



Statistical Modeling

CH.3 - Regression Diagnostics

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Outline

1 Organizational Information

2 Regression Diagnostics

Course Contents

Chylin		
Session	Торіс	
1	Simple Linear Regression	
2	Multiple Linear Regression	
3	Regression Diagnostics (
4	Qualitative Variables as Predictors	
5	Transformation of Variables	
6	Weighted Least Squares	
7	Correlated Errors	
8	Analysis of Collinear Data	
9	Working with Collinear Data	
10	Variable Selection Procedures	
11	Logistic Regression	
12	Further Topics	

Outline

1 Organizational Information

2 Regression Diagnostics

Introduction

- In this chapter we talk about the standard regressions assumptions, the consequences when violating them and how to detect violations so that we can focus on the remainder of the course on methods of how to correct or compensate for violations.
- When those assumptions are violated, the discussed and derived results for making inferences about the regression coefficients do not hold, which essentially means that conclusions drawn on the corresponding models are wrong.
- The majority of the discussed methods are graphical methods which means that they may be somewhat subjective here or there, which needs to be kept in mind when interpreting diagnostic plots.

Overview

- Assumptions about the form of the model.
- 2 Assumptions about the errors.
- 3 Assumptions about the predictors.
- 4 Assumptions about the observations.

The properties of the least squares estimators (BLUE) are based on the discussed assumptions!

Assumption 1: Model

The model that relates Y and X_1, X_2, \ldots, X_p is assumed to be linear in the regression parameters $\beta_0, \beta_1, \ldots, \beta_p$ so that

Model:
$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + ... + \beta_p X_p + \epsilon$$

Observation: $y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + ... + \beta_p x_{ip} + \epsilon_i, i = 1, 2, ..., n$

- This assumption is called the linearity assumption.
- In simple linear regression checking can be done using a scatterplot of Y versus X. For multiple linear regression there are other plotting techniques which we will discuss.
- When the linearity assumptin does not hold, transforming the data may lead to linearity (<u>Transformations are</u> discussed at a later point).

Assumption 2: Errors



- The errors $\epsilon_1, \epsilon_2, \dots, \epsilon_n$ are assumed to be **independently and identically distributed** (iid) normal random variables each with mean zero and commonor variance σ^2 This implies:
 - Normality Assumption: The error ϵ_i , i = 1, 2, ..., n has a normal distribution.
 - The errors $\epsilon_1, \epsilon_2, \ldots, \epsilon_n$ have mean zero.
 - **Constant Variance Assumption:** The errors have the same (but unknown) variance σ^2 . When this assumtion does not hold we have the heteroscedasticity problem.
 - Independent errors Assumption: $\epsilon_1, \epsilon_2, \dots, \epsilon_n$ are independent of each other (pairwise covariances are zero). Violations lead to the *autocorrelation problem*.

Assumption 3: Predictors

- Thre are three assumptions for the predictor variables.
 - The predictor variables X_1, X_2, \ldots, X_p are **nonrandom**. This means the values $x_{1j}, x_{2,j}, \ldots, x_{nj}$ with $j = 1, 2, \ldots, p$ are fixed (which is usually only fully satisfied under experimental conditions). In practice the results presented hold, but results are conditional on the data.
 - The values $x_{1j}, x_{2,j}, \ldots, x_{nj}$ are measured without error (which is hardly ever satisfied). In practice it is sufficient, when the measurement error is small compared to the random error ϵ_i .
 - The predictor variables X_1, X_2, \ldots, X_p arre assumend to be linaerly independent of each other. This assumtion guarantees the uniqueness of the lest squares solution. If this assumption is violated this is to refeered as the *collinearity problem*.

The first two assumptions cannot be checked and do not play a role in our analysis. They have to be kept in mind when collecting data.

Assumption 4: Observations

All observations are equally reliable and have an approximately equal role in determining the regression results. This means that they are equally relied on when drawing conclusions.

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Conclusion

Small or minor violations of the underlying assumptions do not invalidate the inferences or conclusions drawn from the analysis. Gross validations, however, can seriously distort conclusions. It is essential to investigate all signs of assumption validations by *always* checking the structure of the residuals and the data patterns at least using graphs!

