Linear Regression - Part 2

Anders Stockmarr
Course developers: Anders Stockmarr, Elisabeth Wreford Andersen

DTU Department of Applied Mathematics and Computer Science
Section for Statistics and Data Analysis
Technical University of Denmark
anst@dtu.dk

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Plan for this week

04_Multible regression

- **Monday** Statistical inference, and the t-test
- **Tuesday** Simple and Multiple regression
- **Wednesday** ANOVA, ANCOVA, and linear models
- **Thursday** Categorical data, statistical report writing, logistic Regression
- **Friday** Introduction to repeated measures , Principal Component Analysis

Learning objectives

04_Multible regression

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2. Interpret the result from a *multiple linear regression*
3. Understand and use interactions.
4. Do model reduction as backwards selection.

Overview

04_Multible regression

Multiple Linear Regression

04_Multible regression

- The association between several continuous variables.
- Y response / outcome / dependent variable
- $X_1, \ldots, X_p$ explanatory / covariates / independent variables.

Data

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Observations of sets $(x_{1i}, \ldots, x_{pi}, y_i)$ for all $i = 1, \ldots, n$ individuals or units.

Unit	x_1	x_2	$\cdots$	x_p	y
1	x_{11}	x_{12}	$\cdots$	x_{1p}	y_1
2	x_{21}	x_{22}	$\cdots$	x_{2p}	y_2
2	x_{31}	x_{32}	$\cdots$	x_{3p}	y_3
$\vdots$	$\vdots$	$\vdots$	$\ldots$	$\vdots$	$\vdots$
n	x_{n1}	x_{n2}	$\cdots$	x_{np}	y_n

The Multiple Linear Regression (MLR) model

$$Y_i = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \ldots + \beta_p x_{pi} + \varepsilon_i, \qquad \varepsilon_i \sim N(0, \sigma^2)$$

Aim: Identify one (or several) reasonable model(s) that are:

- As simple as possible
- Captures the relevant structures in the data

General rule: Keep variables that contribute — drop variables that don't

Important Issues to Consider

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- Which explanatory variables to include
- Curvature in the response to the explanatory variables
- Interactions between explanatory variables (will return to this)
- Correlation between explanatory variables

Use and Abuse of Multiple Linear Regression?

- Multiple Linear Regression may correspond to the scientific question of interest.
- With multiple explanatory variables, the predictions become more precise (more of the variability is explained).
- Assume that one of the explanatory variables is of greatest interest. There may be another variable connected to both the variable of interest and the outcome:

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  1. It seems that the higher the sales of ice cream the more drowning accidents.

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- Example: Drowning and ice cream sales
  1. It seems that the higher the sales of ice cream the more drowning accidents.
  2. Is this because people eat ice cream at the beach, and then cannot swim?
  3. Or is there a 3rd variable (season) influencing both sale of ice cream and drowning accidents?

Example: Air pollution studies

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How is ozone concentration related to wind speed, air temperature and solar radiation?

- We have 111 observations of ozone, wind speed, temperature and radiation.

The outcome (response) Y is the ozone concentration and the explanatory variables are X_1 radiation (rad), X_2 temperature (temp) and X_3 wind speed.

Always start by plotting the data!

Scatter plot

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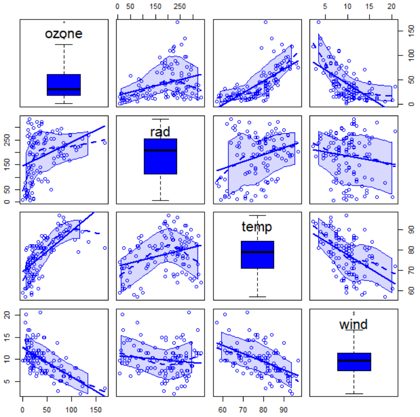
```
library(car)
scatterplotMatrix(~ ozone + rad + temp + wind,
                  diagonal = list(method="boxplot"),data = oz)
```



Overview

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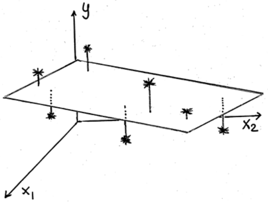
The Regression Model 04_Multible regression

$$Y_i = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \ldots + \beta_p x_{pi} + \varepsilon_i$$

Traditional assumptions:
$\varepsilon_i \sim N(0, \sigma^2)$, independent.



