ETH

Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Applied Statistical Regression

AS 2014

Dr. Marcel Dettling

Institute for Data Analysis and Process Design

Zurich University of Applied Sciences

CH-8401 Winterthur

1 Introduction

1.1 What is Regression?

Regression analysis can be seen as the duct tape of statistics. The reason why it is widely used is because it may yield the answer to an everyday question, namely how a target value of special interest depends on several other factors or causes. Examples are numerous and include:

- how fertilizer and soil quality affects the growth of plants
- how size, location, furnishment and age affect apartment rents
- how age, sex, experience and nationality affect car insurance premiums

In all quantitative settings, regression techniques can provide an answer to these questions. They describe the relation between some *explanatory* or *predictor variables* and a variable of special interest, called the *response* or *target variable*. Regression techniques are of high practical importance, and probably the most widely used statistical methodology.

Example

In an applied research project at ZHAW, we tried to understand and manage the fresh water consumption on board of edelweiss air planes. Fresh water is mostly used in the toilet. Minimizing the carried amount was identified as important, because this reduces the weight of the airplane, and thereby fuel consumption and cost. The project goal was to relate the consumption on the *number of passengers* and *flight duration*, but also on less obvious parameters such as *daytime* and *destination*. Furthermore, it was required to quantify a well-calculated reserve, to set up a simple prediction scheme and to perform operations management on the filling of the tank.

1.2 Regression Mathematics

In the Edelweiss Air example, we can identify the fresh water consumption as the target value and denote it as the *response variable* y. Among the explanatory causes or *predictors* are *number of passengers*, and *flight duration*, plus a few more. These are denoted with $x_1, x_2, ..., x_p$, assuming that there are p predictors. The goal is linking the target to the predictors, which could happen with this model:

$$y = f(x_1, x_2, ..., x_p) + E$$

The target value is obtained as the sum of some function $f(\cdot)$ applied on the predictors, plus an error term E. Why the error? In practice, it is highly unlikely that $f(x_1, x_2, ..., x_p)$ yields an all-case perfect explanation of the fresh water consumption. The error is there to catch the imperfection and summarizes the remaining variation in the response. It is assumed to be *random* and can neither be controlled or predicted. On the other hand, $f(x_1, x_2, ..., x_p)$ is called the *systematic* or *deterministic* part of the regression equation.

The task is thus to learn about the function $f(\cdot)$. In full generality, without any restrictions, this is a very difficult problem: function space is infinite-dimensional, thus there are just too many options such that we could come to a unique solution based on just a few dozens of observations. It has proven practical to be very restrictive with the form of functions $f(\cdot)$ that are considered, i.e. normally, a linear model is assumed:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + ... + \beta_p x_p + E$$

This setup is called *linear modeling*. It boils down to determine some parameters $\beta_0, \beta_1, \beta_2, ..., \beta_p$ from observed data points, a task we call *estimation* in statistics. Please note that this is mathematically much simpler than finding $f(\cdot)$ without imposing any conditions.

One might of course fear that the limitation to linear modeling is too restrictive. However, practice proves this not to be the case, with the main reason being that only the parameters, but not the predictors need to enter linearly. In particular, the following structure is still a linear model:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 (x_1)^2 + \beta_3 \log(x_2) + \beta_4 x_1 x_2 + E$$

For such models, it is possible to estimate the parameters from a relatively low number of data points with the least squares algorithm that will be presented shortly. Using variable transformations as outlined above, linear modeling becomes a very rich and flexible tool. Truly non-linear models are rarely absolutely necessary in practice and most often arise from a theory about the relation between the variables rather than from necessity in an empirical investigation. Of course, the right variable transformations need to be found, but using some simple guidelines and visual displays this is a manageable task, as we will see later.

1.3 Goals with Regression

There are a variety of reasons to perform regression analysis. The two most prominent ones are:

Understanding on the predictor-response relation, i.e. doing inference

In the mortality example outlined in the chapter about multiple linear regression, one is be interested in testing whether air pollution affects mortality, under control of potentially confounding factors such as weather and the socio-demographic variables. We will see that regression, i.e. linear modeling offers tools to answer whether air pollution harms in statistically significant way. Drawing conclusions on true causal relationship, however, is a somewhat different matter.