- Analysing residuals is a simple and effective method for detecting model deficiencies in regression analysis. In most analysis it is probably the most important part of an analysis.
- Residual plots may lead to suggestiosn fo structure or point to information in the data tha tmight be missed or overlooked. Those clues can lead to a better understanding (and possibly a better model) of the underlying process.
- Starting point for the analysis are the ordinary least squares residuals that can be calculated after obtained the fitted values:

$$\hat{y}_{i} = \frac{\hat{\beta}_{0} + \hat{\beta}_{1}x_{i1} + \hat{\beta}_{2}x_{i2} + \ldots + \hat{\beta}_{p}x_{ip}}{e_{i} = y_{i} - \hat{y}_{i}} \text{ for } i = 1, 2, \ldots, n$$

The fitted values can also be written as function of the predictor variables, where p_{ij} only depends on the predictor variables (essentially values from the hat matrix P).

$$\hat{y}_i = p_{i1}y_1 + p_{i2}y_2 + ... + p_{in}y_n$$

When i = j the value prepresents the weight (leverage) given to y_i in determining the i-th fitted value \hat{y}_i . The n leverage values p_1, p_2, \dots, p_n can be obtained by

$$p_{ii} = \underbrace{\frac{1}{n}}_{+} + \underbrace{\frac{(x_i - \bar{x})^2}{\sum (x_i - \bar{x})^2}}_{-}$$



A high laverage value indicates some "extremeness" in X.

- The ordinary least squares residuals e_1 , e_2 , ..., e_p do not have unequal variances $Var(e_i) = \sigma^2(1 p_{ii})$. Analyzing requires standardized residuals by calculating
 - by calculating $z_i = \frac{1}{2}$
- This requires an unbiased estimate for the unknown standard deviation σ of ϵ for which we have two unbiased estimates to choose from

$$\hat{\sigma}^2 = \frac{\sum e_i^2}{n - p - 1} = \frac{SSE}{n - p - 1} \quad \text{with} \quad \hat{\sigma}_{(i)}^2 = \frac{SSE_{(i)}}{(n - 1) - p - 1} = \frac{SSE_{(i)}}{n - p - 2}$$

■ $SSE_{(i)}$ is the sum of squared residuals when the *i*-th observation is left out so that the model is fitted using n-1 observations.

The choice of variance estimates results in two different types of residuals, although both are unbiased estimates.

Internally studentized residuals (using $\hat{\sigma}^2$)

$$r_i = \frac{e_i}{\hat{\sigma}\sqrt{1 - p_{ii}}}$$
 with $\hat{\sigma}^2 = \frac{SSE}{n - p - 1}$

Externally studentized residuals (using $\hat{\sigma}_{(i)}^2$)

$$r_i^* = \frac{e_i}{\hat{\sigma}_{(i)}\sqrt{1-p_{ii}}}$$
 with $\hat{\sigma}_{(i)}^2 = \frac{SSE_{(i)}}{n-p-2}$

Called externally studentized because \hat{e}_{i} not involved in (external to $\hat{\sigma}$



Graphical Methods

Dimensionality:

- One-dimensional graphs, inidcate the distribution of a particular variable (e.g. symmetry, skewedness) and allow identification of outliers.
- Two-dimensional graphs allow exploration of relationships (by pairing variables) and general patterns.

Step in Model Selection Process:

- Graphs before fitting a model, to e.g. correct data errors, seelect variables and preparation for model selection.
- Graphs after fitting a model to check assumptions and assessing the goodness of fit.

