STK4900/9900 - Lecture 5

Program

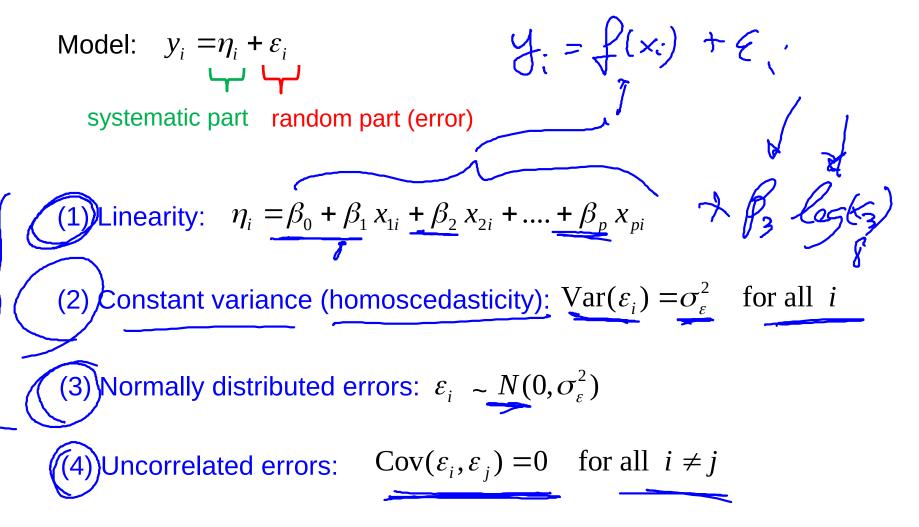
- 1. Checking model assumptions
 - Linearity
- Equal variances
 - Normality
 - Influential observations
 - Importance of model assumptions
 - 2. Selection of predictors
 - Forward and backward selection
 - Criteria for selecting predictors

3. High dimensional regression

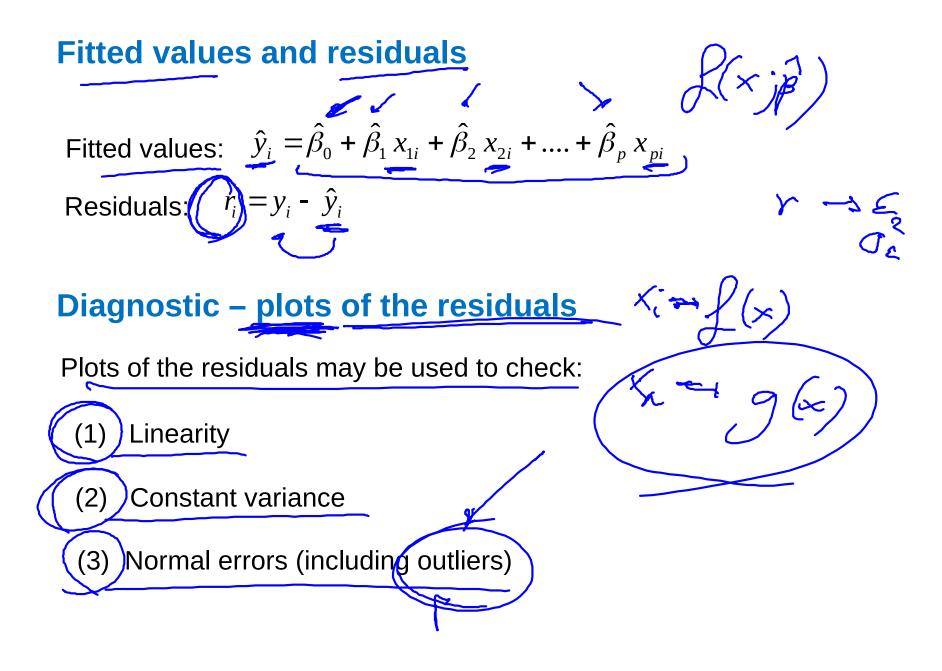
Section 4.7 Chapter 5: only some main points E: N X (O, Ga)

Pa+Fix, +Fix

Assumptions for linear regression



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



(1) Check of linearity

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

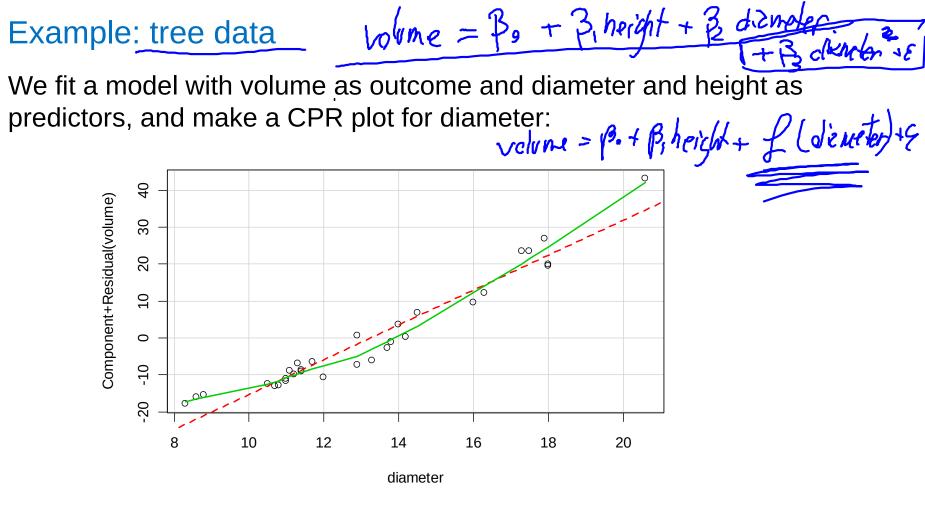
$$\eta_{i} = \beta_{0} + \beta_{1} x_{1i} + \dots + \beta_{j-1} x_{j-1,i} + f_{j}(x_{ji}) + \beta_{j+1} x_{j+1,i} \dots + \beta_{p} x_{pi}$$