Target value prediction as a function of new explanatory variables

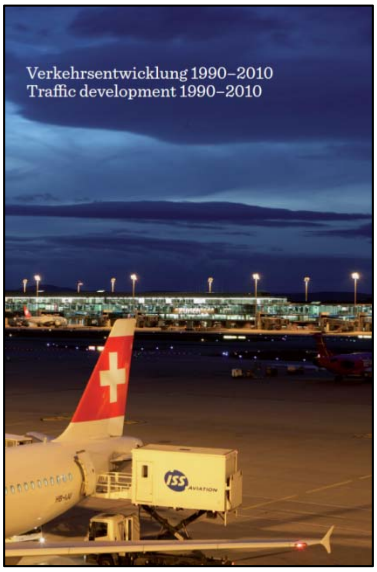
In the fresh water consumption example from above, an airplane crew or the ground staff may want to determine the amount of water that is necessary for a particular flight, given its parameters. Regression analysis, i.e. linear modeling incorporates the previous experience in that matter and yields a quantitative prediction. It also results in prediction intervals which give a hint on the uncertainty such a prediction has. In practice, the latter might be very useful for the amount of reserve water that needs to be loaded.

2 Simple Regression

The term simple regression means that there is a response and only one single predictor variable. This has several practical advantages: we can easily visualize the two variables and their relation in a scatterplot, and the involved mathematics is quite a bit easier. We will first address non-parametric curve fitting, also known as *smoothing*. Later, we proceed to linear modeling which in its most basic form amounts to laying a straight line into the scatterplot. But as we will see, linear modeling can also be used for fitting curves.

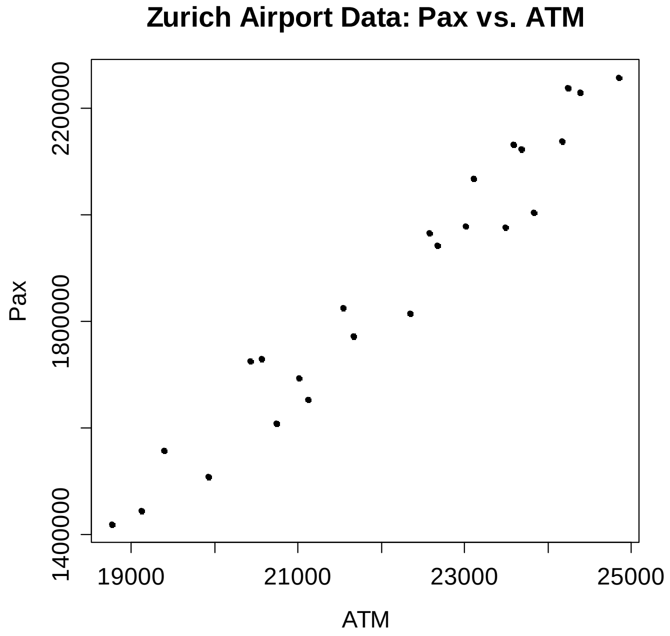
2.1 Example: Zurich Airport Data

The example we consider for developing the methodology is from Zurich Airport. Every month, the number of air traffic movements as well as the number of passengers is reported. The two variables are named *ATM* and *Pax*, with the former being the predictor, and the latter being the response. The goal is to predict passenger figures for future months based on the flight plan, and to quantify the uncertainty in these forecasts. The data are publicly accessible here: http://www.flughafen-zuerich.ch/desktopdefault.aspx/tabid-612/



We could display the figures in a table, but a much better solution is to visualize them in a scatterplot, as shown on the next page. As the first step, we need to import the data into R. Assuming that the data exist in form of an Excel spread sheet; we recommend exporting them in a comma- or tab-separated text file. In R, we can then use the function `read.table()`, respectively one of the tailored versions like `read.csv()` (for comma separation) or `read.delim()` (for tab separation), for importing the data. This will result in a so-called *data frame*, the structure which is most suitable for performing regression analysis in R. In our example, the Zurich Airport Data are stored in a data frame named `unique2010`. For producing a scatterplot, we can employ the generic `plot()` function, where several additional arguments can be set.

```
> plot(Pax ~ ATM, data=unique2010)
> title("Zurich Airport Data: Pax vs. ATM")
```



The question is how the systematic relation between *Pax* and *ATM* can be described. We could imagine that an arbitrary, smooth function $f(\cdot)$ that fits well to the data points, without following them too closely, is a good solution. Another viable and popular option would be to use a straight line for capturing the relation.