Least squares:
Find the $\beta_0, \beta_1, \ldots, \beta_p$ to minimize the sum of the squared distances:
$SS(\beta_0, \beta_1, \ldots, \beta_p) =$
$\sum(y_i - (\beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \ldots + \beta_p x_{pi}))^2$

Matrix Notation

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If $n = 6$ and $p = 3$ then we can write the model using matrix notation:

$$\begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ y_6 \end{pmatrix} = \begin{pmatrix} 1 & x_{11} & x_{12} & x_{13} \\ 1 & x_{21} & x_{22} & x_{23} \\ 1 & x_{31} & x_{32} & x_{33} \\ 1 & x_{41} & x_{42} & x_{43} \\ 1 & x_{51} & x_{52} & x_{53} \\ 1 & x_{61} & x_{62} & x_{63} \end{pmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \beta_3 \end{pmatrix} + \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{pmatrix}$$

Using compact notation we have:

$$\boldsymbol{y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$$

Estimation

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Using Least Squares method for estimation we get:

$$\hat{\beta} = (X^T X)^{-1} X^T Y$$

The estimated uncertainty on the estimate (variance):

$$var(\hat{\beta}) = \sigma^2 (X^T X)^{-1}$$

When we have estimates for $\beta_0, \beta_1 \ldots, \beta_p$ then we can calculate the expected values for the outcome:

$$\hat{y} = X\hat{\beta}$$

The value $\hat{y}_i$ is called the fitted value, or expected value. This corresponds to the value on the regression line.

Estimation continued

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As for simple linear regression we also have the residuals (what is left):

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

Using the matrix notation:

$$\boldsymbol{\hat{\varepsilon}} = \boldsymbol{y} - \boldsymbol{\hat{y}}$$

The model variance $\boldsymbol{\sigma^2}$ is estimated:

$$\boldsymbol{\hat{\sigma}^2} = \boldsymbol{s^2} = \frac{\boldsymbol{\hat{\varepsilon}^T \hat{\varepsilon}}}{\boldsymbol{n - (p+1)}} = \boldsymbol{MSE}$$

Multiple Linear Regression

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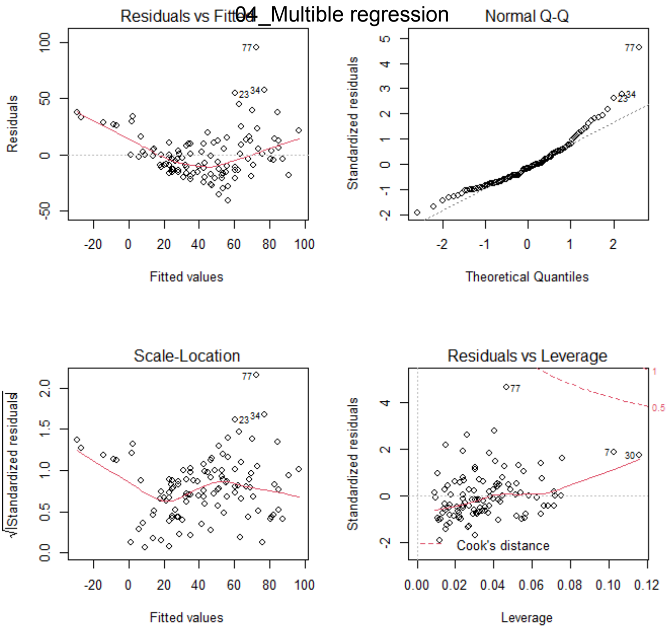
```
reg1 <- lm(ozone ~ rad + temp + wind, data = oz)
summary(reg1)

## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) -64.2321    23.0420   -2.79   0.0063 **
## rad           0.0598     0.0232    2.58   0.0112 *
## temp          1.6512     0.2534    6.52  2.4e-09 ***
## wind         -3.3376     0.6538   -5.10  1.4e-06 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 21.2 on 107 degrees of freedom
## Multiple R-squared:  0.606,Adjusted R-squared:  0.595
## F-statistic: 54.9 on 3 and 107 DF,  p-value: <2e-16
```


04_Multible regression
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Cook's distance
Leverage
77
23
34
70
30
1
0.5

Interpreting the Estimates

04_Multible regression

- It is always important to interpret the model parameters - give an explanation in words of the results.

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- It is always important to interpret the model parameters - give an explanation in words of the results.
- $\hat{\beta}_i$ is the effect of variable X_i on Y, when all other variables are fixed.
- $\hat{\beta}_i$ is a slope. The expected change in Y when X_i changes one unit and the remaining variables are unchanged.

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04_Multible regression

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- $\hat{\beta}_i$ is the effect of variable X_i on Y, when all other variables are fixed.
- $\hat{\beta}_i$ is a slope. The expected change in Y when X_i changes one unit and the remaining variables are unchanged.
- The effect is corrected for the effect of the other explanatory variables.