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

We may the 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})

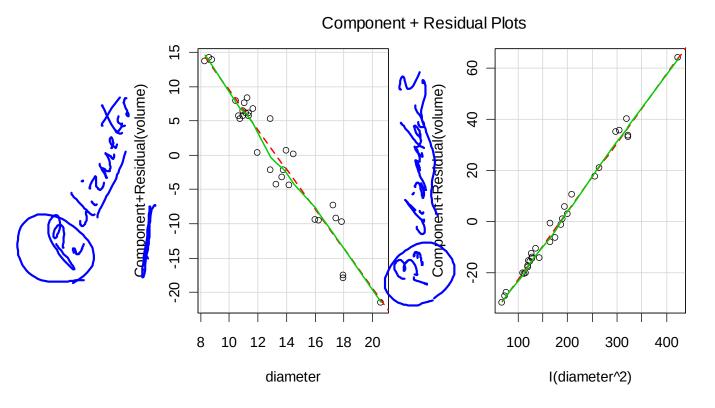
In the text book the plot is denoted a component-plus-residual plot (CPR plot)

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



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

trees=read.table("http://www.uio.no/studier/emner/matnat/math/STK4900/data/trees.txt",header=T) fit.both=lm(volume~diameter+height, data=trees) library(car) crPlots(fit.both, terms=~diameter) We fit a model that also has a second degree term for diameter, and make a CPR plots for diameter and diameter^2



The plots indicate that the linearity assumption is reasonable both for diameter and diameter² (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))

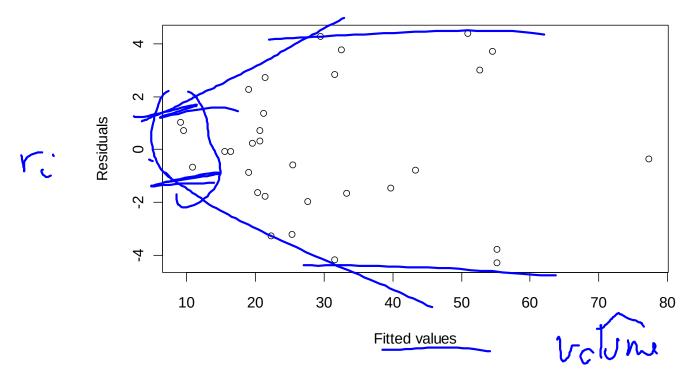
Check of constant variance (homoscedasticity) If the model is correctly specified, there should by no systematic patterns in the residuals A plot of the residuals versus the fitted (or predicted) values may be used to check the assumption of equal variances If the variances increase with the expected outcome, the plot will have a fan like shape (like the right hand plot below) Predicted \ Predicted Y E t١

Homoscedasticity

Heteroscedasticity

Example: tree data

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

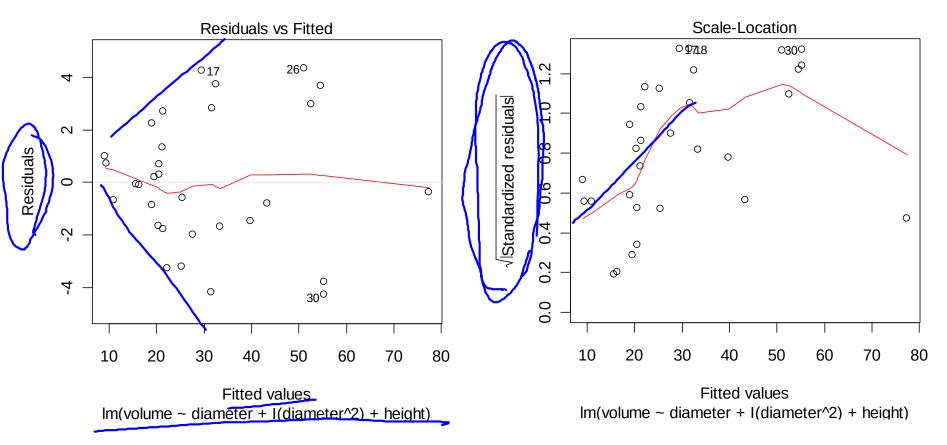


The <u>plot is quite reasonable</u>, but there may be some indication of increasing variances model <- In (volume which be believed in the plot is a laboratory) the indication of the plot is a laboratory in the plot is a laboratory

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

plot(fit.sq,1)

plot(fit.sq,3)



The added line helps to see if there is a pattern in the residuals (which may be due to non-linearities) The added line helps to see if the variance (or standard deviation) is increasing (heteroscedasticity)

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

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

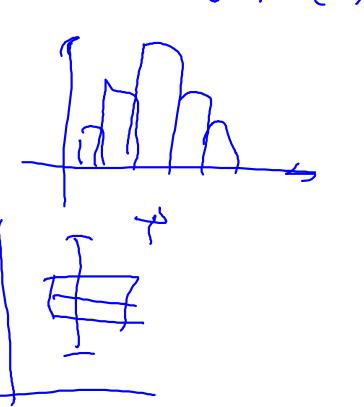
Various plots may be made to check this:

• Histogram of residuals

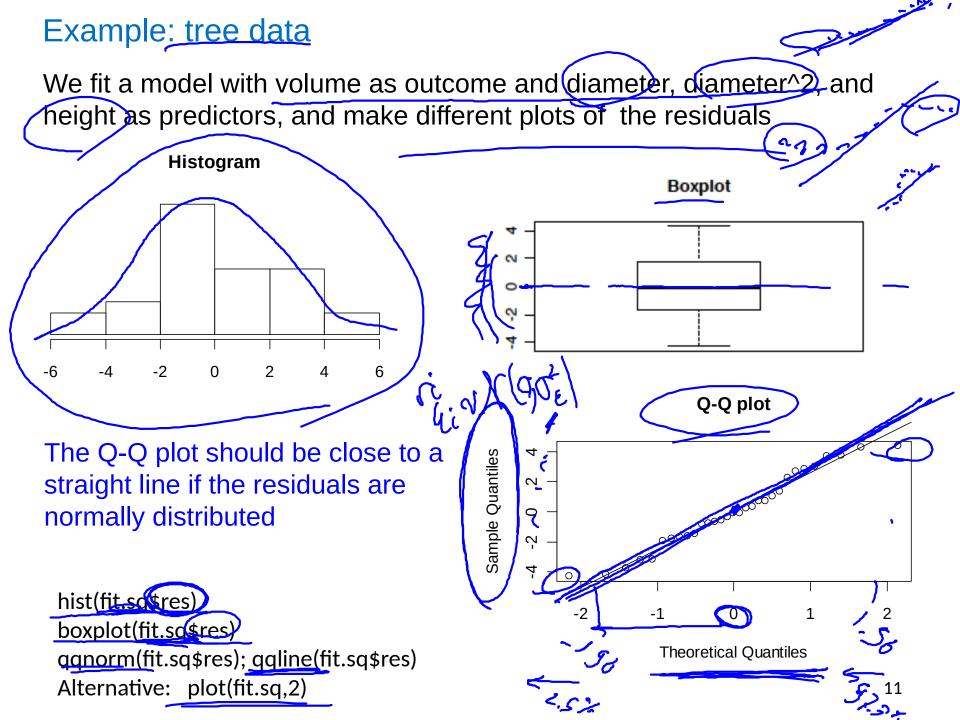
Check of normality

 $(\mathbf{3})$

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



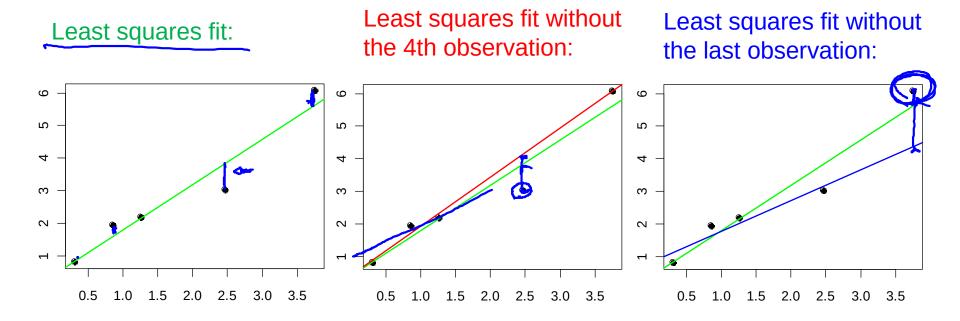
E-N/Q



Influential observations

Consider the	erosion	example:

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

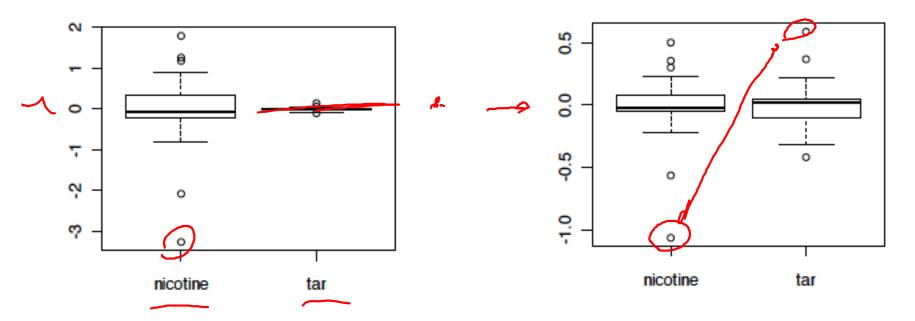


The last observation has a larger influence on the slope estimate than the 4th observation A measure for the influence of an observation is the change in the estimate(s) when the model is fitted leaving out the observation

These "dfbetas" (delete-and-fit-betas) are easily computed in R:

R-commands: fit=lm(erosion~water) summary(fit) dfbeta(fit) # dfbetas	R-output (edited):EstimateStd. Error(Intercept)0.40610.4454water1.39000.2096
The command "dfbetas(fit)" gives standardized dfbetas that may be more appropriate for multiple linear regression when the predictors are on different scales	(Intercept) water 1 -0.0164 0.0059 2 0.2066 -0.0596 3 0.0089 -0.0018 4 -0.0362 -0.1093 5 -0.4386 0.4511