Example: Hamiltons Data

P103

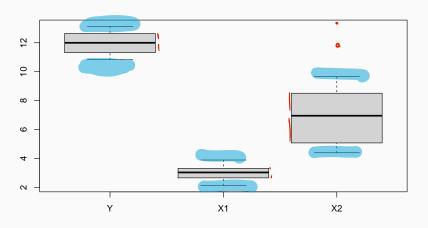
```
##
          Υ
              Х1
                   X2
      12.37 2.23 9.66
      12.66 2.57 8.94
   2
     12.00 3.87 4.40
     11.93 3.10 6.64
   5
     11.06 3.39 4.91
     13.03 2.83 8.52
     13.13 3.02 8.04
   8
     11.44 2.14 9.05
     12.86 3.04 7.71
   10 10.84 3.26 5.11
   11 11.20 3.39 5.05
   12 11.56 2.35 8.51
   13 10.83 2.76 6.59
   14 12.63 3.90 4.90
   15 12.46 3.16 6.96
```

Graphs before fitting a Model

- 1 Boxplot
- 2 Histogram
- 3 Pairsplot

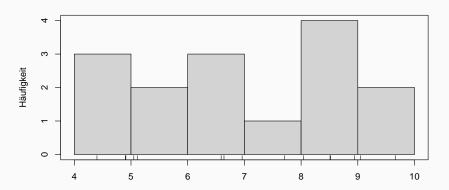
Boxplot

boxplot(P103)

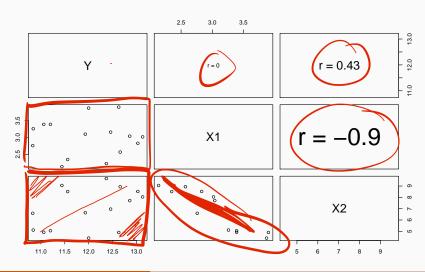


Histogram

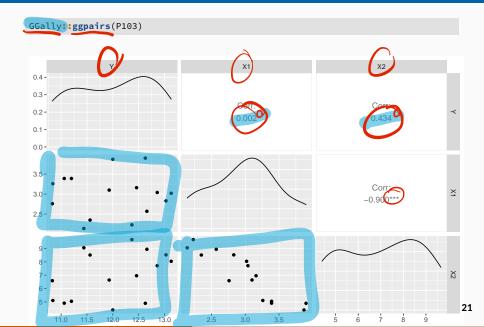
```
hist(P103$X2, main = "", ylab = "Häufigkeit", xlab = "")
rug() 103$X2)
box()
```



pairs(P103, upper.panel=panel.cor)



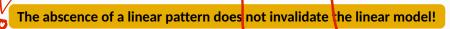
Pairsplot



Pairsplot

Interpretation:

- The pairwise correlation should always be interpreted in conjunction with the scatter plots.
 - The correlation coefficients only measures **linear** dependence.
 - The correlation coefficient is non-robuts and may be substantially influenced by few data points.
- The appearence of the scatter plot only serves as an indication of the results to be expected.
 - In simple linear regression the plot of Y and X is expected to show a linear pattern.
 - In mulitple liinear regression the scatter plots between Y and each X may or may not show a linear pattern.



Graphs after fitting a Model

- 1 Graphs for cheking the linearity and normality assumptions
- 2 Graphs for the detection of ouliers and influential observations
- 3 Diagnostic plots for the effect of variables

Model Fitting lm()

```
1 + X1 + X2, data=P103)
summary (mod)
##
## Call:
## lm(formula = Y ~ 1 + X1 + X2, data = P103)
##
## Residuals:
         Min
                  10
                         Median
                                        30
                                                 Max
## -0.013632 -0.009451 -0.002279 0.008630 0.016325
##
## Coefficients:
               Estimate Std. Error t value Pr(>|t|)
##
## /Totercept) -4.515414 0.061142 -73.85
                                              <2e-16 **
               3.097008 0.012274 252.31
## X1
                                              k2e-16
## X2
               1.031859
                           0.003684 280.08
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
## Residual standard error: 0.01072 on 12 degrees of
## Multiple R-squared: 0.9998, Adjusted R-squared: 10.9998
```

F-statistic: 3.922e+04 on 2 and 12 DF, p-value: 2.ze-16

Model Fitting olsrr::ols_regress()

```
mod <- ols_regress(Y ~ 1 + X1 + X2, data=P103)</pre>
mod
##
                    Model Summary
                   1.000 RMSE
                                           0.011
## R
## R-Squared 1.000 Coef. Var 0.089
                        MSE
## Adj. R-Squared
                  1.000
                                          0.000
## Pred R-Squared 1.000
                         MAE
                                           0.009
  RMSE: Root Mean Square Error
  MSE: Mean Square Error
  MAF: Mean Absolute Error
##
                          ANOVA
##
           Sum of
          Squares
                   DF Mean Square F
                                              Sig.
## Regression 9.007 2 4.504 39222.343
                                                 0.0000
## Residual 0.001 12
                          0.000
## Total
             9.009
                            Parameter Estimates
      model Beta Std. Error Std. Beta t
## (Intercept) -4.515 0.061
                                 -73.851
                                                 0.000
                                                        -4.649
                                                               -4.382
```

