

02323 Introduction to Statistics

Lecture 9: Multiple linear regression

DTU Compute
Technical University of Denmark
2800 Lyngby – Denmark

Agenda

- 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

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

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

Example: Ozone 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
⋮	⋮	⋮	⋮	⋮	⋮
18	131	8.0	76	9	29
20	223	11.5	68	9	30

Example: Ozone concentration

```
## See 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="Ozone", 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, see ?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

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

## 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$noise, xlab="Noise", ylab="Ozone")
cor(Air$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

- 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

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, \dots, x_p
- We are modelling a *linear relation* between Y and x_1, x_2, \dots, x_p , described with the regression model

$$Y_i = \beta_0 + \beta_1 x_{1,i} + \dots + \beta_p x_{p,i} + \varepsilon_i \quad , \quad \varepsilon_i \sim N(0, \sigma^2) \text{ and i.i.d.}$$
- Y_i og ε_i are random variables and $x_{j,i}$ are variables

Least squares estimates

- The coefficient estimates are found by minimizing:

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

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

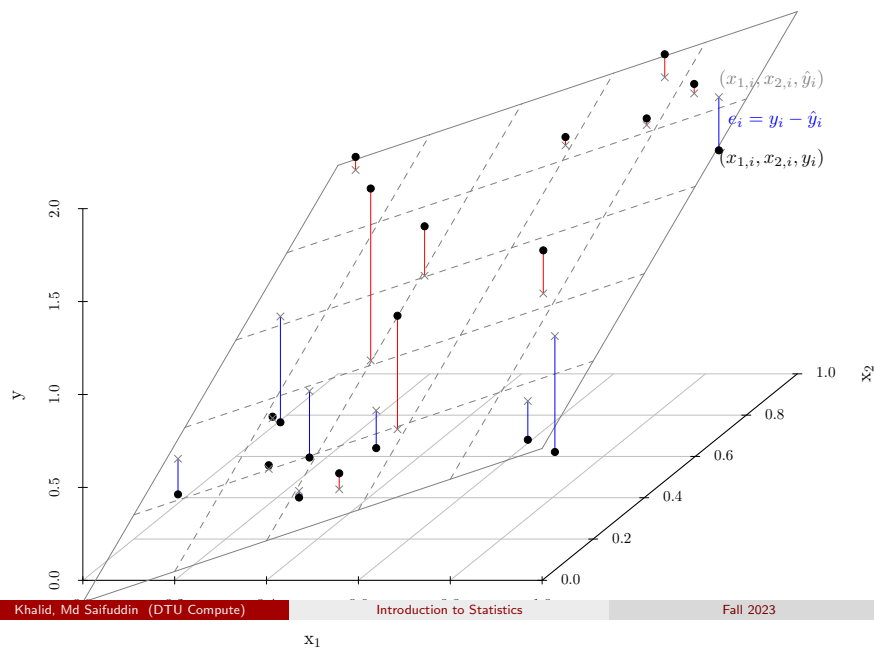
$$\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_{i,1} + \dots + \hat{\beta}_p x_{i,p}$$

- And then the residuals are found as

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

residual = observation – prediction

Least squares estimates - The concept!



Parameter interpretation in MLR (Remark 6.14)

What does $\hat{\beta}_i$ express?

- The expected y -change with 1 unit x_i -change
- The effect of x_i given the other variables
- The effect of x_i corrected for the other variables
- The effect of x_i "other variables being equal"
- The unique effect of x_i
- Depends on what else is in the model!!
- Generally: NOT a causal/intervention effect!!

Computations for MLR - no explicit formulas given!

- Remark 6.6: Extract $\hat{\beta}_i$ and $\hat{\sigma}_{\beta_i}$ from R-output (summary(myfit))
- Theorem 6.2: The t-distribution can be used for inference for parameters
- Methods 6.4 and 6.5: Hypothesis tests and Confidence intervals for parameters based on R-output.
- Everything: **THE SAME** as for **SIMPLE** linear regression!
- (In Section 6.6: Mathematical matrix based expressions including explicit formulas. Not syllabus in course 02402)

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

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))
```

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

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))
```

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

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 can 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

- 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

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

```
#####
## 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
fitWindSqTemperatureSq <- lm(logOzone ~ temperature + temperature2 + wind + windSq + radiation, data=Air)
summary(fitWindSqTemperatureSq)

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

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

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)
```

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

Colinearity

- MLR breaks down if X-data has "exact linear redundancy"
 - 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*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

- 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**

Agenda

- 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**

The overall regression method box 6.16