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

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 β_j 's will be unbiased
- The standard errors can be wrongly estimated
- Confidence intervals and P-values can be flawed
- Prediction intervals 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

volume = kh. 42

Non-linearity:

- soume = height i <u>dismeder</u> + diteter 19 (ag (valum) = log (height) + log (dismeter)+9 $\log(x_{ii})$ Transform X_{ji} , e.g.
- $\log(y_i)$ Transform y_i , e.g.
- Include second order term(s) and/or interaction(s)

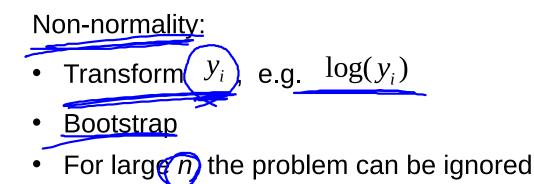
Model misfit and possible improvements

GAM Generalized additive models, 4.10.1, more on slide 20-23)

Heteroscedasticity:

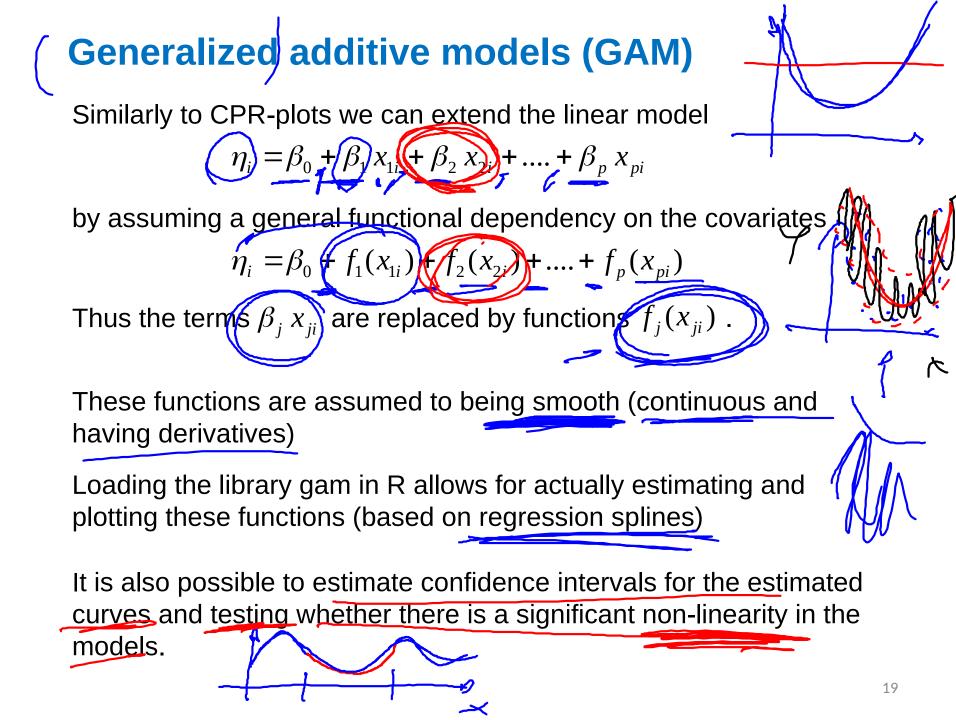
- typically log-transform or root-transform Transform '
- (More advanced: use weighted least-squares or a generalized linear model)

$$\begin{array}{c}
\left(\log\left(y\right) - \frac{1}{B_{n}} + \frac{1}{B_{1}} \times_{1} + \frac{1}{B_{n}} \times_{2} \times_{2} + \frac{1}{B_{n}} \times_{2} \times_{2} + \frac{1}{B_{n}} \times_{2} \times_{$$



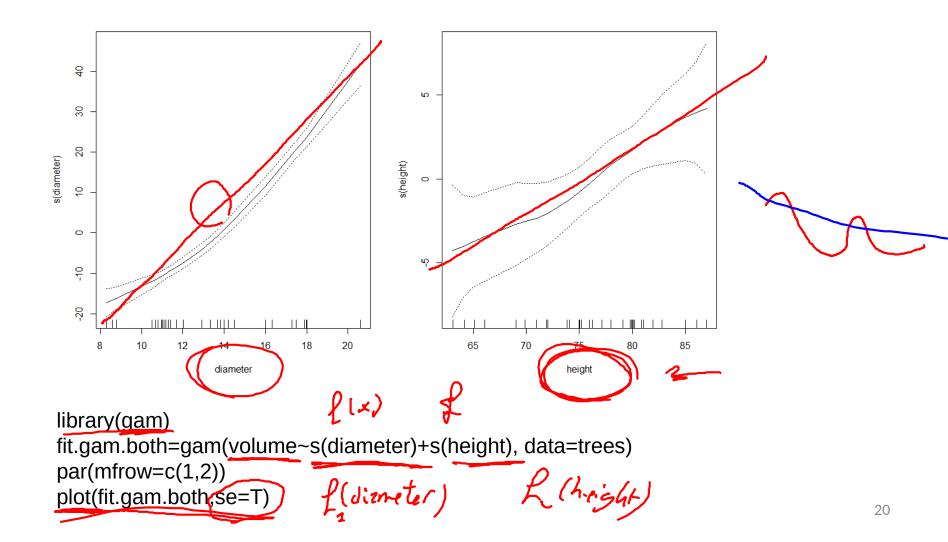
Influential observations:

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



Example GAM: tree data

We fit a model with volume as outcome depending on smooth functions of diameter and height:



Example GAM: tree data (contd)

The functional dependency is specified by writing s(diameter) and s(height) in the model fitting statement. We could (for instance) force the dependency on height to be linear by instead writing

fit.gam.dia=gam(volume~s(diameter)+height, data=trees)

We obtain confidence interval by specifying se=T in the plot command

Here we are not able to force a straight line within the confidence limits for the diameter-function. This indicates that there is a significant non-linearity for this variable.

