Module 2: MULTIPLE LINEAR REGRESSION
Week 2
TMA4315 Generalized linear models H2018

Mette Langaas, Department of Mathematical Sciences, NTNU
– with contributions from Øyvind Bakke and Ingeborg Hem

30.08 and 06.09 [PL], 31.08 and 07.09 [IL]

What to remember?

Model:

$$\mathbf{Y} = X\beta + \varepsilon$$

with full rank design matrix. And classical *normal* linear regression model when

$$\varepsilon \sim N_n(\mathbf{0}, \ ^2\mathbf{I}).$$

Parameter of interest is β and σ^2 is a nuisance. Maximum likelihood estimator

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

has distribution: $\hat{\beta} \sim N_p(\beta, \sigma^2(\mathbf{X}^T\mathbf{X})^{-1})$.

Restricted maximum likelihood estimator for σ^2:

$$\hat{\sigma}^2 = \frac{1}{n-p}(\mathbf{Y} - \mathbf{X}\hat{\beta})^T(\mathbf{Y} - \mathbf{X}\hat{\beta}) = \frac{\mathsf{SSE}}{n-p}$$

with $\frac{(n-p)\hat{\sigma}^2}{\sigma^2} \sim \chi^2_{n-p}$.

Statistic for inference about β_j, c_{jj} is diagonal element j of $(\mathbf{X}^T\mathbf{X})^{-1}$.

$$T_j = \frac{\hat{\beta}_j - \beta_j}{\sqrt{c_{jj}}\hat{\sigma}} \sim t_{n-p}$$

This requires that $\hat{\beta}_j$ and $\hat{\sigma}$ are independent.

Inference

We will consider confidence intervals and prediction intervals, and then test single and linear hypotheses.

Confidence intervals (CI)

In addition to providing a parameter estimate for each element of our parameter vector β we should also report a $(1-\alpha)100\%$ confidence interval (CI) for each element. (We will not consider simultanious confidence regions in this course.)

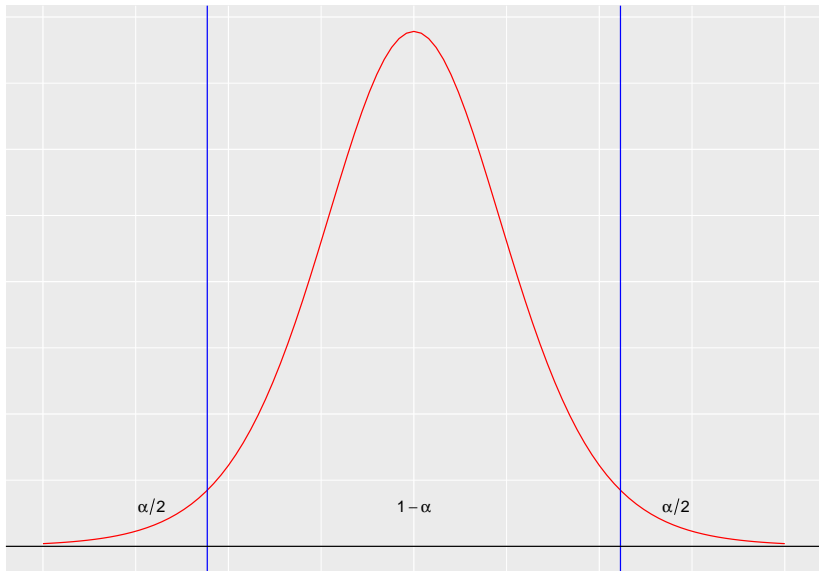We focus on element j of β, called β_j. It is known that

$T_j = \frac{\hat{\beta}_j - \beta_j}{\sqrt{c_{jj}}\hat{\sigma}}$ follows a t-distribution with $n-p$ degrees of freedom.

Let $t_{\alpha/2,n-p}$ be such that $P(T_j > t_{\alpha/2,n-p}) = \alpha/2$.

Since the t-distribution is symmetric around 0, then $P(T_j < -t_{\alpha/2,n-p}) = \alpha/2$. We may then write

$$P(-t_{\alpha/2,n-p} \leq T_j \leq t_{\alpha/2,n-p}) = 1 - \alpha$$

(Blue lines at $\pm t_{\alpha/2, n-p}$.)

