Course 02402 Introduction to Statistics

Lecture 9: Multiple linear regression

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Overview

1. Warm up with some simple linear regression
2. Multiple linear regression
3. Model selection
4. Residual analysis (model validation)
5. Curvilinearity
6. Confidence and prediction intervals
7. Colinearity
8. The overall regression method

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Example: Ozon concentration

We have a set of observations of: logarithm to ozone concentration (log(ppm)), temperature, radiation and wind speed:

ozone	radiation	wind	temperature	month	day
41	190	7.4	67	5	1
36	118	8.0	72	5	2
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
18	131	8.0	76	9	29
20	223	11.5	68	9	30

Example: Ozone concentration

```r
## Se info about  data
?airquality
## Copy the data
Air <- airquality
## Remove rows with at least one NA value
Air <- na.omit(Air)

## Remove one outlier
Air <- Air[-which(Air$Ozone == 1), ]

## Check  the empirical density
hist(Air$Ozone, probability=TRUE, xlab="Ozon", main="")

## Concentrations are positive and very skewed, let's
## log-transform right away:
## (although really one could wait and check residuals from models)
Air$logOzone <- log(Air$Ozone)
## Bedre epdf?
hist(Air$logOzone, probability=TRUE, xlab="log Ozone", main="")

## Make a time variable (R timeclass, se ?POSIXct)
Air$t <- ISOdate(1973, Air$Month, Air$Day)
## Keep only some of the columns
Air <- Air[ ,c(7,4,3,2,8)]
## New names of the columns
names(Air) <- c("logOzone","temperature","wind","radiation","t")

## What's in  Air?
str(Air)
Air
head(Air)
tail(Air)

## Typically one would  begin with a pairs plot
pairs(Air, panel = panel.smooth, main = "airquality data")
```

Example: Ozone concentration

- Let us first analyse the relation between ozone and temperature

- Apply a *simple linear regressions model*

$$Y_i = \beta_0 + \beta_1 x_i + \varepsilon_i \quad , \quad \varepsilon_i \sim N(0, \sigma^2) \text{ og i.i.d.}$$

  where

  - Y_i is the (logarithm of) ozone concentration of observation i
  - x_i is the temperature at observation i

Fit the model in R

```r
################################

## See the relation between ozone and temperature
plot(Air$temperature, Air$logOzone, xlab="Temperature", ylab="Ozon")

## Correlation
cor(Air$logOzone, Air$temperature)

## Fit a simple linear regression model
summary(lm(logOzone ~ temperature, data=Air))

## Add a vector with random values, is there a significant linear relation?
## ONLY for ILLUSTRATION purposes
Air$noise <- rnorm(nrow(Air))
plot(Air$logOzone, Air$noise, xlab="Noise", ylab="Ozon")
cor(Air$logOzone, Air$noise)
summary(lm(logOzone ~ noise, data=Air))
```

Simple linear regression model for the other two

We can also make a simple linear regression model with each of the other two independent variables

```
################################
## With each of the other two independent variables

## Simple linear regression model with the wind speed
plot(Air$logOzone, Air$wind, xlab="logOzone", ylab="Wind speed")
cor(Air$logOzone, Air$wind)
summary(lm(logOzone ~ wind, data=Air))

## Simple linear regression model with the radiation
plot(Air$logOzone, Air$radiation, xlab="logOzone", ylab="Radiation")
cor(Air$logOzone, Air$radiation)
summary(lm(logOzone ~ radiation, data=Air))
```

Overview

Multiple linear regression

- Y is the *dependent variable*
- We are interested in modelling the Y's dependency of the *independent* or *explanatory* variables $x_1, x_2, ..., x_p$
- We are modelling a *linear relation* between Y and $x_1, x_2, ..., x_p$, described with the regression model

  $Y_i = \beta_0 + \beta_1 x_{1,i} + \cdots + \beta_p x_{p,i} + \varepsilon_i \quad , \quad \varepsilon_i \sim N(0, \sigma^2)$ and i.i.

- Y_i og ε_i are random variables and $x_{j,i}$ are variables

Least squares estimates

- The coefficient estimates are found by minimizing:

$$RSS(\beta_0, \beta_1, \ldots, \beta_p) = \sum_{i=1}^{n} [y_i - (\beta_0 + \beta_1 x_{i,1} + \cdots + \beta_p x_{i,p})]^2$$