It is, however, possible to let a straight line go through the intervals for height. This indicates that there is no important non-linearity for this variable.

We can test this more carefully, next slide.

Example GAM: tree data (contd) volume = fi (dizmeter) + f2 (hight) + E

The functional dependency is specified by writing s(diameter) and s(height) in the model fitting statement. We could (for instance) force the dependency on height to be linear by writing s(diameter)+height

Then non-linearities can be tested with standard F-tests:

fit.gam.dia=gam(volume-s)(diameter)+height, data=trees) anova(fit.both,fit.gam.dia,fit.gam.both) Analysis of Variance Table

Model 1: volume ~ diameter + height Model 2: volume \sim s(diameter) + height Model 3: volume \sim s(diameter) + s(height) Res.Df RSS Df Sum of Sq Pr(>F)28 421.92 1 10.13 0.00021 2 25 180.56 3.0000 241.36 3 22 174.73 3.0002 5.84 0.86403 0.24

The non-linearity for diameter is clearly significant, there is no reason to include a non-linear term for height.

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

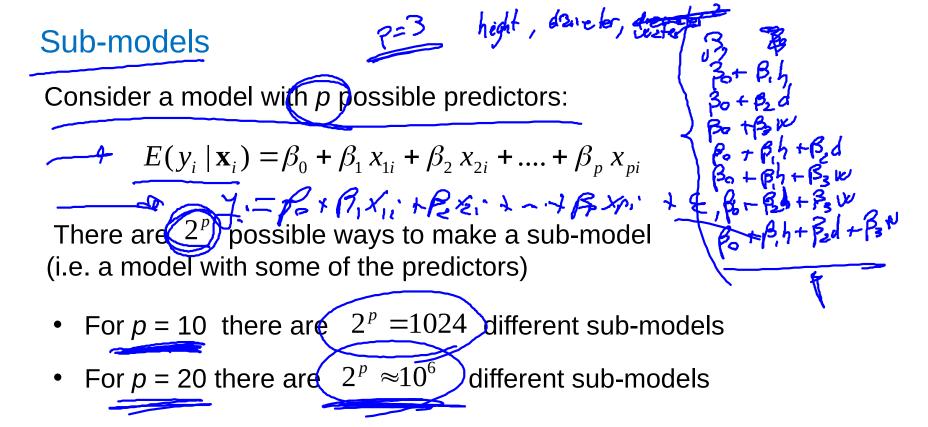
In general we would like to have

- •<u>a simple model</u>
- 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

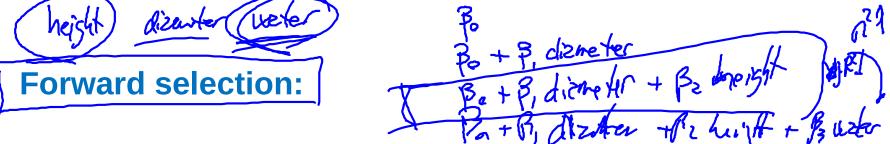


For each numeric covariate one may also include e.g. a quadratic term

Further one may take interactions into account

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

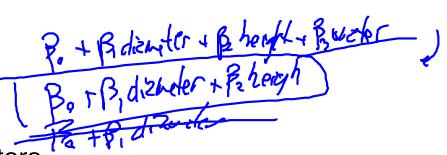
We need strategies for deciding which sub-models to consider



- 1. Fit all *p* models with only one predictor
- 2. Chose 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)

Backward selection:

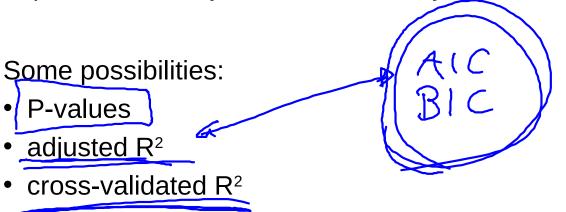


- 1. Fit the model with all *p* predictors
- 2. Compare the model with all predictors with the *p* different models where one predictor has been left out
- 3. Leave out the "least important" predictor
- 4. Compare the model now obtained with the *p* -1 different models where one more predictor has been left out
- 5. Leave out the "least important" predictor
- 6. Continue in this way until a model is obtained that only contains "important" predictors (intercept) 0.81(intercept) 0.0000 (intercept) 0.0000) (intercept) 0.00000) (intercept) 0.0000) (intercept) (

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



P-values

Forward selection:

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

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Backward selection:

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

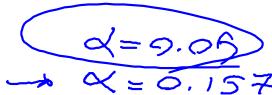
P-values are mainly used when the objective is either

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

P,

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 R²

The coefficient of determination

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

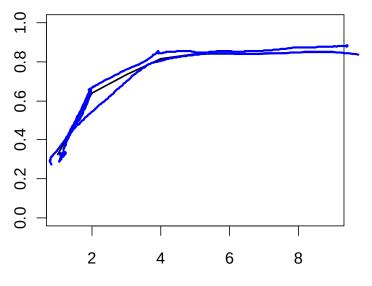
It could be tempting to choose the model with the largest R² But then we would end up with a model including all predictors

