 0.05
## Largest |rstudent|:
##      rstudent unadjusted p-value Bonferonni p
## 308 3.060391      0.0024031      0.75457
```

# QQ Plot

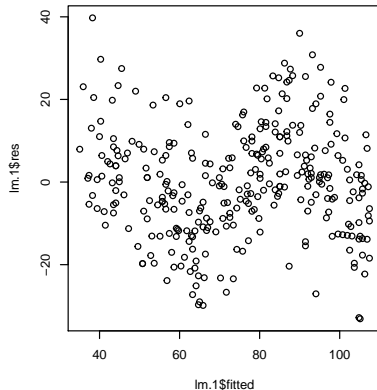
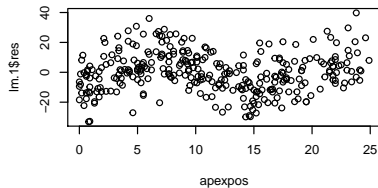
```
qqPlot(lm.1, main="QQ Plot") #qq plot for studentized resid
```



Cook's Distance

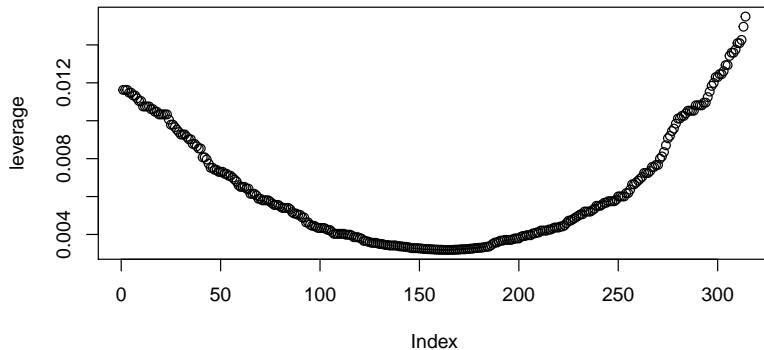
# Plot Residuals

```
# Plots
layout( cbind( c(0,0,1,1,1,1,1,0,0) , rep(2,9) ) )
plot(apexpos, lm.1$res)
plot(lm.1$fitted, lm.1$res)
```



# Leverage Plot

```
leverage = hat(model.matrix(lm.1))  
plot(leverage)
```



# Quadratic Regression

```
apexpos2 = apexpos^2
```

```
lm.2 = lm(fsiq7 ~ apexpos + apexpos2)
```

```
summary(lm.2)
```

```
##
```

```
## Call:
```

```
## lm(formula = fsiq7 ~ apexpos + apexpos2)
```

```
##
```

```
## Residuals:
```

```
##      Min       1Q   Median       3Q      Max
```

```
## -33.939  -8.731  -0.351   7.826  38.618
```

```
##
```

```
## Coefficients:
```

```
##              Estimate Std. Error t value Pr(>|t|)
```

```
## (Intercept) 108.47508    2.05289   52.840 < 2e-16 ***
```

```
## apexpos      -3.17979    0.40087   -7.932 3.91e-14 ***
```

```
## apexpos2      0.01163    0.01644    0.707    0.48
```

```
## ---
```

```
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
##
```

```
## Residual standard error: 13.26 on 311 degrees of freedom
```

```
## Multiple R-squared:  0.6997, Adjusted R-squared:  0.6977
```

```
## F-statistic: 362.2 on 2 and 311 DF, p-value: < 2.2e-16
```

# Get standardized coefficients

```
library(QuantPsyc)  
lm.beta(lm.1)
```

```
##      apexpos  
## -0.8361638
```

## Logistic Regression

```
library(ISLR); data(Default)  
lr.out <- glm(default~.,,family="binomial",data=Default)  
summary(lr.out)
```

Can also use `glm()` to run other types of regression. See `?family`

# Stepwise Selection

## Forward

Efficient, but not guaranteed to find best overall model.

```
library(MASS); library(elasticnet)
data(diabetes)
X <- diabetes$x
Y <- diabetes$y
diabetes2 <- data.frame(cbind(Y,X))

ids <- sample(1:nrow(diabetes2), .5*nrow(diabetes2),replace=FALSE)
diab.train <- diabetes2[ids,]
diab.test <- diabetes2[-ids,]

set.seed(1034)
lmNULL <- lm(Y ~ 1, data=diab.train)
lmFULL <- lm(Y ~ ., data=diab.train)

stepFor <- stepAIC(lmNULL,scope=list(lower=lmNULL,upper=lmFULL),
                  direction="forward")
```

# Forward Results

```
head(stepFor$anova)
```

```
## Stepwise Model Path
## Analysis of Deviance Table
##
## Initial Model:
## Y ~ 1
##
## Final Model:
## Y ~ bmi + ltg + map + hdl + sex
##
##
```

	Step	Df	Deviance	Resid. Df	Resid. Dev	AIC
##	1			220	1320796.6	1923.724
##	2 + bmi	1	491504.234	219	829292.4	1822.867
##	3 + ltg	1	209246.738	218	620045.7	1760.604
##	4 + map	1	23630.751	217	596414.9	1754.017
##	5 + hdl	1	9970.288	216	586444.6	1752.291
##	6 + sex	1	10900.601	215	575544.0	1750.145