- The "predicted" (= "fitted") are found as

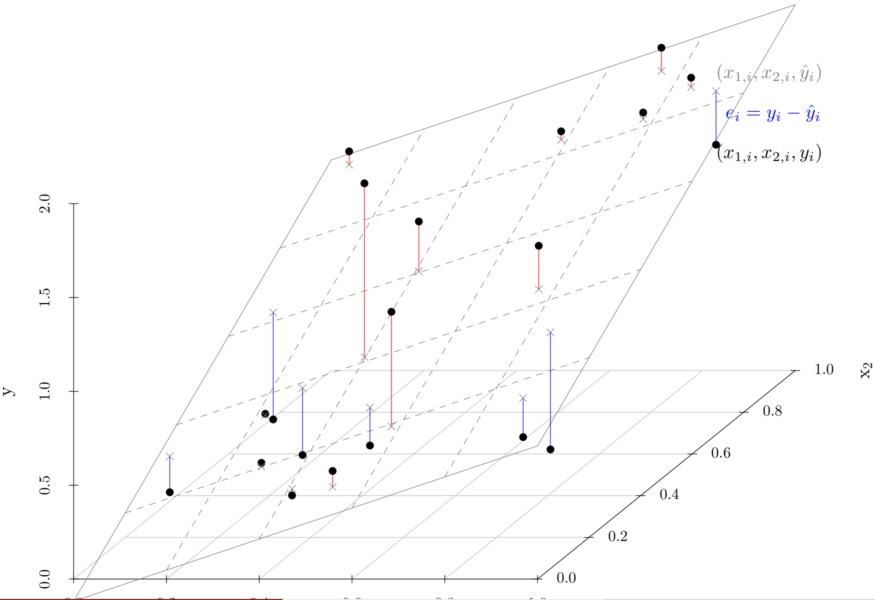
$$\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_{i,1} + \cdots + \hat{\beta}_p x_{i,p}$$

- And then the residuals are found as

$$e_i = y_i - \hat{y}_i$$

$$\text{residual} = \text{observation} - \text{prediction}$$

Least squares estimates - The concept!



Computations for MLR - no explicit formulas given!

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- Everything: THE SAME as for SIMPLE linear regression!
- (In Section 6.6: Mathematical matrix based expressions including explicit formulas. Not syllabus in course 02402)

Parameter interpretation in MLR (Remark 6.14)

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- The effect of x_i "other variables being equal"
- The unique effect of x_i

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- The unique effect of x_i
- Depends on what else is in the model!!
- Generally: NOT a causal/intervention effect!!

Overview

Extend the model (forward selection)

- *Not included in the eNote*
- Start with the *linear regression model* with the most significant independent variable
- *Extend the model* with the remaining independent variables (inputs) one at a time
- *Stop* when there is not any significant extensions possible

```
################################
## Extend the model

## Forward selection:
## Add wind to the model
summary(lm(logOzone ~ temperature + wind, data=Air))
## Add radiation to the model
summary(lm(logOzone ~ temperature + wind + radiation, data=Air))
```

Reduce the model (model reduction or backward selection)

- *Described in the eNote, section 6.5*
- Start with the full model
- Remove the most insignificant independent variable
- Stop when all prm. estimates are significant

```
################################
## Backward selection

## Fit the full model
summary(lm(logOzone ~ temperature + wind + radiation + noise, data=Air))
## Remove the most non-significant input, are all now significant?
summary(lm(logOzone ~ temperature + wind + radiation, data=Air))
```

Model selection

- There is no fully certain method for finding the best model!
- It will require subjective decisions to select a model
- Different procedures: either forward or backward selection (or both), depends on the circumstances
- Statistical measures and tests to compare model fits
- In this course only backward selection is described

Overview

Residual analysis (model validation)

- Model validation: Analyze the residuals to check that the assumptions is met
- $e_i \sim N(0, \sigma^2)$ is independent and identically distributed (i.i.d.)
- Same as for the simple linear regression model

Assumption of normal distributed residuals

- Make a qq-normalplot (normal score plot) to see if they seem normal distributed

```
################################
## Assumption of normal distributed residuals

## Save the selected fit
fitSel <- lm(logOzone ~ temperature + wind + radiation, data=Air)

## qq-normalplot
qqnorm(fitSel$residuals)
qqline(fitSel$residuals)
```

Assumption of identical distribution of residuals

- Plot the residuals (e_i) versus the predicted (fitted) values ($\hat{y}_i$)

```
##################################
## Plot the residuals vs. predicted values

plot(fitSel$fitted.values, fitSel$residuals, xlab="Predicted values",
     ylab="Residuals")
```

- Seems like the model kan be improved!
- Plot the residuals vs. the independent variables

```
##################################
## Plot the residuals vs. the independent variables

par(mfrow=c(1,3))
plot(Air$temperature, fitSel$residuals, xlab="Temperature")
plot(Air$wind, fitSel$residuals, xlab="Wind speed")
plot(Air$radiation, fitSel$residuals, xlab="Radiation")
```

Overview

Curvilinear model

If we want to estimate a model of the type

$$Y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \varepsilon_i$$

we can use a multiple linear regression model

$$Y_i = \beta_0 + \beta_1 x_{i,1} + \beta_2 x_{i,2} + \varepsilon_i$$

where

- $x_{i,1} = x_i$
- $x_{i,2} = x_i^2$

and apply the same methods as for multiple linear regression.