The Estimates from the MLR

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```
##               Estimate Std..Error   Lower  Upper p.value
## (Intercept)   -64.23      23.04 -109.91 -18.55 0.00628
## rad             0.06       0.02    0.01   0.11 0.01124
## temp            1.65       0.25    1.15   2.15 < 0.001
## wind           -3.34       0.65   -4.63  -2.04 < 0.001
```

And the variance is estimated by:

$$\hat{\sigma}^2 = 21.2^2 = 449.44$$

The Intercept $= \hat{\beta}_0$ is the expected ozone when wind=0, rad=0 and temp=0, not so interesting.

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The Intercept $= \hat{\beta}_0$ is the expected ozone when wind=0, rad=0 and temp=0, not so interesting.
temp $= \hat{\beta}_2$ is a slope. The ozone level increases by 1.65 when the temperature increases by 1 for fixed wind and radiation.

Overview

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Building a MLR

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- Perhaps this model was too simple.
- We want to include radiation, temperature and wind but we don't know whether it is reasonable with linear effects.
- Perhaps we need a curve.

GAM

04_Multible regression

- This morning we talked about adding squared terms of continuous explanatory variables. After looking at residual plots and seeing a non-random shape.

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04_Multible regression

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04_Multible regression

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- In many cases, however, we have one or more continuous explanatory variables, but no a priori reason to choose one particular parametric form over another for describing the shape of the relationship between the response variable and the explanatory variable(s).
- Generalized additive models (GAMs) are useful in such cases because they allow us to capture the shape of a relationship between y and x without having to chose a particular parametric form beforehand.

GAM

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- We are replacing the linear form in the regression model

$$\sum_j \beta_j X_j$$

- By the sum of smooth functions

$$\sum_j s_j(X_j)$$

- The functions s_j are unspecified smooth functions estimated using a non-parametric smoother

GAM for the ozone example

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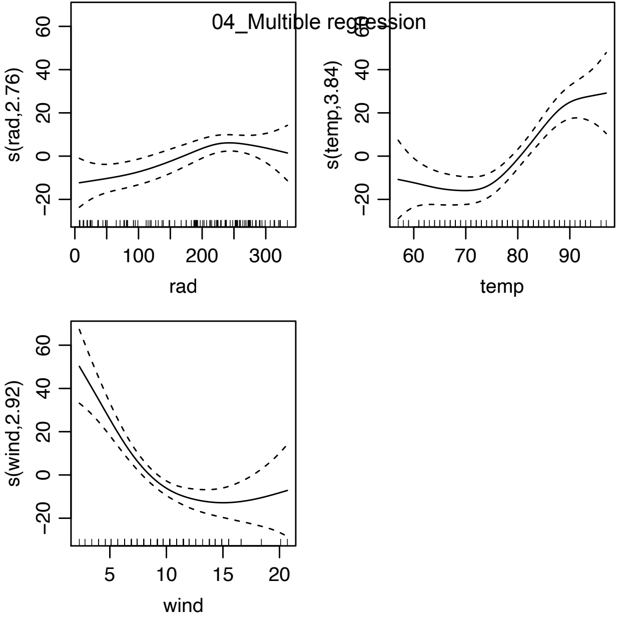
```
library(mgcv)
par(mfrow = c(2,2), mgp = c(2,0.7,0), mar =
c(3,3,1,1))
model <- gam(ozone ~ s(rad) + s(temp) + s(wind), data = oz)
plot(model)
par(mfrow = c(1,1))
```


04_Multible regression
s(rad,2.76)
rad
0
100
200
300
-20
0
20
40
60
s(temp,3.84)
temp
60
70
80
90
s(wind,2.92)
wind
5
10
15
20

Ideas from GAM

04_Multible regression

- The confidence intervals are sufficiently narrow to suggest that the curvature in the relationship between ozone and temperature is real
- The curvature of the relationship with wind is questionable
- A linear model may well be all that is required for solar radiation

What if the effect of temperature depends on wind speed?

We had the model

$$y_i = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \beta_3 x_{3i} + \varepsilon_i$$

Where y_i is the observed ozone concentration i, x_{1i} the radiation, x_{2i} the temperature and x_{3i} the wind speed.
We are assuming that temperature and wind have an **additive effect** on the ozone concentration.
The effect of temperature is assumed the same for all wind speeds.

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We are assuming that temperature and wind have an **additive effect** on the ozone concentration.
The effect of temperature is assumed the same for all wind speeds.
Perhaps the additive model is too simple, we can include a **multiplicative term** (also called an interaction).

$$y_i = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + +\beta_3 x_{3i} + \beta_4 (x_{2i} \cdot x_{3i}) + \varepsilon_i$$

where β_4 accounts for the **interaction** between temperature and wind.

Taylor expansion of real functions

Why is a multiplicative term a relevant idea?

- Power series expansion of a smooth one-dimensional function:

$$f(x) = f(x_0) + \sum_{n=1}^{\infty} a_n (x - x_0)^n, \qquad a_n = f^{(n)}(x_0) n!$$

- 1^{st} order Taylor expansion:

$$\begin{aligned} f(x) =& f(x_0) + f'(x_0) \cdot (x - x_0) + r_1(x - x_0) \\ =& \underbrace{f(x_0) - f'(x_0) \cdot x_0}_{\alpha} + \underbrace{f'(x_0)}_{\beta} \cdot x + r_1(x - x_0) \\ =& \alpha + \beta x + r_1(x - x_0) \end{aligned}$$

Taylor expansion of real functions

- If the relation between Y and x is really f:

$$Y = \alpha + \beta x + \varepsilon$$

$\varepsilon = r_1(x - x_0) + \epsilon$ covers both model aberrations and stochasticity.

- If the model aberration is too big to be handled by the general uncertainty ε, we may resort to a finer model description, Taylor expansion to the 2^{nd} order (here in arbitrary dimensions):

$$\begin{aligned} f(x) =& f(x_0) + < f'(x_0), x - x_0 > \\ &+ \frac{1}{2}(x - x_0)^T \cdot f''(x_0) \cdot (x - x_0) + r_2(x - x_0) \end{aligned}$$

- The matrix in the second term contains the coefficients to the 2^{nd} order multiplicative model terms.

Trees

04_Multible regression

- We need to get some ideas about which interactions to include.

Trees

04_Multible regression

- We need to get some ideas about which interactions to include.
- Trees can help identify interactions
- Good for initial data inspection
- The splits that gives the largest reduction in variance for each part.
- At the leaves we have the mean value in that subset of the data

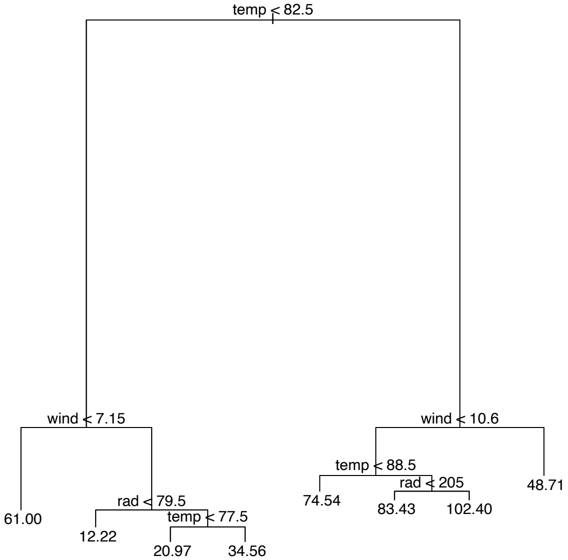
Tree in example

04_Multible regression