Inserting $T_j = \frac{\hat{\beta}_j - \beta_j}{\sqrt{c_{jj}}\hat{\sigma}}$ and solving so β_j is in the middle gives:

$$P(\hat{\beta}_j - t_{\alpha/2, n-p}\sqrt{c_{jj}}\hat{\sigma} \le \beta_j \le \hat{\beta}_j + t_{\alpha/2, n-p}\sqrt{c_{jj}}\hat{\sigma}) = 1 - \alpha$$

A $(1 - \alpha)\%$ CI for β_j is when we insert numerical values for the upper and lower limits: $[\hat{\beta}_j - t_{\alpha/2, n-p}\sqrt{c_{jj}}\hat{\sigma}, \hat{\beta}_j + t_{\alpha/2, n-p}\sqrt{c_{jj}}\hat{\sigma}]$.

CIs can be found in R using `confint` on an `lm` object. (Here
dummy variable coding is used for `location`, with average as
reference location.)

```
library(gamlss.data)
fit = lm(rent ~ area + location + bath + kitchen + cheating
confint(fit)
```

```
##                     2.5 %       97.5 %
## (Intercept) -44.825534    0.8788739
## area          4.354674    4.8029443
## location2    28.579849   49.9405909
## location3    92.970636  159.1443278
## bath1        52.076412   96.0311030
## kitchen1     94.907671  145.9621578
## cheating1   144.427555  178.4000215
```

Prediction intervals

Remember, one aim for regression was to "construct a model to predict the reponse from a set of (one or several) explanatory variables- more or less black box".

Assume we want to make a prediction (of the response - often called Y_0) given specific values for the covariates - often called $\mathbf{x}_0$. An intuitive point estimate is $\widehat{Y}_0 = \mathbf{x}_0^T \widehat{\beta}$ - but to give a hint of the uncertainty in this prediction we also want to present a prediction interval for the Y_0.

First, we assume that the unobserved response at covariate $\mathbf{x}_0$ is independent of our previous observations and follows the same distribution, that is $Y_0 \sim N(\mathbf{x}_0^T\beta, \sigma^2)$. Further,

$$\hat{Y}_0 = \mathbf{x}_0^T\hat{\beta} \sim N(\mathbf{x}_0^T\beta, \sigma^2\mathbf{x}_0^T(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{x}_0).$$

Then, for $Y_0 - \mathbf{x}_0^T\hat{\beta}$ we have

$\mathsf{E}(Y_0 - \mathbf{x}_0^T\hat{\beta}) = 0$ and $\mathsf{Var}(Y_0 - \mathbf{x}_0^T\hat{\beta}) = \mathsf{Var}(Y_0) + \mathsf{Var}(\mathbf{x}_0^T\hat{\beta}) = \sigma^2 + \sigma^2\mathbf{x}_0^T($

so that

$$Y_0 - \mathbf{x}_0^T\hat{\beta} \sim N(0, \sigma^2(1 + \mathbf{x}_0^T(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{x}_0))$$

Inserting our REML-estimate for σ^2 gives

$$T = \frac{Y_0 - \mathbf{x}_0^T\hat{\beta}}{\hat{\sigma}\sqrt{1 + \mathbf{x}_0^T(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{x}_0}} \sim t_{n-p}.$$

Then, we start with

$$P(-t_{\alpha/2,n-p} \leq \frac{Y_0 - \mathbf{x}_0^T \hat{\beta}}{\hat{\sigma}\sqrt{1 + \mathbf{x}_0^T(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{x}_0}} \leq t_{\alpha/2,n-p}) = 1 - \alpha$$

and solve so that Y_0 is in the middle, which gives

$$P(\mathbf{x}_0^T\hat{\beta} - t_{\alpha/2,n-p}\hat{\sigma}\sqrt{1 + \mathbf{x}_0^T(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{x}_0} \leq Y_0 \leq \mathbf{x}_0^T\hat{\beta} + t_{\alpha/2,n-p}\hat{\sigma}\sqrt{1 +$$

A $(1-\alpha)\%$ PI for Y_0 is when we insert numerical values for the upper and lower limits:

$$[\mathbf{x}_0^T\hat{\beta} - t_{\alpha/2,n-p}\hat{\sigma}\sqrt{1 + \mathbf{x}_0^T(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{x}_0}, \mathbf{x}_0^T\hat{\beta} +$$
$$t_{\alpha/2,n-p}\hat{\sigma}\sqrt{1 + \mathbf{x}_0^T(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{x}_0}].$$

PIs can be found in R using `predict` on an `lm` object, but make sure that `newdata` is a `data.frame` with the same names as the original data.