Model Presentation: Stargazer

```
mod <- lm(Y ~ 1 + X1 + X2, data=P103)
stargazer::stargazer(mod, header=FALSE, single.row = T)</pre>
```

Table 2

		Dependent variable:
		Y
	X1	3.09 *** (0.012)
	X2	1.032**** (0.004)
	Constant	-4.515 ^{***} (0.061)
	Observations	15
	R^2	1.000
	Adjusted R ²	1.000
	Residual Std. Error	0.011 (df = 12)
	F Statistic	39,222.340*** (df = 2; 12)
	Note:	*p<0.1; **p<0.05; ***p<0.01

Model Presentation: Texreg

```
mod <- lm(Y ~ 1 + X1 + X2, data=P103)</pre>
texreg(mod)
```

	Model 1
(Intercept)	-4.52***
	(0.06)
X1	3.10***
	(0.01)
X2	1.03***
	(0.00)
R^2	1.00
Adj. R ²	1.00
Num. obs.	15
***n / 0 001·	**n < 0.01· *n < 0.05

Table 3: Statistical models

Linearity and Normality

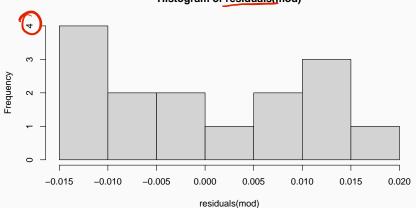
- Residual Histogram: Under the assumptions the histogram should resemble a normal distribution with symmetric shape and most observations around the center and few observations in the tails.
- QQ-Plot: Plot of the residuals versus the normals scores, which are what we would expect to obtain if the residuals were taken from a normal distribution. Under normality this plot should resemble a (nearly) straight line.
- Residuals vs. Predictors: The residuals should be uncorrelated with each of the predictors. If the assumptions hold, the plot should be a random scatter of points. Any pattern indicates a violation of an assumption, which often can be fixed using transformations.
- Residuals vs. Fitted: The residuals should also be uncorrelated with the fitted values, therefore this plot should also be a random scatter of points.

Histogram



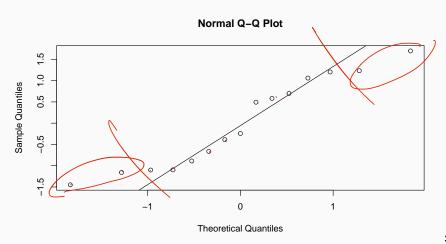


Histogram of residuals(mod)



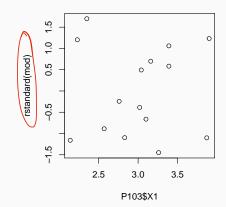
QQ-Plot (Standardized Residuals)

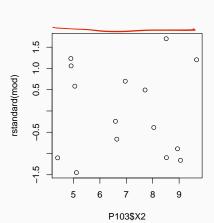
```
qqnorm(rstandard(mod))
qqline(rstandard(mod))
```



Standardized Residuals vs. Predictors

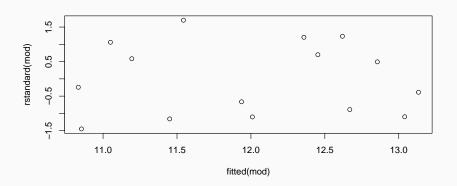
```
par(mfrow=c(1,2))
plot(y=rstandard(mod),x=P103$X1)
plot(y=rstandard(mod),x=P103$X2)
```





Standardized Residuals vs. fitted Values

```
par(mfrow=c(1,1))
plot(y=rstandard(mod), x=fitted(mod))
```