```r
library(tree)
model<-tree(ozone~., data = oz)
plot(model)
text(model)
```

Tree in example

04_Multible regression



Trees

04_Multible regression

- If the number of covariates is large, the single tree method will no longer work. One will then need to resort to sparse methodology.
- One such bases itself on the Random Forest methodology, selecting subsets of covariates at random and construct corresponding trees.
- Selection of interacting terms, after correcting for correlation/dependence, can be made following *Behr et al 2022*, `https://doi.org/10.1073/pnas.2118636119`.
- The procedure by *Behr et al 2022* is, however, outside the scope of this course.

Ideas from the tree

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- Temperature is by far the most important
- Wind speed important at both high and low values. Low wind is associated to higher mean ozone levels.
- Possible interaction between wind and temperature and wind and radiation.

Overview

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New model for the ozone data

04_Multible regression

- We are now ready with a more complex model for the ozone data.
- We will include curvature for wind and temperature and interactions between wind and temperature and wind and radiation.

$$\begin{aligned} y_i &= \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + +\beta_3 x_{3i} + \beta_4 x_{2i}^2 + \beta_5 x_{3i}^2 \\ &+ \beta_6 (x_{2i} \cdot x_{3i}) + \beta_7 (x_{1i} \cdot x_{3i}) + \varepsilon_i \end{aligned}$$

- y_i=ozone, x_{1i}=radiation, x_{2i}=temp, x_{3i}=wind and $\varepsilon_i \sim N(0, \sigma^2)$.

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04_Multible regression

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$$
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&+ \beta_6 (x_{2i} \cdot x_{3i}) + \beta_7 (x_{1i} \cdot x_{3i}) + \varepsilon_i
\end{aligned}
$$

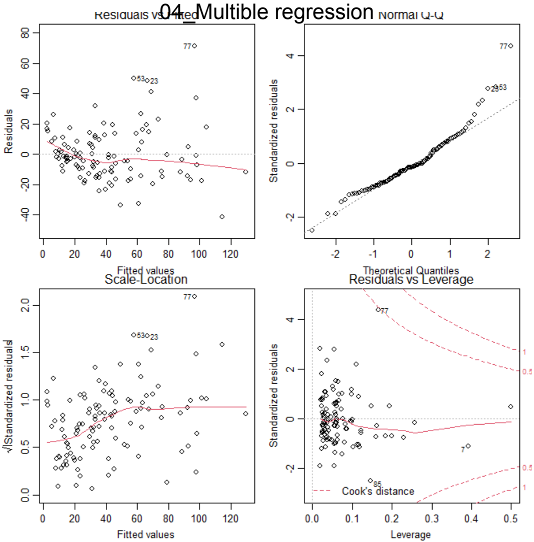
- y_i=ozone, x_{1i}=radiation, x_{2i}=temp, x_{3i}=wind and $\varepsilon_i \sim N(0, \sigma^2)$.
- The next step is to simplify the model
- We must not forget to check the underlying assumptions!

The new model

04_Multible regression

```
reg2 <- lm(ozone ~ rad + temp + wind + I(temp^2) +
             I(wind^2) + temp:wind + rad:wind, data = oz)
summary(reg2)

## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept) 514.40147  193.78358    2.65   0.0092 **
## rad           0.21295    0.06928    3.07   0.0027 **
## temp        -10.65404    4.09489   -2.60   0.0106 *
## wind        -27.39197    9.61700   -2.85   0.0053 **
## I(temp^2)     0.06780    0.02241    3.03   0.0031 **
## I(wind^2)     0.61940    0.14577    4.25  4.7e-05 ***
## temp:wind     0.16967    0.09446    1.80   0.0754 .
## rad:wind     -0.01356    0.00609   -2.23   0.0281 *
##
## Residual standard error: 17.9 on 103 degrees of freedom
## Multiple R-squared:  0.729,Adjusted R-squared:  0.711
## F-statistic: 39.6 on 7 and 103 DF,  p-value: <2e-16
```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Fitted values
Residuals vs Leverage
Standardized residuals
Cook's distance
Leverage

Work with the person next to you

04_Multible regression

- Use the model with interaction.
- What is the expected ozone concentration:
  - If the level of radiation is 100, temperature is 60 and wind speed is 20.
  - If the level of radiation is 185, temperature is 80 and wind speed is 10.
  - If the level of radiation is 185, temperature is 80 and wind speed is 5.

Overview

04_Multible regression

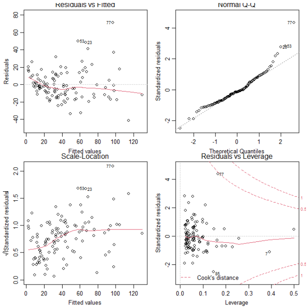
Model Check in detail 04_Multible regression

As in the simple linear regression we must check our model assumptions before we interpret our model too much. We have to check:

- Normal residuals (observed - fitted), using qq-plots.
- Variance homogeneity (one σ^2), residual plots against fitted values.
- Linear effect of $X_1, \dots X_p$, residual plots against each covariate.

Model Check in example 04_Multible regression

```
par(mfrow=c(2, 2))
plot(reg2, which=1:4)
```



- The model check still did not look good!
- Problem with variance homogeneity.

Model Check in example 04_Multible regression

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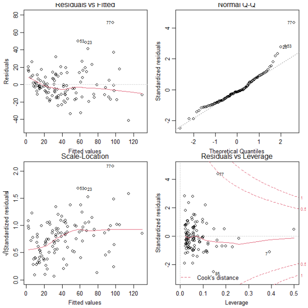
```



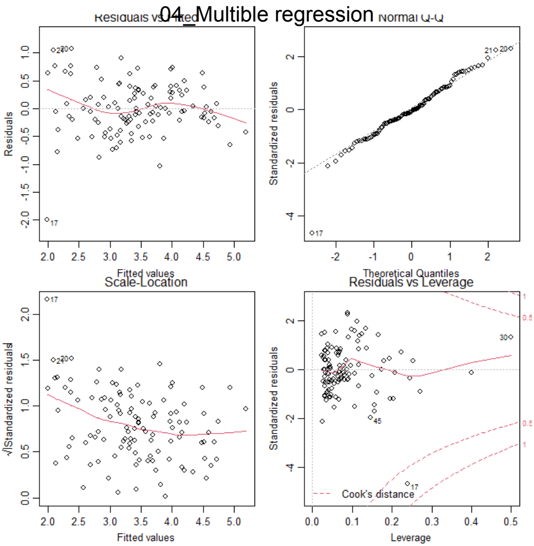
- The model check still did not look good!
- Problem with variance homogeneity.
- What should we do?

New model for log(ozone)

04_Multible regression

- We need to start from scratch with all the original explanatory variables included.
- We would expect the curvature to have changed.
- We can run a new GAM and do a new Tree;
- With just a few explanatory variables, we can also choose brute force and include all 2nd order effects.
- The new starting model should be:

```
reg3 <- lm(log(ozone) ~ rad + temp + wind + I(temp^2) +
             I(wind^2) + I(rad^2) +
             rad:temp + rad:wind +
             temp:wind,data = oz)
```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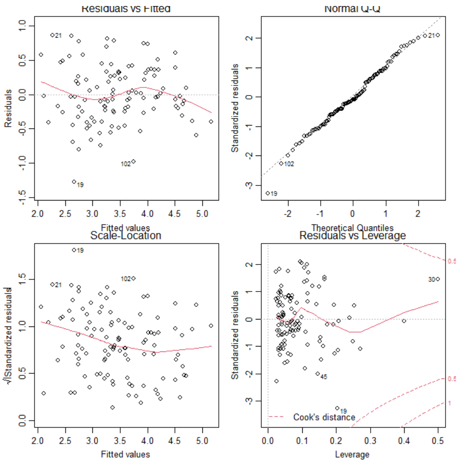
Removing Outlier

