

# STK4900/9900 - Lecture 5

## Program

1. Checking model assumptions
    - Linearity
    - Equal variances
    - Normality
    - Influential observations
    - Importance of model assumptions
  2. Selection of predictors
    - Forward and backward selection
    - Criteria for selecting predictors
- Section 4.7
  - Chapter 5: only some main points

## Assumptions for linear regression

$$\text{Model: } y_i = \eta_i + \varepsilon_i$$


  
 systematic part    random part (error)

(1) **Linearity:**  $\eta_i = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \dots + \beta_p x_{pi}$

(2) **Constant variance (homoscedasticity):**  $\text{Var}(\varepsilon_i) = \sigma_\varepsilon^2$  for all  $i$

(3) **Normally distributed errors:**  $\varepsilon_i \sim N(0, \sigma_\varepsilon^2)$

(4) **Uncorrelated errors:**  $\text{Cov}(\varepsilon_i, \varepsilon_j) = 0$  for all  $i \neq j$

We will here focus on the three first assumptions and return to the 4th in the second part of the course

## Fitted values and residuals

Fitted values:  $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_{1i} + \hat{\beta}_2 x_{2i} + \dots + \hat{\beta}_p x_{pi}$

Residuals:  $r_i = y_i - \hat{y}_i$

## Diagnostic – plots of the residuals

Plots of the residuals may be used to check:

- (1) Linearity
- (2) Constant variance
- (3) Normal errors (including outliers)

## (1) Check of linearity

Assume that the correct form of the systematic part of the model is

$$\eta_i = \beta_0 + \beta_1 x_{1i} + \dots + \beta_{j-1} x_{j-1,i} + f_j(x_{ji}) + \beta_{j+1} x_{j+1,i} + \dots + \beta_p x_{pi}$$

i.e. the model is linear in all predictors, except possibly for the  $j$ -th

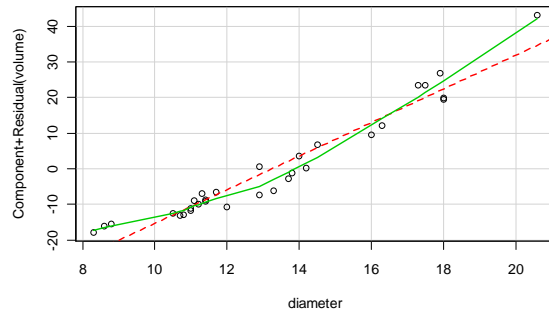
We may estimate the function  $f_j(x)$  based on a plot of the *partial residuals*  $\hat{\beta}_j x_{ji} + r_i$  versus the values of the predictor ( $x_{ji}$ )

In the text book the plot is denoted a component-plus-residual plot (CPR plot)

To obtain a CPR plot in R, we have to use the "car" library

## Example: tree data

We fit a model with volume as outcome and diameter and height as predictors, and make a CPR plot for diameter:

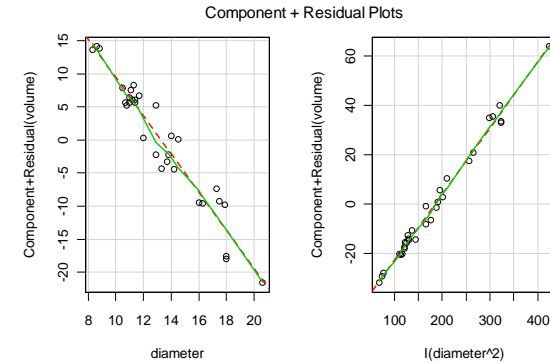


The plot indicates that a second degree polynomial may be more appropriate

```
trees=read.table("http://www.uio.no/studier/emner/matnat/math/STK4900/v11/trees.txt",header=T)
fit.both=lm(volume~diameter+height, data=trees)
library(car)
crPlots(fit.both, terms=~diameter)
```

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We fit a model that also has a second degree term for diameter, and make a CPR plots for diameter and diameter<sup>2</sup>