Leverage, Influence and Outliers



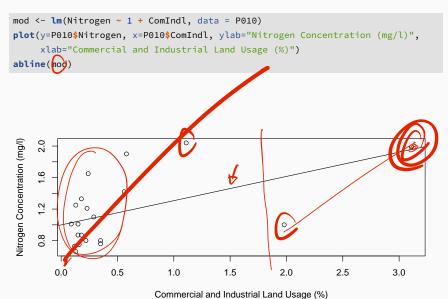
- We want to ensure that the model is not overly determined by one or a few observations. In multiple linear regression this cannot be simply detected graphically.
- When identifying influential data points (points that drag the regression line in their direction) looking a residuals does not necessarily help.
- Influential points can be identified, when the regression coefficients (fitted values, t-Tests, etc) change heavily, when we omit these points while estimating the model.

Outliers

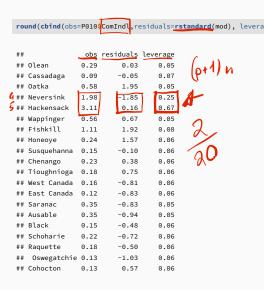
- Outliers in the Response Variable: Observations with large standardized residuals are outliers in the response variable as they lie far from the fitted line (in Y direction). Outliers indicate a model failure for these observations.
- Outliers in the Predictors: Outliers can also occur in the X-Space. The leverage values p_{ii} allow to measure these discrepancies (based on distance from \bar{x}) and are called **high-leverage** points. It should be checked if those points are also **influential** before they are treated.

Inspecting the residuals is necessary but not sufficient as high-leverage points (usually twice the average size of (p+1)/n) usually have small residuals.

Example: River Data



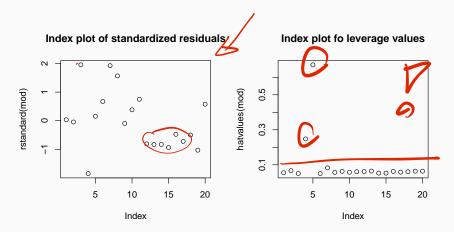
Example: River Data



A small residual value is desireable and the standardized residuals show no outlier. However, the small residual is not due to a good fits, but due to high leverage of the observations for Neversink and Hackensack.

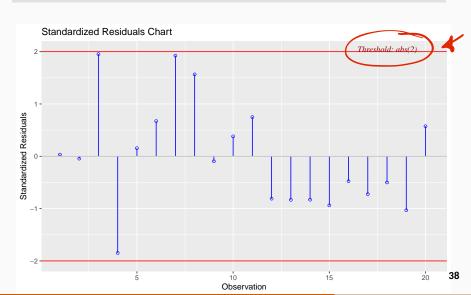
Example: River Data

```
par(mfrow=c(1,2))
plot(rstandard(mod), main="Index plot of standardized residuals")
plot(hatvalues(mod), main="Index plot fo leverage values")
```



Example: River Data





Influence

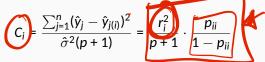
- The influence of an observations my be measured by the effects on the fit when iti is omitted from the data in the fitting process.
- $\hat{eta}_{0(i)}, \hat{eta}_{1(i)}, \dots, \hat{eta}_{p(i)}$ denote the regression coefficients obtained when the *i*-th observation sis deleted. $\hat{y}_{1(i)}, \hat{y}_{2(i)}, \dots, \hat{y}_{n(i)}$ and $\hat{\sigma}_{(i)}^2$ denote the predicted values and residual mean square error when dropping the *i*-th observation respectively. The resulting observation equation for the models follows by

$$\hat{y}_{m(i)} = \hat{\beta}_{0(i)} + \hat{\beta}_{1(i)}x_{m1} + \ldots + \hat{\beta}_{p(i)}x_{mp}$$

Measures to assess influence usually look at differences produced in $\hat{\beta}_j$ $\hat{\beta}_{j(i)}$ or $\hat{y}_j - \hat{y}_{j(i)}$.