We want to predict the rent - with PI - for an apartment with area 50 m^2, location 2 ("good"), nice bath and kitchen and with central heating:

```
library(gamlss.data)
fit = lm(rent ~ area + location + bath + kitchen + cheating
newobs = rent99[1, ]
newobs[1, ] = c(NA, NA, 50, NA, 2, 1, 1, 1, NA)
predict(fit, newdata = newobs, interval = "prediction", typ
```

```
##        fit      lwr      upr
## 1 602.1298 315.5353 888.7243
```

Questions:
1. When is a prediction interval of interest?
2. Explain the result from `predict` above. What are `fit`, `lwr`, `upr`?
3. What is the interpretation of a 95% prediction interval?

Single hypothesis testing set-up

In single hypothesis testing we are interesting in testing one null hypothesis against an alternative hypothesis. In linear regression the hypothesis is often about a regression parameter β_j:

$$H_0 : \beta_j = 0 \text{ vs. } H_1 : \beta_j \neq 0$$

Remark: we implicitly say that our test is done given that the other variables are present in the model, that is, the other β_is $(j \neq i)$ are not zero.

Two types of errors:

▶ "Reject H_0 when H_0 is true"="false positives" = "type I error" ="miscarriage of justice". These are our *fake news*, which are very important for us to avoid.

▶ "Fail to reject H_0 when H_1 is true (and H_0 is false)"="false negatives" = "type II error"= "guilty criminal go free".

We choose to reject H_0 at some significance level α if the p-value of the test (see below) is smaller than the chosen significance level. We say that : Type I error is "controlled" at significance level α, which means that the probability of miscarriage of justice (Type I error) does not exceed α.

Q: Draw a 2 by 2 table showing the connection between

▶ "truth" (H_0 true or H_0 false) - rows in the table, and
▶ "action" (reject H_0 and accept H_0) - columns in the table,

and place the two types of errors in the correct position within the table.

What else should be written in the last two cells?

Hypothesis test on β_j (t-test)

In linear regression models our test statistic for testing $H_0 : \beta_j = 0$ is

$$T_0 = \frac{\hat{\beta}_j - 0}{\sqrt{c_{jj}}\hat{\sigma}_\varepsilon} \sim t_{n-2}$$

where $c_{jj}\hat{\sigma}_\varepsilon^2 = \widehat{\text{Var}}(\hat{\beta}_j)$.

Inserted observed values (and estimates) we have t_0.

We would in a two-sided setting reject H_0 for large values of abs(t_0). We may rely on calculating a p-value.

The p-value

A p-value is a test statistic satisfying $0 \leq p(\mathbf{Y}) \leq 1$ for every vector of observations $\mathbf{Y}$.

▶ Small values are interpreted as evidence that H_1 is true(-ish).

▶ In single hypothesis testing, if the p-value is less than the chosen significance level (chosen upper limit for the probability of committing a type I error), then we reject the null hypothesis, H_0. The chosen significance level is often referred to as α.

▶ A p-value is *valid* if

$$P(p(\mathbf{Y}) \leq \alpha) \leq \alpha$$

for all α, $0 \leq \alpha \leq 1$, whenever H_0 is true, that is, if the p-value is valid, rejection on the basis of the p-value ensures that the probability of type I error does not exceed α.

▶ If $P(p(\mathbf{Y}) \leq \alpha) = \alpha$ for all α, $0 \leq \alpha \leq 1$, the p-value is called an *exact* p-value.

In our linear regression we use the t-distibution to calculate
p-values for our two-sided test situation $H_0 : \beta_j = 0$
vs. $H_1 : \beta_j \neq 0$. Assume we have observed that our test statistic
T_0 takes the numerical value t_0. Since the t-distribution is
symmetric around 0 we have

$$p\text{-value} = P(T_0 > \text{abs}(t_0)) + P(T_0 < -\text{abs}(t_0)) = 2 \cdot P(T_0 > \text{abs}(t_0)).$$

We reject H_0 if our calculated p-value is below our chosen
signficance level. We often choose as significance level $\alpha = 0.05$.

Munich rent index hypothesis test

We look at print-out using summary from fitting lm.

```
library(gamlss.data)
fit = lm(rent ~ area + location + bath + kitchen + cheating
knitr::kable(summary(fit)$coefficients, digits = 3)
```

	Estimate	Std. Error	t value	$Pr(>|t|)$
(Intercept)	-21.973	11.655	-1.885	0.059
area	4.579	0.114	40.055	0.000
location2	39.260	5.447	7.208	0.000
location3	126.057	16.875	7.470	0.000
bath1	74.054	11.209	6.607	0.000
kitchen1	120.435	13.019	9.251	0.000
cheating1	161.414	8.663	18.632	0.000

Q (and A):