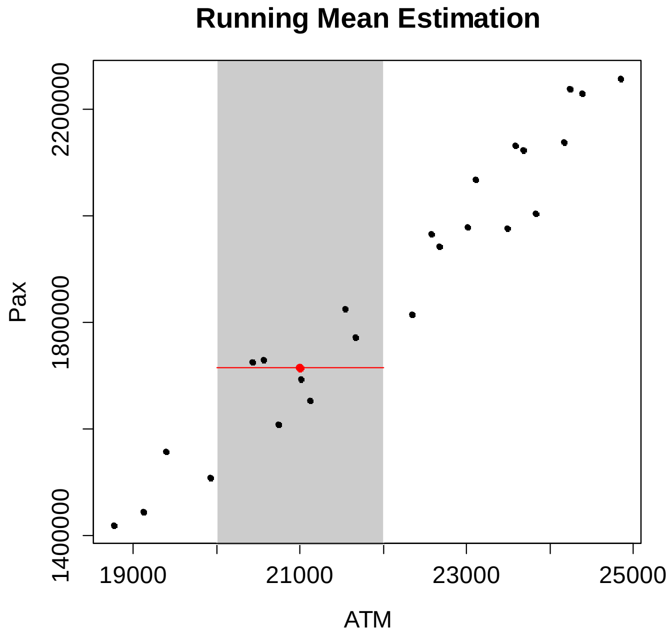
The advantages of smoothing are its flexibility and the fact that less assumptions are made on the form of the relation. This comes with the price that the functional form generally remains unknown, and that we can overfit, i.e. adapt too much to the data. With linear modeling, we have the benefit that formal inference on the relation is possible and that the efficiency is better, i.e. less data are required for a good estimate. The downside of the parametric approach is that it is only sensible if the relation is linear, and that it might falsely imply causality.

2.2 Scatterplot Smoothing

We start out with the smoothing approach. The goal here is to visualize the relation between *Pax* and *ATM*, but we are not after the functional form of $f(\cdot)$. Because there is no parametric function that describes the response-predictor relation, smoothing is also known as *non-parametric regression analysis*.

2.2.1 Running Mean Estimation

A simple yet intuitive smoother is the *running mean*. In colloquial language it involves taking a fixed width window on the x-axis, and compute the mean over all the within-window data point's y-values. That value then is the estimate for the function value at the window center.



The above illustration shows the running mean estimate at $ATM = 21'000$ with window width $\lambda = 2000$. The y-values of all the observations which fall into the grey highlighted region are averaged, which yields a value of $1'716'195$. The respective point is marked by the red symbol in the plot. The grey window is the slid over the x-axis which defines the running mean smooth. In mathematical notation, the running mean estimate for the unknown function $f(\cdot)$ denoted as $\hat{f}_\lambda(\cdot)$, is defined as follows:

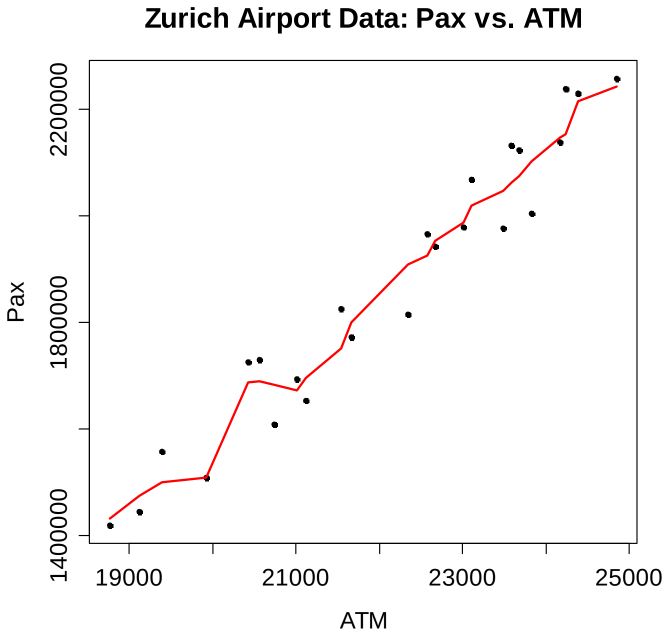
$$\hat{f}_\lambda(x) = \frac{\sum_{i=1}^{n} w_i y_i}{\sum_{i=1}^{n} w_i}, \text{ with weights } w_i = \begin{cases} 1 & if \ |x - x_i| \le \lambda / 2 \\ 0 & else \end{cases}.$$