The plots indicate that the linearity assumption is reasonable both for diameter and diameter<sup>2</sup> (i.e. linearity in the parameters)

```
fit.sq=lm(volume~diameter+I(diameter^2)+height, data=trees)
crPlots(fit.sq, terms=~diameter+I(diameter^2))
```

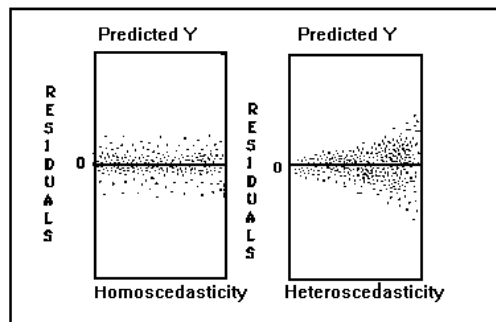
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## (2) Check of constant variance (homoscedasticity)

If the model is correctly specified, there should be no systematic patterns in the residuals

A plot of the residuals versus the fitted (or predicted) values may be used to check the assumption of equal variances

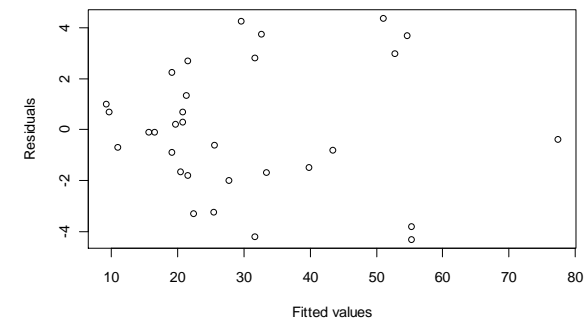
If the variances increase with the expected outcome, the plot will have a fan like shape (like the right hand plot below)



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## Example: tree data

We fit a model with volume as outcome and diameter, diameter<sup>2</sup>, and height as predictors, and plot the residuals versus the fitted values

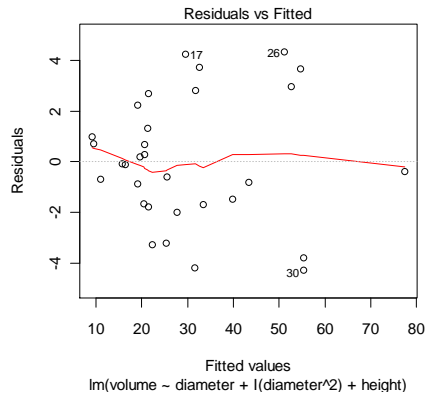


The plot is quite reasonable, but there may be some indication of increasing variances

```
fit.sq=lm(volume~diameter+I(diameter^2)+height, data=trees)
plot(fit.sq$fit, fit.sq$res, xlab="Fitted values", ylab="Residuals")
```

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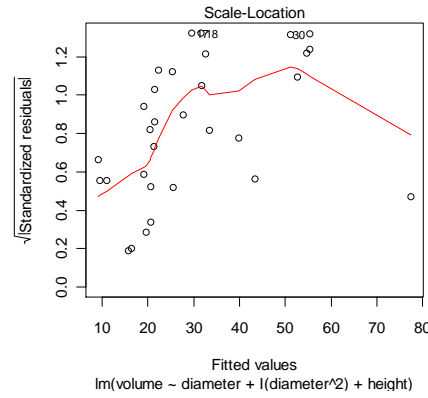
plot(fit.sq,1)



The added line helps to see if there is a pattern in the residuals (which may be due to non-linearities)

The fitted lines may not be trusted where there is little data (i.e. in the right-hand part of the plots above)

plot(fit.sq,3)



The added line helps to see if the variance (or standard deviation) is increasing

### (3) Check of normality

If the model is correctly specified, the residuals should behave as a sample from a normal distribution with mean zero

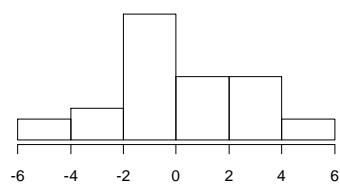
Various plots may be made to check this:

- Histogram of residuals
- Boxplot of residuals
- Normal Q-Q plot of residuals

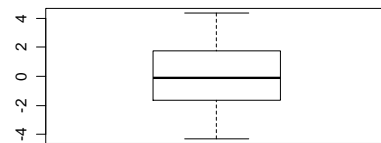
### Example: tree data

We fit a model with volume as outcome and diameter, diameter<sup>2</sup>, and height as predictors, and make different plots of the residuals

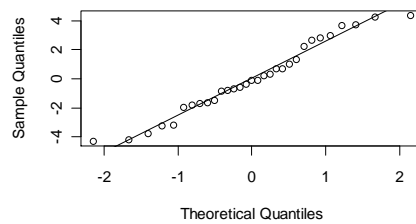
Histogram



Boxplot



Q-Q plot



The Q-Q plot should be close to a straight line if the residuals are normally distributed

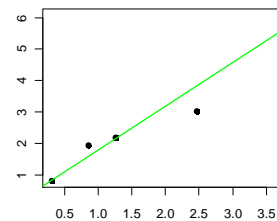
```
hist(fit.sq$res)
boxplot(fit.sq$res)
qqnorm(fit.sq$res); qqline(fit.sq$res)
Alternative: plot(fit.sq,2)
```

### Influential observations

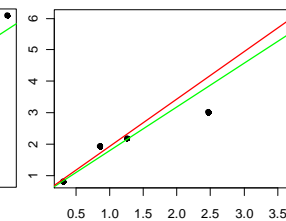
Consider the erosion example:

Amount of water ( <i>l/s</i> )	0.31	0.85	1.26	2.47	3.75
Erosion ( <i>kg</i> )	0.82	1.95	2.18	3.02	6.07

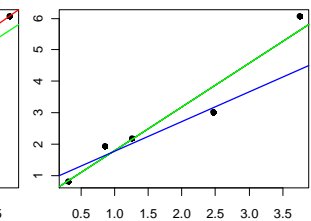
Least squares fit:



Least squares fit without the 4th observation:



Least squares fit without the last observation:



The last observation has a larger influence on the slope estimate than the 4th observation

A measure for the influence of an observation is the change in the estimate(s) when the model is fitted leaving out the observation

These "dfbetas" are easily computed in R:

**R-commands:**

```
fit=lm(erosion~water)
summary(fit)
dfbeta(fit) # dfbetas
```

**R-output (edited):**

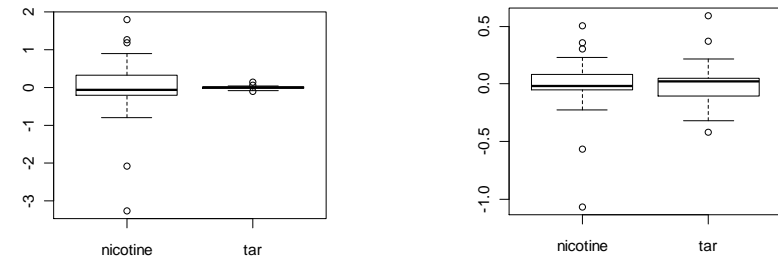
	Estimate	Std. Error
(Intercept)	0.4061	0.4454
water	1.3900	0.2096

**The command**

"dfbetas(fit)" gives standardized dfbetas that may be more appropriate for multiple linear regression when the predictors are on different scales

	water
1	-0.0164
2	0.2066
3	0.0089
4	-0.0362
5	-0.4386

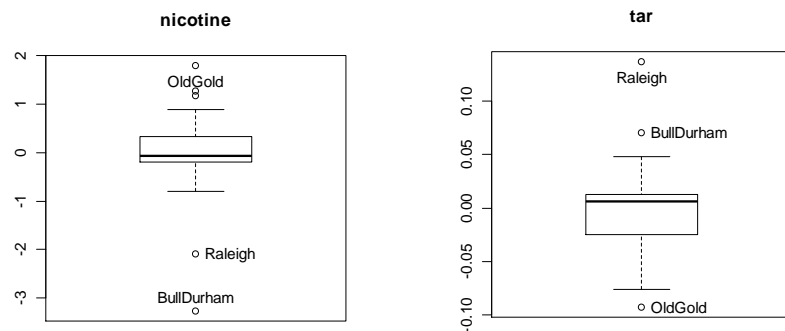
Boxplots of dfbetas (left) and standardized dfbetas (right) for the cigarette data (omitting the intercept, which usually is of less interest)