1. Where is hypothesis testing performed here, and which are the hypotheses rejected at level 0.01?

2. Will the test statistics and p-values change if we change the regression model?

3. What is the relationship between performing an hypothesis test and constructing a CI interval? Remember:

```
library(gamlss.data)
fit = lm(rent ~ area + location + bath + kitchen + cheating
confint(fit)

##                   2.5 %      97.5 %
## (Intercept) -44.825534   0.8788739
## area          4.354674   4.8029443
## location2    28.579849  49.9405909
## location3    92.970636 159.1443278
## bath1        52.076412  96.0311030
## kitchen1     94.907671 145.9621578
```

Testing linear hypotheses in regression

We study a normal linear regression model with $p = k + 1$ covariates, and refer to this as model A (the larger model). We then want to investigate the null and alternative hypotheses of the following type(s):

$$
\begin{aligned}
H_0 : \beta_j &= 0 \text{ vs. } H_1 : \beta_j \neq 0 \\
H_0 : \beta_1 &= \beta_2 = \beta_3 = 0 \text{ vs. } H_1 : \text{ at least one of these } \neq 0 \\
H_0 : \beta_1 &= \beta_2 = \cdots = \beta_k = 0 \text{ vs. } H_1 : \text{ at least one of these } \neq 0
\end{aligned}
$$

We call the restricted model (when the null hypotesis is true) model B, or the smaller model.

These null hypotheses and alternative hypotheses can all be rewritten as a linear hypothesis

$$H_0 : \mathbf{C}\beta = \mathbf{d} \text{ vs. } \mathbf{C}\beta \neq \mathbf{d}$$

by specifying $\mathbf{C}$ to be a $r \times p$ matrix and $\mathbf{d}$ to be a column vector of length p.

The test statistic for performing the test is called F_{obs} and can be formulated in two ways:

$$F_{obs} = \frac{\frac{1}{r}(SSE_{H_0} - SSE)}{\frac{SSE}{n-p}} \tag{1}$$

$$F_{obs} = \frac{1}{r}(\mathbf{C}\hat{\beta} - \mathbf{d})^\mathsf{T}[\hat{\sigma}^2\mathbf{C}(\mathbf{X}^\mathsf{T}\mathbf{X})^{-1}\mathbf{C}^\mathsf{T}]^{-1}(\mathbf{C}\hat{\beta} - \mathbf{d}) \tag{2}$$

where SSE is from the larger model A, SSE_{H_0} from the smaller model B, and $\hat{\beta}$ and $\hat{\sigma}^2$ are estimators from the larger model A.

Testing a set of parameters - what is $\mathbf{C}$ and $\mathbf{d}$?

We consider a regression model with intercept and five covariates, $x_1, \ldots, x_5$. Assume that we want to know if the covariates x_3, x_4, and x_5 can be dropped (due to the fact that none of the corresponding β_js are different from zero). This means that we want to test:

$$H_0 : \beta_3 = \beta_4 = \beta_5 = 0 \text{ vs. } H_1 : \text{ at least one of these } \neq 0$$

This means that our $\mathbf{C}$ is a 6×3 matrix and $\mathbf{d}$ a 3×1 column vector

$$\mathbf{C} = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \text{ and } \mathbf{d} \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

Testing one regression parameter

If we set $\mathbf{C} = (0, 1, 0, \cdots, 0)^T$, a row vector with 1 in position 2 and 0 elsewhere, and $\mathbf{d} = (0, 0, \ldots, 0)$, a column vector with 0s, then we test

$$H_0 : \beta_1 = 0 \text{ vs. } H_1 : \beta_1 \neq 0.$$

Now $\mathbf{C}\hat{\beta} = \beta_1$ and $\mathbf{C}(\mathbf{X}^\mathsf{T}\mathbf{X})^{-1}\mathbf{C}^\mathsf{T} = c_{11}$, so that F_{obs} then is equal to the square of the t-statistics for testing a single regression parameter.

$$F_{obs} = (\hat{\beta}_1 - 0)^T [\hat{\sigma}^2 c_{jj}]^{-1} (\hat{\beta}_1 - 0) = T_1^2$$

Repeat the argument with β_j instead of β_1.

Remark: Remember that $T_\nu^2 = F_{1,\nu}$.

Testing "significance of the regression"

If we set $\mathbf{C} = (0, 1, 1, \cdots, 1)^T$, a row vector with 0 in position 1 and 0 elsewhere, and $\mathbf{d} = (0, 0, \dots, 0)$, a column vector with 0s, then we test

$H_0 : \beta_1 = \beta_2 = \cdots = \beta_k = 0$ vs. $H_1 :$ at least one different from zero.