Cook's Distance

- Cook's distance measures the difference between the regression coefficients obtained from the full data and the regression coefficients obtained by deleting the i-th observation.
- The influence of the *i*-th observation for i = 1, ..., n is given by

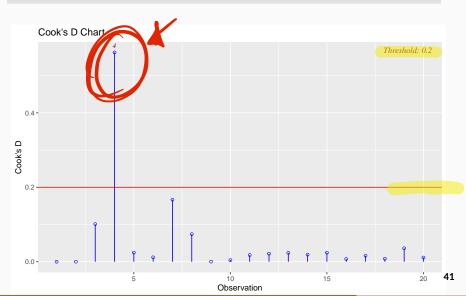


- Cook's distance is a product of the sqaured residual and the so called **potential funciton** $p_{ii}/(1-p_{ii})$.
- If C_i is large omitting a datapoint causes large changes in the model. Points are said to be influential when their Cook's distance meets or exceeds the 50% point of the *F*-distribution with p+1 and n-p-1 degrees of freedom. A rule of thumb is do investiage points where $C_i \ge 1$.

Cook's Distance

OLSTY

ols_plot_cooksd_chart(mod)



Welsch and Kuh Measure (DFITS)

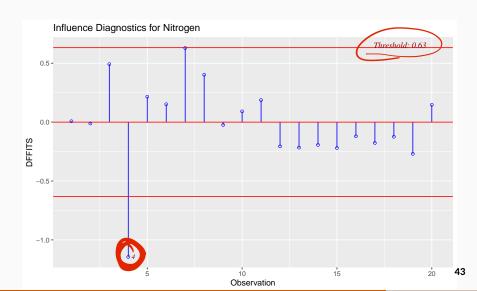
■ The measure proposed by Welsch and Kuh is the scaled difference between the *i*-th fitted value obtained from the full data and the *i*-th fitted value obtained by deleting the respective observation.

DFITS_i =
$$\frac{\hat{y}_i - \hat{y}_{i(i)}}{\widehat{\sigma_{(i)}^2} \sqrt{p_{ii}}} = r_i^* \sqrt{\frac{p_{ii}}{1 - p_{ii}}}$$

- Points with $|DFITS_i| > 2\sqrt{(p+1)/(n-p-1)}$ are usually classified as influential.
- C_i and $DFITS_i$ are functions of the residual and levrage values. It is often sufficient to inspect either the Cook's distance or DFITS.

Welsch and Kuh Measure (DFITS)

ols_plot_dffits(mod)



What to do with outliers?



- Outliers and influential observations should not routinely be deleted or automatically down-weighted.
- Points with high leverage and high influence are not necessarily bad observations! They can be an indication of model mispecification (e.g. non-linearity in the data) or show that the data did not come from a normal polulation. In those cases they may be the most informative data points.
- Each outlier should be inspected with care and checked individually.
 If data points are removed this should be documented in the research including reasons for the decision.
- Antoher option is to use <u>robust regression</u> where less weight is given to data points with high leverage.

Role of Variables in Regression Models

- Predictors are usually sequentially introduced into a regression equaiton.
- Given a model that contains ρ predictors, what is the effect of deleting (or adding) one of the variables from (or to) the model?
- One indication can be obtained by the t-test. If the t-value is large in absolute terms, the variables retained, otherwise omitted.
- **The results of the t-test are only valid if the underlying assumptions hold, tehrefore additinal graphs should be inspected when deciding wether or not to include a variable in the regresison model.

Example: Scottish Hills Races Data

P120

##		Time	Distance	Climb	
##	Greenmantle New Year Dash	965	2.5	650	
##	Carnethy	2901	6.0	2500	
##	Craig Dunain	2019	6.0	900	
##	Ben Rha	2736	7.5	800	
##	Ben Lomond	3736	8.0	3070	
##	Goatfell	4393	8.0	2866	
##	Bens of Jura	12277	16.0	7500	
##	Cairnpapple	2182	6.0	800	
##	Scolty	1785	5.0	800	
##	Traprain Law	2385	6.0	650	
##	Lairig Ghru	11560	28.0	2100	
##	Dollar	2583	5.0	2000	
##	Lomonds of Fife	3900	9.5	2200	
##	Cairn Table	2648	6.0	500	
##	Eildon Two	1616	4.5	1500	
##	Cairngorm	4335	10.0	3000	
##	Seven Hills of Edinburgh	5905	14.0	2200	
##	Knock Hill	4719	3.0	350	
##	Black Hill	1045	4.5	1000	
##	Creag Beag	1954	5.5	600	
##	Kildoon	957	3.0	300	
##	Meall Ant-Suiche	1674	3.5	1500	
##	Half Ben Nevis	2859	6.0	2200	
##	Cow Hill	1076	2.0	900	
##	North Berwick Law	1121	3.0	600	
##	Creag Dubh	1573	4.0	2000	