It may be useful to inspect observations that have a large influence on the estimates

```
cigarettes=read.table("http://www.uio.no/studier/emner/matnat/math/STK4900/v11/cigarettes.txt",
header=T)
fit.cig=lm(CO~nicotine+tar,data=cigarettes)
boxplot(dfbeta(fit.cig))
boxplot(dfbetas(fit.cig))
```

We may use the identify-command to find the cigarette brands that have a large influence on the estimates (for one estimate at a time)



```
R-commands for the the j-th estimate (with j=2, i.e. nicotine)
fit=lm(CO~nicotine+tar,data=cigarettes)
db=dfbeta(fit)
j=2
boxplot(db[,j])
identify(rep(1,dim(db)[1]),db[,j], labels=cigarettes$brand)
```

### The importance of model assumptions

Without linearity of the predictors we have a wrong specification of the systematic part of the model:

- The effect of a predictor may be wrongly estimated
- A predictor may be important, but we do not know
- **Serious nonlinearity jeopardizes the analysis**

If the variances are not equal (and/or the errors are correlated):

- The estimates of the  $\beta_j$ 's will be unbiased
- The standard errors are wrongly estimated
- **Confidence intervals and P-values are flawed**

If the errors are not normal – but the other model assumptions are true:

- Estimates of standard errors are valid
- Test statistics are not exactly t- and F-distributed, but for large  $n$  they are approximately so
- **The distributional assumptions are not critical**

A few influential observations may, however, have large effects on the estimates. How these are treated may be critical for the conclusions on the relations between covariates and response

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## Model misfit and possible improvements

Non-linearity:

- Transform  $x_{ji}$ , e.g.  $\log(x_{ji})$
- Transform  $y_i$ , e.g.  $\log(y_i)$
- Include second order term(s) and/or interaction(s)

Heteroscedasticity:

- Transform  $y_i$ , typically log-transform
- (More advanced: use weighted least-squares or a generalized linear model)

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Non-normality:

- Transform  $y_i$ , e.g.  $\log(y_i)$
- For large  $n$  the problem can be ignored

Influential observations:

- Check the coding of the observations
- Run the regression without the influential observations  
How different are the estimates?

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## Selection of predictors

When there are a number of predictors, a choice has to be made on which ones to include in a regression model

In general we would like to have

- a simple model
- with good empirical fit

These two aims may be conflicting and the trade-off between them may depend on the objectives of the study

**Possible objectives:**

- Study the effect of one predictor while adjusting for the effects of the other predictors (the predictor of main interest should always be included in the model)
- Identify important predictors for an outcome
- Predict the outcome for a new unit where only the values of the predictors are available

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## Sub-models

Consider a model with  $p$  possible predictors:

$$E(y_i | \mathbf{x}_i) = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \dots + \beta_p x_{pi}$$

There are  $2^p$  possible ways to make a sub-model (i.e. a model with some of the predictors)

- For  $p = 10$  there are  $2^p = 1024$  different sub-models
- For  $p = 20$  there are  $2^p \approx 10^6$  different sub-models

For each numeric covariate one may also include e.g. a quadratic term

Further one may take interactions into account

Except for small values of  $p$  it is not feasible to investigate all possible sub-models

We need strategies for deciding which sub-models to consider

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## Forward selection:

1. Fit all  $p$  models with only one predictor
2. Choose the predictor that "contributes most"
3. Run  $p - 1$  regressions with this predictor and another one
4. Choose the model that "fits" best
5. Continue adding predictors until "no improvement"

Since predictors that have been included on an earlier stage need not continue to be important later on, step 4 can be supplemented with deletion of predictors that no longer contribute (stepwise regression)

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## Backward selection:

1. Fit the model with all  $p$  predictors
2. Compare the model with all predictors with the  $p$  different models where one predictor has been left out
3. Leave out the "least important" predictor
4. Compare the model now obtained with the  $p - 1$  different models where one more predictor has been left out
5. Leave out the "least important" predictor
6. Continue in this way until a model is obtained that only contains "important" predictors

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## Criteria for inclusion / exclusion

When using forward or backward selection, one needs a criterion for when to include/exclude a predictor

Different criteria may be used, and the choice between them may depend on the objectives of the study

Some possibilities:

- P-values
- adjusted  $R^2$
- cross-validated  $R^2$

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## P-values

Forward selection:

- include at each step the most significant predictor (lowest P-value)

Backward selection:

- exclude at each step the least significant predictor (largest P-value)

P-values are mainly used when the objective is either

- to study the effect of one predictor while adjusting for the effects of the other predictors
- to identify important predictors for an outcome

Need to decide a cut-off for when to include/exclude a predictor

Often 5% is used, but the text book recommends a more liberal cut-off (combined with backward selection) when the aim is to correct for possible confounders

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## Ordinary R<sup>2</sup>

The coefficient of determination

$$R^2 = \frac{MSS}{TSS} = 1 - \frac{RSS}{TSS}$$

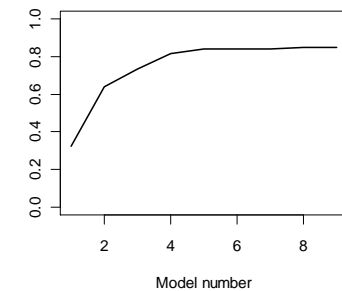
measures the proportion of the total variability in the outcomes that is accounted for by the predictors in the model

It could be tempting to choose the model with the largest R<sup>2</sup>

But then we would end up with a model including all predictors

Example of R<sup>2</sup> from practical exercise 14.e

Maximum for the largest model



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The adjusted R<sup>2</sup>

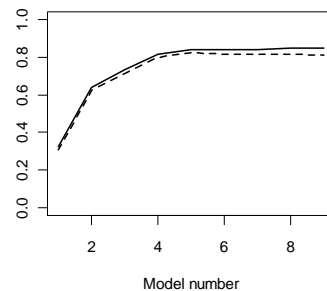
$$R_{\text{adj}}^2 = 1 - \frac{RSS/(n-p-1)}{TSS/(n-1)}$$

penalizes including more predictors

The adjusted R<sup>2</sup> will have a maximum over the different models considered, and it may therefore be used to select predictors

Example of adjusted R<sup>2</sup> from practical exercise 14.e (dashed line)

Maximum for model 5



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## Cross validation

A drawback with R<sup>2</sup> and adjusted R<sup>2</sup> is that the observations are used twice:

- estimate the  $\beta_j$ 's
- evaluate the predictions of the  $y_i$ 's:  
$$\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_{1i} + \hat{\beta}_2 x_{2i} + \dots + \hat{\beta}_p x_{pi}$$

Idea:

- Estimate the regression model without using the observation  $y_i$
- Predict  $y_i$  using the obtained estimates  
Denote this prediction  $\hat{y}_i^{(-i)}$

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## Cross validated $R^2$

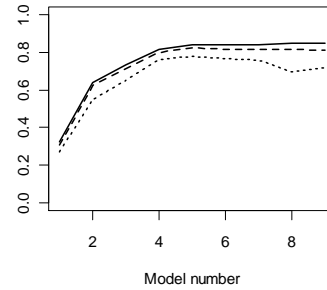
$$R_{cv}^2 = 1 - \frac{\sum_{i=1}^n (y_i - \hat{y}_i^{(-i)})^2}{\sum_{i=1}^n (y_i - \bar{y})^2}$$

The cross-validated  $R^2$  will have a maximum over the different models considered, and it may therefore be used to select predictors

Example of crossvalidated  $R^2$   
from practical exercise 14.e  
(dotted line)

Maximum for model 5, which is the  
same as for the adjusted  $R^2$

But often the cross-validated  $R^2$  will give  
smaller models than the adjusted  $R^2$



We have described "leave-one-out" cross validation.  
Alternative versions of cross-validation exist, e.g. 10-fold cross validation