This means we test if at least one of the regression parameters (in addition to the intercept) is different from 0. The small model is then the model with only the intercept, and for this model the SSE_{H_0} is equal to SST (sums of squares total, see below). Let SSE be the sums-of-squares of errors for the full model. If we have k regression parameters (in addition to the intercept) then the F-statistic becomes

$$F_{obs} = \frac{\frac{1}{k}(\mathsf{SST} - \mathsf{SSE})}{\frac{\mathsf{SSE}}{n-p}}$$

with k and $n - p$ degrees of freedom under H_0.

Is the regression significant?

```
summary(fit)$fstatistic
```

```
##      value      numdf      dendf
##   420.0427     6.0000  3075.0000
```

Relation to Wald test

Since $\mathsf{Cov}(\hat{\beta}) = \sigma^2(\mathbf{X}^T\mathbf{X})^{-1}$, then $\mathsf{Cov}(\mathbf{C}\hat{\beta}) = \mathbf{C}\sigma^2(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{C}^T$, so that $\mathbf{C}\hat{\sigma}^2(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{C}^T$ can be seen as an estimate of $\mathsf{Cov}(\mathbf{C}\hat{\beta})$. Therefore, F_{obs} can be written

$$F_{obs} = \frac{1}{r}(\mathbf{C}\hat{} - \mathbf{d})^{\mathsf{T}}[\widehat{\mathsf{Cov}}(\mathbf{C}\hat{\beta})]^{-1}(\mathbf{C}\hat{} - \mathbf{d}) = \frac{1}{r}W$$

where W is a so-called Wald test. It is known that $W \sim \chi_r^2$ asymptotically as n becomes large. We will study the Wald test in more detail later in this course.

It can in general be shown that

$$rF_{r,n-p} \stackrel{n \to \infty}{\longrightarrow} \chi_r^2.$$

That is, if we have a random variable F that is distributed as Fisher with r (numerator) and $n - p$ (denominator) degrees of freedom, then when n goes to infinity (p kept fixed), then rF is approximately χ^2-distributed with r degrees of freedom. Also, if our error terms are not normally distributed then we can assume that when the number of observation becomes very large then $rF_{r,n-p}$ is approximately χ_r^2.

Focus on likelihood: Likelihood ratio test and deviance

The likelihood ratio test

An alternative to the Wald test is the likelihood ratio test (LRT), which compares the likelihood of *two models*.
We use the following notation. A: the larger model and B: the smaller model (under H_0), and the smaller model is nested within the larger model (that is, B is a submodel of A).

▶ First we maximize the likelihood for model A (the larger model) and find the parameter estimate $\hat{\beta}_A$. The maximum likelihood is achieved at this parameter estimate and is denoted $L(\hat{\beta}_A)$.

▶ Then we maximize the likelihood for model B (the smaller model) and find the parameter estimate $\hat{\beta}_B$. The maximum likelihood is achieved at this parameter estimate and is denoted $L(\hat{\beta}_B)$.

The likelihood of the larger model (A) will always be larger or equal to the likelihood of the smaller model (B). Why?

The likelihood ratio statistic is defined as

$$-2 \ln \lambda = -2(\ln L(\hat{\beta}_B) - \ln L(\hat{\beta}_A))$$

(so, -2 times small minus large).

Under weak regularity conditions the test statistic is approximately χ^2-distributed with degrees of freedom equal the difference in the number of parameters in the large and the small model. This is general - and not related to the GLM! More in TMA4295 Statistical Inference!

P-values are calculated in the upper tail of the χ^2-distribution.

Observe: to perform the test you need to fit both the small and the large model.

Notice: asymptotically the Wald and likelihood ratio test statistics have the same distribution, but the value of the test statistics might be different.

```
# TRY OUT BOTH Wald and LRT
```

The LRT can be performed using `anova()`.

Deviance (something new!)

The *deviance* is used to assess model fit and also for model choice, and is based on the likelihood ratio test statistic. It is used for all GLMs in general - and replaces using SSE in multiple linear regression.

Saturated model: If we were to provide a perfect fit to our data t This "imaginary model" is called the *saturated* model. This would be a model where each observation was given its own parameter.

Candidate model: The model that we are investigated can be thought of as a *candidate* model. Then we maximize the likelihood and get $\hat{\beta}$.