04_Multible regression

```
reg3 <- update(reg3, data=oz[-17,])
```



Model Estimates

04_Multible regression

```
summary(reg3)

Coefficients:
               Estimate Std. Error t value Pr(>|t|)
(Intercept)  1.378e+01  5.064e+00   2.721  0.00768 **
rad         -1.670e-05  5.470e-03  -0.003  0.99757
temp        -2.208e-01  1.076e-01  -2.051  0.04287 *
wind        -6.291e-01  2.425e-01  -2.594  0.01092 *
I(temp^2)    1.270e-03  6.014e-04   2.111  0.03725 *
I(wind^2)    1.038e-02  3.608e-03   2.876  0.00493 **
I(rad^2)    -1.353e-05  6.260e-06  -2.161  0.03308 *
rad:temp     9.794e-05  6.208e-05   1.578  0.11780
rad:wind    -3.984e-05  1.552e-04  -0.257  0.79794
temp:wind    4.429e-03  2.385e-03   1.857  0.06628 .
```

Overview

04_Multible regression

Testing

04_Multible regression

- When we finally have a satisfactory starting model then we often want to simplify.
- Sometimes we have specific questions, i.e.
  - Does the crime rate depend on the level of education?
  - Did the intervention make the children eat more healthily?
- Other times we have a lot of variables and are mainly looking for structures in the data.

Model selection

04_Multible regression

- It is not trivial to chose a good starting model. Often it is a combination of theoretical knowledge and/or practical experience, and then the hypotheses we want to test.

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04_Multible regression

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- Sometimes we have a large amount of data with many variables and not much knowledge. Here we will often take a more exploratory approach with some sensible strategies, and an automated approach when looking for a model.
- Be cautious when using automated approaches. If the number of variables is not too large, then it is better to think it through and keep an eye on what is happening.

Model selection

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- It is not trivial to chose a good starting model. Often it is a combination of theoretical knowledge and/or practical experience, and then the hypotheses we want to test.
- Sometimes we have a large amount of data with many variables and not much knowledge. Here we will often take a more exploratory approach with some sensible strategies, and an automated approach when looking for a model.
- Be cautious when using automated approaches. If the number of variables is not too large, then it is better to think it through and keep an eye on what is happening.
- A rule of thumb: The number of parameters in the model should be less than (number of observations)/5.

Backwards and Forwards selection

Backwards

- Start with the largest model, the most complex, and remove variables which are not significant, one at a time. Continue until all variables are significant.

Backwards and Forwards selection

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- Start with the largest model, the most complex, and remove variables which are not significant, one at a time. Continue until all variables are significant.

Forwards

- Start with the model that only includes an intercept. Add a variable one at a time starting with the most significant. Continue until none of the remaining variables are significant.

Tests of main effects and interactions

Never remove a main effect if it is part of an interaction

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Tests of main effects and interactions

Never remove a main effect if it is part of an interaction

In R the function drop1() will help you not to make mistakes.

Never remove a lower order term if it is part of a higher order term

You don't know if there is (evidence of) an interaction unless you look for it

Model reduction in example

04_Multible regression

```
drop1(reg3,test="F")

Single term deletions
Model:
log(ozone) ~ rad + temp + wind + I(temp^2) + I(wind^2) + I(rad^2) +
             rad:temp + rad:wind + temp:wind
          Df Sum of Sq    RSS     AIC F value   Pr(>F)
<none>                 19.020 -173.05
I(temp^2)  1   0.84769 19.867 -170.25  4.4570 0.037253 *
I(wind^2)  1   1.57299 20.593 -166.31  8.2704 0.004925 **
I(rad^2)   1   0.88826 19.908 -170.03  4.6703 0.033077 *
rad:temp   1   0.47342 19.493 -172.35  2.4891 0.117796
rad:wind   1   0.01253 19.032 -174.98  0.0659 0.797937
temp:wind  1   0.65574 19.675 -171.32  3.4477 0.066284 .
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Model reduction in example

04_Multible regression

```
drop1(reg3,test="F")

Single term deletions
Model:
log(ozone) ~ rad + temp + wind + I(temp^2) + I(wind^2) + I(rad^2) +
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          Df Sum of Sq    RSS     AIC F value   Pr(>F)
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I(rad^2)   1   0.88826 19.908 -170.03  4.6703 0.033077 *
rad:temp   1   0.47342 19.493 -172.35  2.4891 0.117796
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temp:wind  1   0.65574 19.675 -171.32  3.4477 0.066284 .
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Notice the use of test="F". We will remove rad:wind.