Extend the ozone model with appropriate curvilinear regression

```r
################################
## Extend the ozone model with appropriate curvilinear regression

## Make the squared wind speed
Air$windSq <- Air$wind^2
## Add it to the model
fitWindSq <- lm(logOzone ~ temperature + wind + windSq + radiation, data=Air)
summary(fitWindSq)

## Equivalently for the temperature
Air$temperature2 <- Air$temperature^2
## Add it
fitTemperatureSq <- lm(logOzone ~ temperature + temperature2 + wind + radiation, data=Air)
summary(fitTemperatureSq)

## Equivalently for the radiation
Air$radiation2 <- Air$radiation^2
## Add it
fitRadiationSq <- lm(logOzone ~ temperature + wind + radiation + radiation2, data=Air)
summary(fitRadiationSq)

## Which one was best?
## One could try to extend the model further
fitWindSqTemperaturSq <- lm(logOzone ~ temperature + temperature2 + wind + windSq + radiation, data=Air)
summary(fitWindSqTemperaturSq)

## Model validation
qqnorm(fitWindSq$residuals)
qqline(fitWindSq$residuals)
plot(fitWindSq$residuals, fitWindSq$fitted.values, pch=19)
```

Overview

Confidence and prediction intervals for the plane, Method 6.9:

Extract Confidence and prediction intervals for the plane by `R`-function `predict`. Options for `confidence` og `prediction` exist.

```
################################
## Confidence and prediction intervals for the curvilinear model

## Generate a new data.frame with constant temperature and radiation, but with varying wind speed
wind<-seq(1,20.3,by=0.1)
AirForPred <- data.frame(temperature=mean(Air$temperature), wind=wind,
                         windSq=wind^2, radiation=mean(Air$radiation))

## Calculate confidence and prediction intervals (actually bands)
CI <- predict(fitWindSq, newdata=AirForPred, interval="confidence", level=0.95)
PI <- predict(fitWindSq, newdata=AirForPred, interval="prediction", level=0.95)

## Plot them
plot(wind, CI[,"fit"], ylim=range(CI,PI), type="l",
     main=paste("At temperature =",format(mean(Air$temperature),digits=3),
                "and radiation =", format(mean(Air$radiation),digits=3)))
lines(wind, CI[,"lwr"], lty=2, col=2)
lines(wind, CI[,"upr"], lty=2, col=2)
lines(wind, PI[,"lwr"], lty=2, col=3)
lines(wind, PI[,"upr"], lty=2, col=3)
## legend
legend("topright", c("Prediction","95% confidence band","95% prediction band"), lty=c(1,2,2), col=1:3)
```

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- MLR breaks down if X-data has "exact linear redundancy"
    - Example: Both height in cm and height in m is in the data.

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  - Example: Both height in cm and height in m is in the data.
- Interpretation and model stability is challenged if X-data has "near redundancy" patterns
  - Example: Both weight and BMI are in the X-data (highly correlated)
- With e.g. two highly correlated x-variables:
  - Together in the model for y none of them may have a unique effect
  - Separately they may have a strong effect each of them

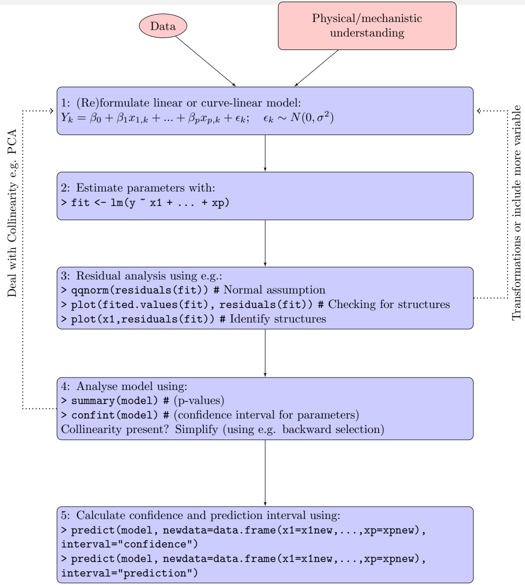
Colinearity - an illustration in R

```
################################
## See problems with highly correlated inputs

## Generate values for MLR
n <- 100
## First variable
x1 <- sin(0:(n-1)/(n-1)*2*2*pi) + rnorm(n, 0, 0.1)
plot(x1, type="b")
## The second variable is the first plus a little noise
x2 <- x1 + rnorm(n, 0, 0.1)
## x1 and x2 are highly correlated
plot(x1,x2)
cor(x1,x2)
## Simulate an MLR
beta0=20; beta1=1; beta2=1; sigma=1
y <- beta0 + beta1 * x1 + beta2 * x2 + rnorm(n,0,sigma)
## See scatter plots for y vs. x1, and y vs. x2
par(mfrow=c(1,2))
plot(x1,y)
plot(x2,y)
## Fit an MLR
summary(lm(y ~ x1 + x2))

## If it was an experiment and the effects could be separated in the design
x1[1:(n/2)] <- 0
x2[(n/2):n] <- 0
## Plot them
plot(x1, type="b")
lines(x2, type="b", col="red")
## Now very low correlation
cor(x1,x2)
## Simulate MLR again
y <- beta0 + beta1 * x1 + beta2 * x2 + rnorm(n,0,sigma)
## and fit MLR
summary(lm(y ~ x1 + x2))
```

It is important how experiments are designed!

Overview

The overall regression method box 6.16



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