RSS

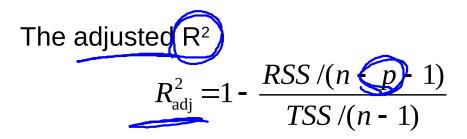
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Example of R² from practical exercise 14.e

Maximum for the largest model



R²1

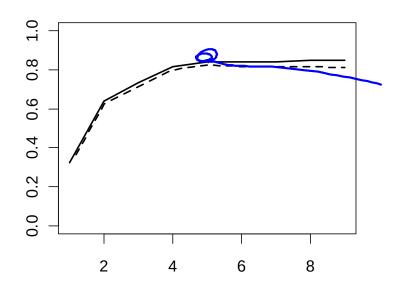


penalizes including more predictors

The adjusted \mathbb{R}^2 will have a maximum over the different models considered, and it may therefore be used to select predictors

Example of adjusted R² from practical exercise 14.e (dashed line)

Maximum for model 5



Cross validation

A drawback with R² and adjusted R² is that the observations are used twice:

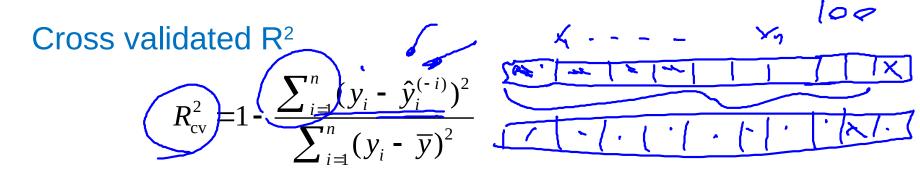
- estimate the β_j 's
- evaluate the predictions of the y_i 's : $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_{1i} + \hat{\beta}_2 x_{2i} + \dots + \hat{\beta}_p x_{pi}$

Idea:

• Estimate the regression model without using the observation y_i

Y3, ×2,

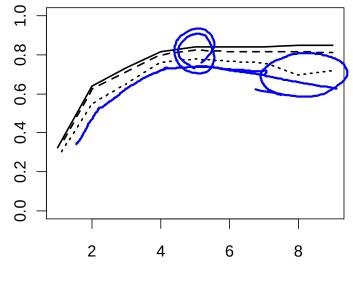
• Predict y_i using the obtained estimates Denote this prediction $\hat{y}_i^{(-i)}$



The cross-validated R² will have a maximum over the different models considered, and it may therefore be used to select predictors

Example of crossvalidated R² from practical exercise 14.e (dotted line)

Maximum for model 5, which is the same as for the adjusted R² But often the cross-validated R² will give smaller models than the adjusted R²



Model number

We have described "l<u>eave-one-out"</u> cross validation. Alternative versions of cross-validation exist, e.g. 10-fold cross validation High-dimensional regression

The regression methods we have studied, require p ≤ n; fewer covariates than observations.

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> High-dimensional regression: p > n; more covariates than observations

Examples: <u>Genomics</u>

p=23.000 gene expressions, or p=1.000.000 SNPs n=200 patients

Astrophysics

p=50.000 stellar
 spectral features
 n=10.000 spectra

Other examples? Psychology, Chemometrics, Marketing ++ 33 Remember the multiple linear regression model:

Data:
$$(y_i, x_{1i}, x_{2i}, ..., x_{pi})$$
 $i = 1, ..., n$
 $y_i = \text{outcome for unit no. } i$
 $x_{ji} = \text{predictor (covariate) no. } j$ for unit no. i
Model:
 $(y_i) = E(y_i | \mathbf{x}_i) + \varepsilon_i$
 $= \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + + \beta_p x_{pi} + \varepsilon_i$
 $\text{systematic part (linear predictor)}$
The least squares estimators from Lecture 3 are not unique when $(p > n)$ We need some regularization to find estimates for the p+1 coefficients!

For p < n, in Ordinary Least Squares (OLS) regression, we are minimizing the MSE

MSE =
$$(y - X_0\beta_0 - X_1\beta_1 - \dots - X_p\beta_p)^2 = (y - X\beta)^2$$

resulting in

$$\hat{\beta} = \operatorname{argmin}_{\beta} \left(y - X\beta \right)^2$$

We can constrain the regression coefficients in order to stabilize estimation and shrink or even eliminate the coefficients of unimportant predictors. Works also when p > n!

$$L_{2} \text{ penalty } \hat{\beta} = \operatorname{argmin}_{\beta} (y - X\beta)^{2} + \lambda \|\beta\|_{2}^{2} \text{ Ridge}$$

$$Penalty \text{ parameter}$$

$$L_{1} \text{ penalty } \hat{\beta} = \operatorname{argmin}_{\beta} (y - X\beta)^{2} + \lambda \|\beta\|_{1} \text{ Lasso}$$