The *deviance* is then defined as the likelihood ratio statistic, where we put the saturated model in place of the larger model A and our candidate model in place of the smaller model B:

$$D = -2(\ln L(\text{candidate model}) - \ln L(\text{saturated model}))$$

For the maximal model, we have parameters $\theta_1, \ldots, \theta_n$, where $\theta_i = E[Y_i]$ The log-likelihood for this model is

$$l(\hat{\beta}, \sigma^2) = -\frac{n}{2}\ln(2\pi) - \frac{n}{2}\ln\sigma^2 - \frac{1}{2\sigma^2}(\mathbf{y}-\theta)^T(\mathbf{y}-\theta) = -\frac{n}{2}\ln(2\pi) - \frac{n}{2}\ln\sigma^2$$

(because $\hat{\theta}_i = y_i$, something you may work out for yourselves)

The deviance is then

$$D = -2\left(-\frac{n}{2}\ln(2\pi\sigma^2) - \frac{1}{2\sigma^2}(\mathbf{y} - \mathbf{X}\hat{\beta})^T(\mathbf{y} - \mathbf{X}\hat{\beta}) - (-\frac{n}{2}\ln(2\pi\sigma^2))\right)$$
$$= \frac{1}{\sigma^2}(\mathbf{y} - \mathbf{X}\hat{\beta})^T(\mathbf{y} - \mathbf{X}\hat{\beta})$$

Note the connection with the RSS! Under the null hypothesis that the model fits the data well, $D \sim \chi^2_{n-p}$ exactly (in this case).

Analysis of variance decomposition and coefficient of determination, R^2

It is possible to decompose the total variability in the data, called SST (sums-of-squares total), into a part that is explained by the regression SSR (sums-of-squares regression), and a part that is not explained by the regression SSE (sums-of-squares error, or really residual).

Let $\bar{Y} = \frac{1}{n} \sum_{i=1}^{n} Y_i$, and $\hat{Y}_i = \mathbf{x}_i^T \hat{\beta}$. Then,

$$\text{SST} = \text{SSR} + \text{SSE}$$

$$\text{SST} = \sum_{i=1}^{n} (Y_i - \bar{Y})^2 = \mathbf{Y}^T (\mathbf{I} - \frac{1}{n} \mathbf{1} \mathbf{1}^T) \mathbf{Y}$$

$$\text{SSR} = \sum_{i=1}^{n} (\hat{Y}_i - \bar{Y})^2 = \mathbf{Y}^T (\mathbf{H} - \frac{1}{n} \mathbf{1} \mathbf{1}^T) \mathbf{Y}$$

$$\text{SSE} = \sum_{i=1}^{n} (Y_i - \hat{Y}_i)^2 = \sum_{i=1}^{n} \hat{\varepsilon}_i^2 = \mathbf{Y}^T (\mathbf{I} - \mathbf{H}) \mathbf{Y}.$$

Based on this decomposition we may define the *coefficient of determination* (R^2) as the ratio between SSR and SST, that is

$$R^2 = \text{SSR/SST} = 1 - \text{SSE/SST}$$

1. The interpretation of this coefficient is that the closer it is to 1 the better the fit to the data. If $R^2 = 1$ then all residuals are zero - that is, perfect fit to the data.

2. In a simple linear regression the R^2 equals the squared correlation coefficient between the reponse and the predictor. In multiple linear regression R^2 is the squared correlation coefficient between the observed and predicted response.

3. If we have two models M1 and M2, where model M2 is a submodel of model M1, then

$$R^2_{M_1} \geq R^2_{M_2}.$$

This can be explained from the fact that $\text{SSE}_{M_1} \leq \text{SSE}_{M_2}$. (More in the Theoretical questions.)

Analysis of variance tables - with emphasis on sequential Type I ANOVA

It is possible to call the function `anova` on an `lm`-object. What does that function do?

```
library(gamlss.data)
fit1 = lm(rent ~ area + location + bath, data = rent99)
anova(fit1)
## Analysis of Variance Table
##
## Response: rent
##               Df   Sum Sq  Mean Sq  F value    Pr(>F)
## area           1 40299098 40299098 1668.142 < 2.2e-16 ***
## location       2  1635047   817524   33.841 2.901e-15 ***
## bath           1  1676825  1676825   69.410 < 2.2e-16 ***
## Residuals   3077 74334393    24158
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1
```

What is produced is a *sequential* table of *the reductions in residual sum of squares (SSE) as each term in the regression formula is added in turn*. This type of ANOVA is often referred to as "Type 1" (not to be confused with type I errors).