Model reduction in example


```
reg4 <- update(reg3, ~. -rad:wind)
drop1(reg4, test = "F")

Single term deletions

Model:
log(ozone) ~ rad + temp + wind + I(temp^2) + I(wind^2) + I(rad^2) +
    rad:temp + temp:wind
          Df Sum of Sq    RSS     AIC F value   Pr(>F)
<none>                 19.032 -174.98
I(temp^2)  1   0.83641 19.869 -172.25  4.4387 0.037611 *
I(wind^2)  1   1.56240 20.595 -168.30  8.2914 0.004864 **
I(rad^2)   1   0.88847 19.921 -171.96  4.7150 0.032243 *
rad:temp   1   0.56397 19.596 -173.77  2.9929 0.086687 .
temp:wind  1   0.66581 19.698 -173.20  3.5333 0.063029 .
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Model reduction in example

04_Multible regression

```
reg4 <- update(reg3, ~. -rad:wind)
drop1(reg4, test = "F")

Single term deletions

Model:
log(ozone) ~ rad + temp + wind + I(temp^2) + I(wind^2) + I(rad^2) +
    rad:temp + temp:wind
          Df Sum of Sq    RSS     AIC F value   Pr(>F)
<none>                 19.032 -174.98
I(temp^2)  1   0.83641 19.869 -172.25  4.4387 0.037611 *
I(wind^2)  1   1.56240 20.595 -168.30  8.2914 0.004864 **
I(rad^2)   1   0.88847 19.921 -171.96  4.7150 0.032243 *
rad:temp   1   0.56397 19.596 -173.77  2.9929 0.086687 .
temp:wind  1   0.66581 19.698 -173.20  3.5333 0.063029 .
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

We will remove rad:temp. We will continue like this until all variables are significant

Model reduction in example


```
reg4 <- update(reg4, ~. -rad:temp)
drop1(reg4, test = "F")

Single term deletions

Model:
log(ozone) ~ rad + temp + wind + I(temp^2) + I(wind^2) + I(rad^2) +
    temp:wind
          Df Sum of Sq    RSS     AIC F value   Pr(>F)
<none>                 19.596 -173.77
rad        1   1.58795 21.184 -167.20  8.2655 0.004919 **
I(temp^2)  1   1.27863 20.875 -168.81  6.6554 0.011310 *
I(wind^2)  1   1.60681 21.203 -167.10  8.3636 0.004679 **
I(rad^2)   1   0.69249 20.289 -171.95  3.6045 0.060450 .
temp:wind  1   0.57900 20.175 -172.56  3.0138 0.085580 .
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Model reduction in example

04_Multible regression

```
reg4 <- update(reg4, ~. -rad:temp)
drop1(reg4, test = "F")

Single term deletions

Model:
log(ozone) ~ rad + temp + wind + I(temp^2) + I(wind^2) + I(rad^2) +
    temp:wind
          Df Sum of Sq    RSS     AIC F value   Pr(>F)
<none>                 19.596 -173.77
rad        1   1.58795 21.184 -167.20  8.2655 0.004919 **
I(temp^2)  1   1.27863 20.875 -168.81  6.6554 0.011310 *
I(wind^2)  1   1.60681 21.203 -167.10  8.3636 0.004679 **
I(rad^2)   1   0.69249 20.289 -171.95  3.6045 0.060450 .
temp:wind  1   0.57900 20.175 -172.56  3.0138 0.085580 .
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

We will remove temp:wind.

Model reduction in example

04_Multible regression

```
reg4 <- update(reg4, ~. -temp:wind)
drop1(reg4, test = "F")

Single term deletions

Model:
log(ozone) ~ rad + temp + wind + I(temp^2) + I(wind^2) + I(rad^2)
          Df Sum of Sq    RSS     AIC F value    Pr(>F)
<none>                 20.175 -172.56
rad        1   1.44844 21.623 -166.94  7.3948 0.0076784 **
temp       1   0.33447 20.509 -172.75  1.7076 0.1942126
wind       1   2.32037 22.495 -162.59 11.8462 0.0008361 ***
I(temp^2)  1   0.69977 20.875 -170.81  3.5725 0.0615534 .
I(wind^2)  1   1.09518 21.270 -168.75  5.5913 0.0199242 *
I(rad^2)   1   0.57877 20.754 -171.45  2.9548 0.0886278 .
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Model reduction in example

04_Multible regression

```
reg4 <- update(reg4, ~. -temp:wind)
drop1(reg4, test = "F")

Single term deletions

Model:
log(ozone) ~ rad + temp + wind + I(temp^2) + I(wind^2) + I(rad^2)
          Df Sum of Sq    RSS     AIC F value    Pr(>F)
<none>                 20.175 -172.56
rad        1   1.44844 21.623 -166.94  7.3948 0.0076784 **
temp       1   0.33447 20.509 -172.75  1.7076 0.1942126
wind       1   2.32037 22.495 -162.59 11.8462 0.0008361 ***
I(temp^2)  1   0.69977 20.875 -170.81  3.5725 0.0615534 .
I(wind^2)  1   1.09518 21.270 -168.75  5.5913 0.0199242 *
I(rad^2)   1   0.57877 20.754 -171.45  2.9548 0.0886278 .
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

We will remove the squared effect of rad.