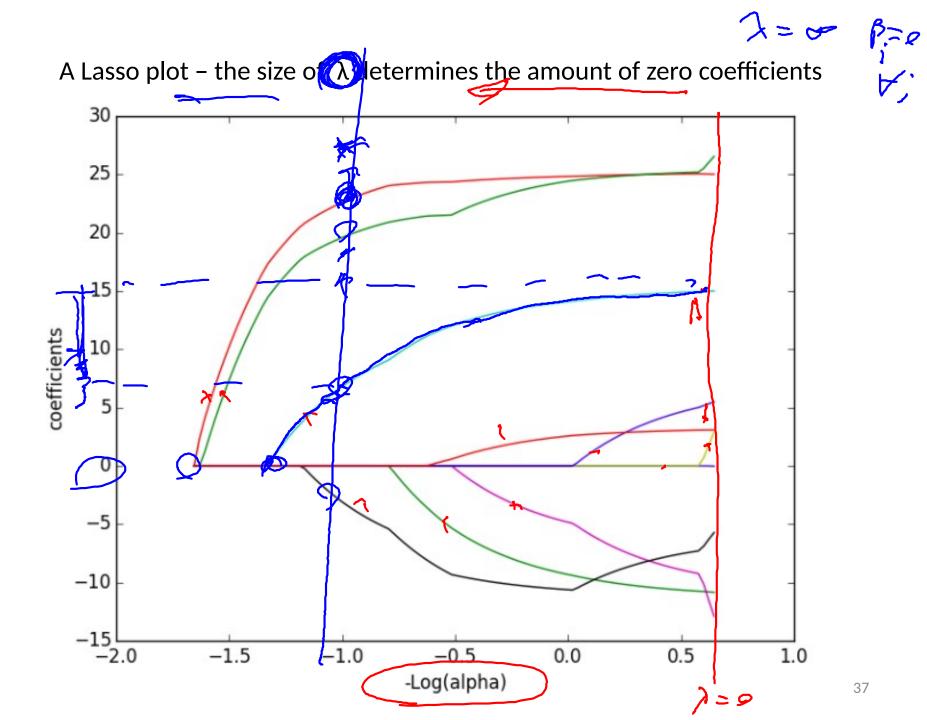


$$PRSS_{\lambda}^{lasso}(\beta) = \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j \right)$$

Smiller get A Salition

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- Lasso leads to shrinkage of the coefficients, but even more important, it zeros out the coefficients of the unimportant variables variable selection!
- This is due to the shape of the L1 penalty
- Challenging optimization problem, several fast algorithms



Ridge regression

$$PRSS_{\lambda}^{ridge}(\beta) = \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij} \beta_j \right)^2 + \lambda \sum_{j=1}^{p} \beta_j^2$$

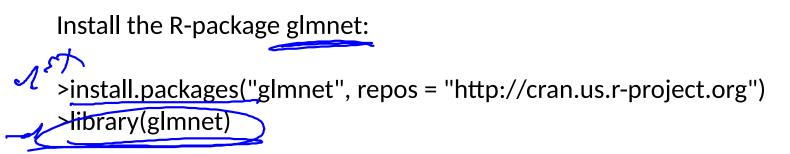
 β_1

5

- Ridge regression only shrinks the coefficients, introducing bias, but reducing variance of the estimators.
- No variable selection



Lasso assumes what we call *sparsity*: That only a few of the p covariates matter. If sparsity is true, Lasso will recover it (theorems etc Norks very well night be chosen by the data via (K-fold) Cross Validation. Lasso and/or Ridge in R: Recommend the package glmnet (incl. linear, logistic, Poisson, Cox regression) ea Cri X e105



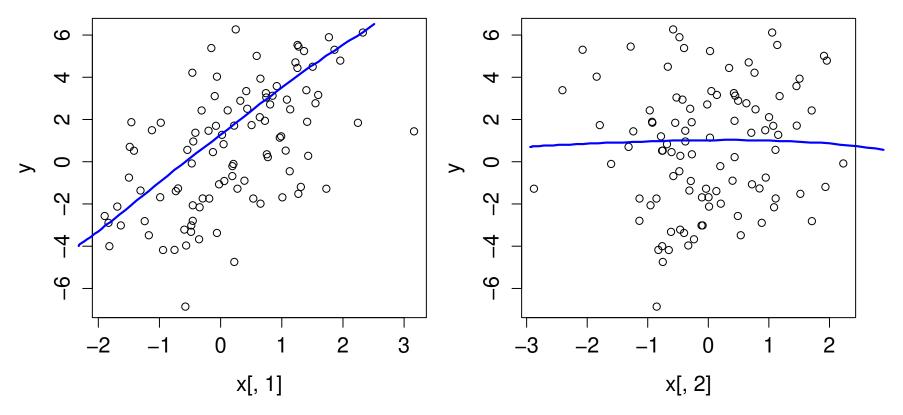
Data should be organized in a vector \mathbf{y} (n x 1) (the response variable) and a matrix \mathbf{x} (n x p) (the p predictor variables)