We can produce the same table by fitting larger and larger regression models.

```
library(gamlss.data)
fit = lm(rent ~ area + location + bath + kitchen + cheating
fit0 <- lm(rent ~ 1, data = rent99)
fit1 <- update(fit0, . ~ . + area)
fit2 <- update(fit1, . ~ . + location)
fit3 <- update(fit2, . ~ . + bath)
```

```
anova(fit0, fit1, fit2, fit3, test = "F")
# anova(fit0,fit1) # compare model 0 and 1 - NOT sequential
# anova(fit0,fit5) # compare model 0 and 5 - NOT sequential

## Analysis of Variance Table
##
## Model 1: rent ~ 1
## Model 2: rent ~ area
## Model 3: rent ~ area + location
## Model 4: rent ~ area + location + bath
##   Res.Df        RSS Df Sum of Sq         F    Pr(>F)
## 1   3081 117945363
## 2   3080  77646265  1  40299098 1668.142 < 2.2e-16 ***
## 3   3078  76011217  2   1635047   33.841 2.901e-15 ***
## 4   3077  74334393  1   1676825   69.410 < 2.2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1
```

If we had changed the order of adding the covariates to the model, then our anova table might also change. You might check that if you want.

See the last page of the classnotes 04.09.2017 for mathematical notation on the sequential test in `anova`, and details on the print-out comes next - NEW: now with formulas!

When running `anova` on one fitted regression the F-test in `anova`
is calculated as for "testing linear hypotheses" - but with a slight
twist. Our large model is still the full regression model (from the
fitted object), but the smaller model is replaced by the *the change
from one model to the next*.

Let SSE be the sums-of-squares-error (residual sums of squares)
from the full (large, called A) model - this will be our denominator
(as always). For our rent example the denominator will be
SSE/(n-p)=64819547/3075 (see above).

The logic is that the full model provides an estimate of σ^2: the
others may not.

For the numerator we are not comparing one small model with the full (large) one, we are instead looking at the change in SSE between two (smaller) models (called model B1 and B2). So, now we have in the numerator the difference in SSE between models B1 and B2, scaled with the difference in number of parameters estimated in model B1 and B2 ="number in B2 minus in B1" (which is the same as the difference in degrees of freedom for the two models).

This means that the test statistics we use are:

$$F_0 = \frac{\frac{\text{SSE}_{B1} - \text{SSE}_{B2}}{\text{df}_{B1} - \text{df}_{B2}}}{\frac{\text{SSE}_A}{\text{df}_A}}$$

Remark: notice that the denominator is just the $\hat{\sigma}^2$ from the larger model A.

This makes our F-test statistic: $f_0 = \frac{40299098/1}{64819547/3075} = 1911.765$ (remember that we swap from capital to small letters when we insert numerical values).

To produce a p-value to the test that

H_0 : "Model B1 and B2 are equally good" vs H_1 : "Model B2 is better t[

and then the $F \sim \text{df}_{B1} - \text{df}_{B2}, \text{df}_A$.

In our example we compare to an F-distribution with 1 and 3075 degrees of freedom. The p-value is the "probability of observing a test statistic at least as extreme as we have" so we calculate the p-value as $P(F > f_0)$. This gives a p-value that is practically 0.

If you then want to use the asymptotic version (relating to a chi-square instead of the F), then multiply your F-statistic with $\text{df}_{B1} - \text{df}_{B2}$ and relate to a χ^2 distribution with $\text{df}_{B1} - \text{df}_{B2}$ degrees of freedom, where $\text{df}_{B1} - \text{df}_{B2}$ is the difference in number of parameters in models B1 and B2. In our example $\text{df}_{B1} - \text{df}_{B2} = 1$.

For the anova table we do this sequentially for all models from starting with only intercept to the full model A. This means you need to calculate SSE and df for models of all sizes to calculate lots of these F_0s. Assume that we have 4 covariates that are added to the model, and call the 5 possible models (given the order of adding the covariates)

▶ model 1: model with only intercept
▶ model 2: model with intercept and covariate 1
▶ model 3: model with intercept and covariate 1 and covariate 2
▶ model 4: model with intercept and covariate 1 and covariate 2 and covariate 3
▶ model 5: model with intercept and covariate 1 and covariate 2 and covariate 3 and covariate 4

Fit a linear model (lm) for each model 1-5, and store SSE and degrees of freedom=df (number of observations minus number of covariates estimated) for each of the models. Call these SSE_1 to SSE_5 and df_1 to df_5.

The anova output has columns: Df Sum Sq Mean Sq F value Pr(>F) and one row for each covariate added to the model.