Model reduction in example

04_Multible regression

```
reg4 <- update(reg4, ~. -I(rad^2))
drop1(reg4, test = "F")

Single term deletions

Model:
log(ozone) ~ rad + temp + wind + I(temp^2) + I(wind^2)
          Df Sum of Sq    RSS     AIC F value    Pr(>F)
<none>                 20.754 -171.45
rad        1    4.1707 24.924 -153.31 20.8996 1.339e-05 ***
temp       1    0.2728 21.027 -172.02  1.3669 0.2450244
wind       1    2.3402 23.094 -161.70 11.7269 0.0008827 ***
I(temp^2)  1    0.6390 21.393 -170.12  3.2022 0.0764518 .
I(wind^2)  1    1.0639 21.818 -167.95  5.3312 0.0229249 *
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Model reduction in example

04_Multible regression

```
reg4 <- update(reg4, ~. -I(rad^2))
drop1(reg4, test = "F")

Single term deletions

Model:
log(ozone) ~ rad + temp + wind + I(temp^2) + I(wind^2)
          Df Sum of Sq    RSS     AIC F value    Pr(>F)
<none>                 20.754 -171.45
rad        1    4.1707 24.924 -153.31 20.8996 1.339e-05 ***
temp       1    0.2728 21.027 -172.02  1.3669 0.2450244
wind       1    2.3402 23.094 -161.70 11.7269 0.0008827 ***
I(temp^2)  1    0.6390 21.393 -170.12  3.2022 0.0764518 .
I(wind^2)  1    1.0639 21.818 -167.95  5.3312 0.0229249 *
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

We will remove the squared effect of temp.

Model reduction in example

04_Multible regression

```
reg4 <- update(reg4, ~. -I(temp^2))
drop1(reg4, test = "F")

Single term deletions

Model:
log(ozone) ~ rad + temp + wind + I(wind^2)
          Df Sum of Sq    RSS     AIC F value    Pr(>F)    
<none>                 21.393 -170.12                      
rad        1    3.9973 25.390 -153.27 19.6192 2.325e-05 ***
temp       1   11.5647 32.958 -124.58 56.7617 1.807e-11 ***
wind       1    3.3253 24.718 -156.22 16.3212  0.000102 ***
I(wind^2)  1    1.6759 23.069 -163.82  8.2258  0.004993 ** 
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Model reduction in example

04_Multible regression

```
reg4 <- update(reg4, ~. -I(temp^2))
drop1(reg4, test = "F")

Single term deletions

Model:
log(ozone) ~ rad + temp + wind + I(wind^2)
          Df Sum of Sq    RSS     AIC F value    Pr(>F)    
<none>                 21.393 -170.12                      
rad        1    3.9973 25.390 -153.27 19.6192 2.325e-05 ***
temp       1   11.5647 32.958 -124.58 56.7617 1.807e-11 ***
wind       1    3.3253 24.718 -156.22 16.3212  0.000102 ***
I(wind^2)  1    1.6759 23.069 -163.82  8.2258  0.004993 ** 
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

We will stop the model reduction as all variables are statistically significant.

Words of caution

04_Multible regression

- Do not blindly use automatic stepwise variable selection procedures
- Don't confuse and combine model search and selection with *confirmatory hypothesis testing*; we need a fitting and sensible model for the latter
- The model space is often very large — there may be more than one model that may explain the data equally well
- Always consider the use of interactions, polynomials and transformations; even though you may decide against them in the end.

Words of caution

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- The model space is often very large — there may be more than one model that may explain the data equally well
- Always consider the use of interactions, polynomials and transformations; even though you may decide against them in the end.

Model selection is an art — it takes practice to master

Final Model

04_Multible regression

We have subsequently removed $rad : wind$, $rad : temp$, $temp : wind$, rad^2, and $temp^2$ through backwards selection. Coefficients in final model:

```
Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept)  1.1932358  0.5990022   1.992 0.048963 *
rad          0.0022097  0.0004989   4.429 2.33e-05 ***
temp         0.0419157  0.0055635   7.534 1.81e-11 ***
wind        -0.2208189  0.0546589  -4.040 0.000102 ***
I(wind^2)    0.0068982  0.0024052   2.868 0.004993 **
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Common issues arising in MLR

04_Multible regression

- Differences in the measurement scales of the explanatory variables, leading to large variation in the sums of squares and hence to an ill-conditioned matrix.
    - Can consider **standardizing**, i.e. subtracting the mean and dividing by the standard deviation.
- Multicollinearity, in which there is a near-linear relation between two of the explanatory variables (nearly the same information), leading to unstable parameter estimates.
    - Perhaps choose only one of several colinear variables, or use PCA (Lecture 10)
- Parameter proliferation where quadratic and interaction terms soak up more degrees of freedom than our data can afford.
    - Careful selection of interaction and quadratic terms, for example through the methods discussed today, trees and GAM.

Learning objectives

04_Multible regression

After this session you should be able to:

1. Understand what a *multiple linear regression* (MLR) models is and be able to fit it to data
2. Interpret the result from a *multiple linear regression*
3. Understand and use interactions.
4. Do backwards selection.

Overview

04_Multible regression

2 Exercises for Multiple linear regression

04_Multible regression

1. Process: Understand process loss as a function of other continuous variables
2. Cheese: Describe the taste of matured cheese as a function of chemical descriptors.