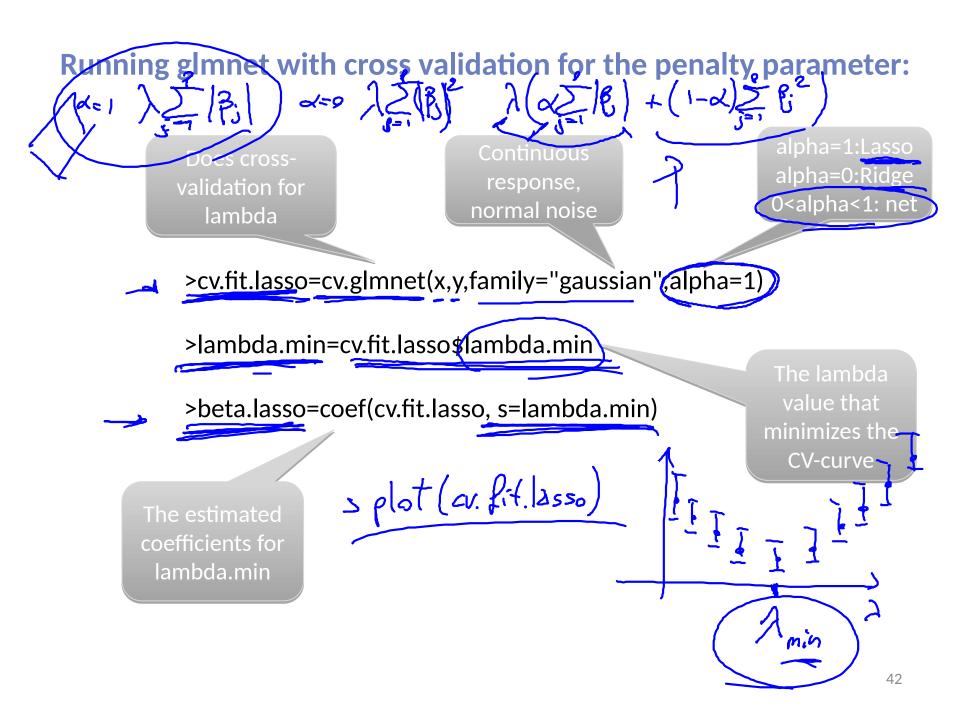
💽 gl	mnet_start.R 🗙	x ×					
$\langle \phi d \rangle$							
	V1	V2	V3	V4	V5	V6	V7
1	0.27385621	-0.036672202	0.85472694	0.967524215	1.41548975	0.52340587	0.56268818
2	2.24481689	-0.546030016	0.23406507	-1.335030427	1.31307582	0.52127458	-0.6100346
3	-0.12542303	-0.606878202	-0.85392169	-0.148777203	-0.66468279	0.60661641	0.16172065
4	-0.54357344	1.108358273	-0.10424799	1.016526228	0.69990418	1.65501642	0.48996346
5	-1.45939839	-0.274494523	0.11190596	-0.851787700	0.31528387	1.05074928	1.38635753
6	1.06320807	-0.753523175	-1.38255341	1.076226985	0.37003310	1.49872124	-0.3604525
7	0.11584499	-0.966302384	0.27417918	0.018531025	-0.21038723	0.54408945	-2.5054893
2	0.38970673	0.399794284	-0.46666982	0.477628120	0.84829129	0.25743529	-0.0994948

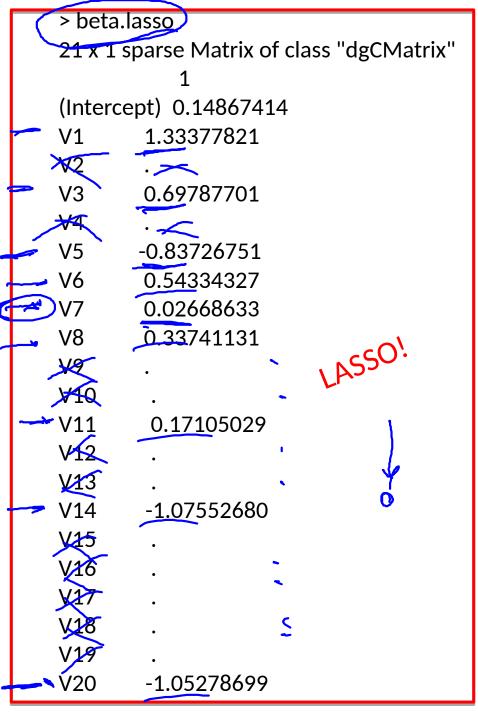
This is a piece of an example of a data matrix \mathbf{x} , with 20 predictors measured for 100 subjects (so here p < n, for comparison with OLS)

/gimnet	mnet_start.R 🗶	x x y x -
$\langle \mathbf{r} \mathbf{c} \rangle$	1	100 observations of 1 variables
	V1	
1	-1.27488603	And this is the corresponding y
2	1.84342510	And this is the corresponding y ,
3	0.45923632	with 100 responses
4	0.56404074	
5	1.87296326	
6	0.52753173	
7	2.43465887	
Q	-0 89459612	Two first predicto

dictors:







	OLS	
	Estimate Pr(> t)	
(Interce	pt) 0.109068 0.347598	
x1	<u>1.38</u> 1072 < 2e-16 ***	_:
x2	0.025016 0.811399	ŭ
х3	0.767490 9.68e-10 ***	no
x4	0.066767 0.537749	с Г
x5	-0.905978 7.07e-12 ***	þ
x6	0.618388 2.28e-08 ***	OLS cannot be found!
x7	0.124492 0.248793	Ĕ
x8	0.401052 0.000138 ***	car -
x9	-0.036556 0.732835	S S
x10	0.136530 0.212670 🕚	С
x11	0.251597 0.026115 *) e
x12	-0.069913 0.532250	Æ
x13	-0.049396 0.660097	C
x14	-1.164018 < 2e-16 ***	^
x15	-0.147334 0.254664	19
x16	-0.051572 0.644480	ō
x17	-0.055904 0.597418	<u> </u>
x18	0.057081 0.591626	NB
x19	-0.006423 0.944577	~
x20	-1.148534 2.08e-14 ***	40
		43