Example: Scottish Hills Races Data

lapply(P120, summary)

```
## $Time
                   Median
                                Mean 3rd Qu.
##
      Min. 1st Qu.
              1680
                       2385
                                3473
##
       957
                                        4118
                                                 12277
##
  $Distance
      Min. 1st Qu.
                     Median
                                Mean 3rd Qu.
##
                                                 Max.
                      6.000
                               7.529
                                       8.000
##
     2.000
             4.500
                                               28.000
##
  $Climb
##
      Min. 1st Qu.
                     Median
                                Mean 3rd Qu.
                                                 Max.
                       1000
                                1815
                                        2200
##
       300
                725
                                                 7500
```

Example: Scottish Hills Races Data

```
mod <- lm(Time ~ 1 + Distance + Climb, data=P120)
summary(mod)
##
## Call:
## lm(formula = Time ~ 1 + Distance + Climb, data = P120)
##
## Residuals:
      Min
             10 Median
                           30
                                 Max
## -973.0 -427.7 -71.2 142.2 3907.3
##
## Coefficients:
               Estimate Std. Error t value Pr(>|t|)
##
## (Intercept) 539.4829
                          258.1607 -2.090 0.0447 *
## Distance
                           36.0684 10.343 9.866-12 ***
               373.0727
                            0.1231 5.387 6.444-06 ***
## Climb
                 0.6629
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
## Residual standard error: 880.5 on 32 degrees of freedom
## Multiple R-squared: 0.9191, Adjusted R-squared: 0.914
## F-statistic: 181.7 on 2 and 32 DF, p-value: < 2.2e-16
```

Added-Variable Plot

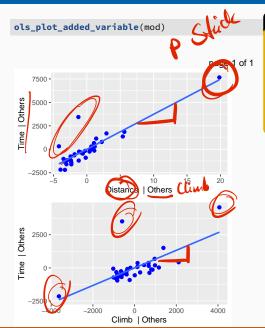
- The added-variable plot enables us to see the magnitude of the regression coefficient of the new variable that is bein considered for inclusion.
- The slope of the least squares line representing the points int he plot is equal to the estimated regression coefficient of the new variable. Additionally the plot shows data points that may be influential for this magnitude.

Added-Variable Plot



- The added variable plot is a plot between two pairs of residuals: the residuals when Y is regressed on predictors except X versus the residuals when regressing X_i on all other predictors.
 - First set of residuals corresponds to the remainder of Y that can not be explained by the other regressors.
 - Second set of residuals corresponds to the part of X_j that cannot be explained by the other predcitors.
 - The resulting slope is equal to $\hat{\beta}_j$ and essentially a visualization that is equivalent to the interpretation as partial regression coefficient.

Added-Variable Plot



Your turn

Do both variables contribute significantly to the model? Is there anything unuasual that should be investigated further?

Effects of an additional Predictor

- When a new regressor is introduced two questions should be answerd:
 - Is the regression coefficient of the new variable significant (different from zero)?
 - Does the ontroduction fo the new variable substantially change the regressions coefficients that are already in the model.

Effects of an additional Predictor

- **Option A:** insignificant and almost no change in coefficients → Should not be included unless theory dicates inclusion.
- **Option B:** significant and subtantial changes in coefficients. \rightarrow Should be included, but needs to be checked for collinearity.
- Option C: significant but no substantial coefficient changes → Ideal condition as variable is uncorrelated with other regressors, variable should be retained.
- **Option D:** insignificant but substantial coefficient changes → indicates collinearity, corective actions are required before discussion.