For example

model 2 vs model 1: Df=df_1-df_2, Sum Sq=SSE_1-SSE_2, Mean Sq=Sum Sq/Df, F value=(Mean Sq)/(SSE_5/df_5)=f_0, Pr(>F)=pvalue=$P(F > f_0)$.

model 3 vs model 2: Df=df_2-df_3, Sum Sq=SSE_2-SSE_3, Mean Sq=Sum Sq/Df, F value=(Mean Sq)/(SSE_5/df_5)=f_0, Pr(>F)=pvalue=$P(F > f_0)$.

In R the p-value is calculated as `1-pf(f0,Df)` or as `1-pchisq(Df*f0,Df)` if the asymptotic chisquare distribution is used.

This is what is presented - a sequential record of the effect of

**Q*: What if you change the order of the covariates into the model?

A competing way of thinking is called *type 3 ANOVA* and instead of looking sequentially at adding terms, we (like in `summary`) calculated the contribution to a covariate (or factor) given that all other covariates are present in the regression model. Type 3 ANOVA is available from library `car` as function `Anova` (possible to give type of anova as input).

Check : Take a look at the print-out from `summary` and `anova` and observe that for our rent data the p-values for each covariate are different due to the different nature of the H_0s tested (sequential vs. "all other present").

If we had orthogonal columns for our different covariates the type 1 and type 3 ANOVA tables would have been equal.

Quality measures

To assess the quality of the regression we can report the R^2 coefficient of determination. However, since adding covariates to the linear regression can not make the SSE larger, this means that adding covariates can not make the R^2 smaller. This means that SSE and R^2 are only useful measures for comparing models with the same number of regression parameters estimated.

If we consider two models with the same model complexity then SSE can be used to choose between (or compare) these models. But, if we want to compare models with different model complexity we need to look at other measures of quality for the regression.

R^2 adjusted (corrected)

$$R^2_{\mathsf{adj}} = 1 - \frac{\frac{SSE}{n-p}}{\frac{SST}{n-1}} = 1 - \frac{n-1}{n-p}(1 - R^2)$$

Choose the model with the *largest* R^2_{adj}.

AIC Akaike information criterion

AIC is one of the most widely used criteria, and is designed for likelihood-based inference. Let $l(\widehat{\beta}_M, \tilde{\sigma}^2)$ be the maximum of the log-likelihood of the data inserted the maximum likelihood estimates for the regression and nuisance parameter. Further, let $|M|$ be the number of estimated regression parameters in our model.

$$\text{AIC} = -2 \cdot l(\widehat{\beta}_M, \tilde{\sigma}^2) + 2(|M| + 1)$$

For a normal regression model:

$$\text{AIC} = n \ln(\tilde{\sigma}^2) + 2(|M| + 1) + C$$

where C is a function of n (will be the same for two models for the same data set). Remark that $\tilde{\sigma}^2 = SSE/n$ - our ML estimator (not our unbiased REML), so that the first term in the AIC is just a function of the SSE. For MLR the AIC and the Mallows Cp gives the same result when comparing models.

Choose the model with the minimum AIC.

BIC Bayesian information criterion.

The BIC is also based on the likelihood (see notation above).

$$\text{BIC} = -2 \cdot l(\widehat{\beta}_M, \tilde{\sigma}^2) + \ln(n) \cdot (|M| + 1)$$

For a normal regression model:

$$\text{BIC} = n \ln(\tilde{\sigma}^2) + \ln(n)(|M| + 1)$$

Choose the model with the minimum BIC.
AIC and BIC are motivated in very different ways, but the final result for the normal regression model is very similar. BIC has a larger penalty than AIC ($\log(n)$ vs. 2), and will often give a smaller model (=more parsimonious models) than AIC. In general we would not like a model that is too complex.

Model selection strategies

▶ All subset selection: use smart "leaps and bounds" algorithm, works fine for number of covariates in the order of 40.

▶ Forward selection: choose starting model (only intercept), then add one new variable at each step - selected to make the best improvement in the model selection criteria. End when no improvement is made.

▶ Backward elimination: choose starting model (full model), then remove one new variable at each step - selected to make the best improvement in the model selection criteria. End when no improvement is made.

▶ Stepwise selection: combine forward and backward.

R packages

```r
install.packages(c("gamlss.data", "tidyverse", "GGally", "N
```

References and further reading

▶ Slightly different presentation (more focus on multivariate normal theory): Slides and written material from TMA4267 Linear Statistical Models in 2017, Part 2: Regression (by Mette Langaas).

▶ And, same source, but now [Slides and written material from TMA4267 Linear Statistical Models in 2017, Part 3: Hypothesis testing and ANOVA] (http://www.math.ntnu.no /emner/TMA4267/2017v/TMA4267V2017Part3.pdf)