```
pred.for<- predict(stepFor,diab.test)
cor(pred.for,diab.test$Y)**2
```

```
## [1] 0.4468704
```



# Stepwise Selection

## Backward

```
library(MASS);set.seed(1034)
stepBack <- stepAIC(lmFULL,direction="backward")

stepBack$anova
```

```
pred.back<- predict(stepBack,diab.test)

cor(pred.back,diab.test$Y)**2
```

```
## [1] 0.4520348
```

Tomorrow we will talk about methods that are thought to be more optimal and have in a sense replaced stepwise selection.

Next is Smoothing

# Smoothing

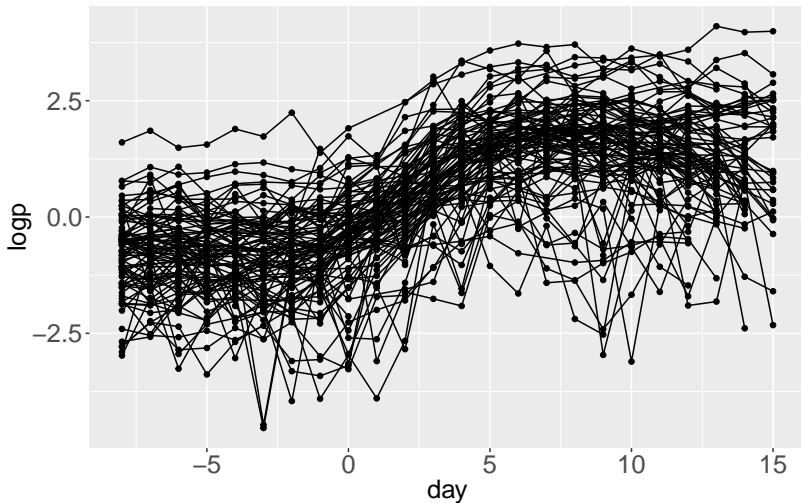
Download example data from Jin-Ting Zhang's website

```
library(data.table)
progdta <- fread("http://www.stat.nus.edu.sg/~zhangjt/books/Chapman/datasets/r
names(progdta) = c("group", "subject", "cycle", "day", "logp", "missing")

# Delete missing data
progdta = progdta[progdta$missing==0,]
```

## Plot Data

```
library(ggplot2)
ggplot(data=prodata, aes(x=day,y=logp,group=cycle)) + geom_point() + geom_line
  theme(axis.text=element_text(size=18),axis.title=element_text(size=18))
```



## Smoothing Cont'd

Obviously the data are not linear, and any linear model will misfit badly and violate assumptions

First, we will fit polynomials to the data

```
# Extract first cycle data only for illustration  
data1 = progdata[progdata$cycle==1,]  
attach(data1)
```

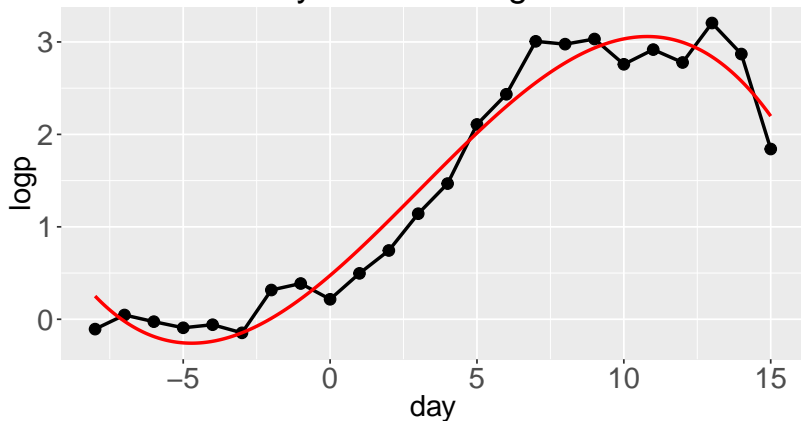
Fitting polynomials to the first cycle data  
Dependent variable: logp (log progesterone level)  
Predictor variable: day (day since ovulation)

```
degree = 3 # degree of polynomial (highest power)  
fit = lm(logp~poly(day,degree),data=data1) # fitted model  
  
# get predictions from fitted model  
time = seq(-8,15,by=0.01) # time points to evaluate the fitted model  
# time points and polynomial evaluated at the time points  
newdata = data.frame(day=time,fity=predict(fit,newdata=data.frame(day=time)))
```

## Plot Estimated Model

```
ggplot(data=data1,aes(x=day,y=logp)) + geom_point(size=3) + geom_line(size=1) +  
  geom_line(data=newdata,aes(x=day,y=fity),color="red",size=1) + ggtitle(paste  
  theme(axis.text=element_text(size=18),axis.title=element_text(size=18),title
```

Polynomial of degree 3



# Splines

```
library(fda)

# Create spline basis object
degree = 3 # degree of polynomial
myrange = c(-8,15) # range of the predictor variable
myknots = c(-8,-5,12,15)
# knot locations, the first element should be equal to the first element in
# myrange and the last element should be equal to the second element in myrange.

# create b-spline basis functions to fit splines
mybasisobj = create.bspline.basis(range=myrange,norder=degree+1,breaks=myknots)
myfdbj = smooth.basis(argvals=data1$day,y=data1$logp,mybasisobj) # fitted spline

# get fitted predictions
time = seq(myrange[1],myrange[2],by=0.01) # time points to evaluate the fitted spline
# time points and polynomial evaluated at the time points
newdata = data.frame(day=time,fity=eval.fd(evalarg=time,fdbj=myfdbj$fd))
```

## Evaluate the fitted curve

```
ggplot(data=data1,aes(x=day,y=logp)) + geom_point(size=3) +  
  geom_line(size=1) + geom_line(data=newdata,aes(x=time,y=fity),color="red",size=2) +  
  geom_vline(xintercept = myknots,size=1,color="white") +  
  geom_vline(xintercept = myknots,size=1,color="black",linetype="dashed") +  
  ggtitle(paste('Spline of degree ',degree)) +  
  theme(axis.text=element_text(size=18),axis.title=element_text(size=18),title=element_text(size=18))
```

Spline of degree 3