The parameter λ is the window width and controls the amount of smoothing. Small values mean close adaptation to the data, while large values indicate averaging over more data points and thus a smoother solution. In R, running mean smoothing can be done with function `ksmooth()`:

```
> fit <- ksmooth(unique2010$ATM,unique2010$Pax, kernel="box",
                 bandwidth=1000, n.points=24, x.points=
                 unique2010$ATM)
```

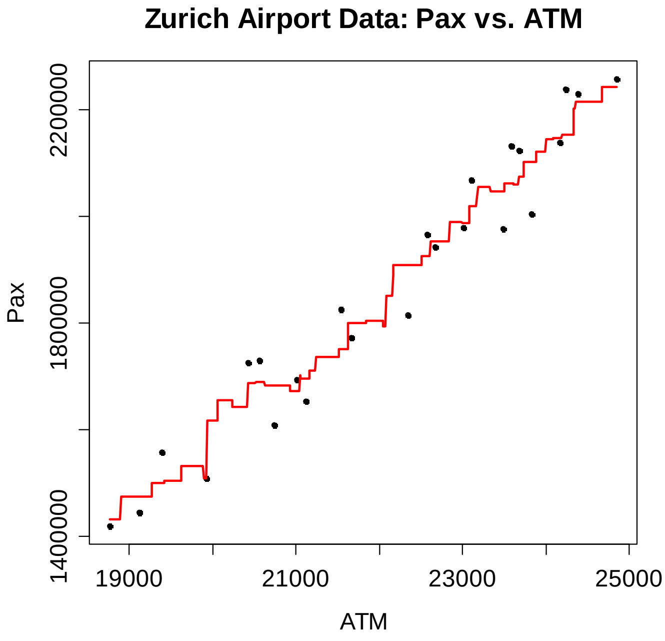
The argument `kernel="box"` tells R to use a rectangular kernel, and the `bandwidth=1000` argument steers the window width. Finally, `n.points` and `x.points` regulate at how many and which x-values the estimate is computed. We chose to do that for the observed *ATM* values. The solution can be plotted:

```
> plot(Pax ~ ATM, data=unique2010, main="...")
> title("Zurich Airport Data: Pax vs. ATM")
> lines(fit, col="red", lwd=2)
```



Perhaps a little more smoothing is required here, because we would hardly believe in a (systematic) relation that shows a decrease in passengers if the number of air traffic movements raises from 20’500 to 21’000. However, we leave this as an exercise to the reader. To point out an important drawback of running mean estimation, we increase the number of evaluation points to 1000 that uniformly cover the range of *ATM* and then plot the result:

```
> fit <- ksmooth(unique2010$ATM,unique2010$Pax, kernel="box",
                 bandwidth=1000, n.points=1000)
```



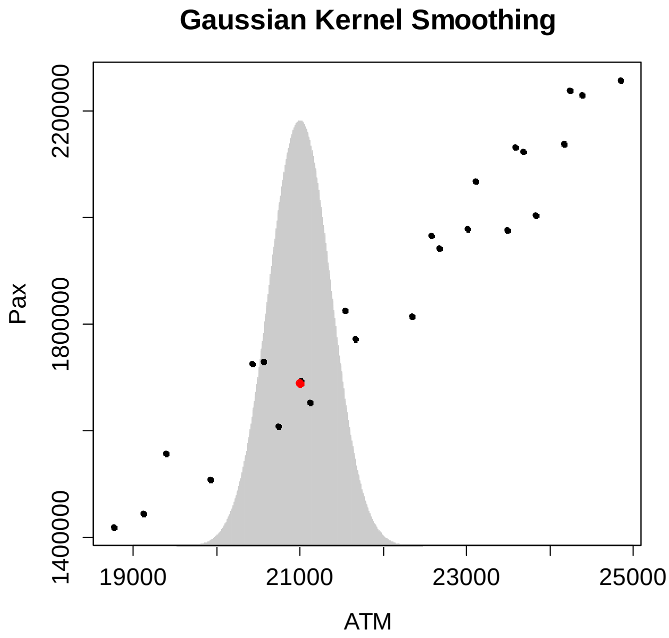
We obtain a function that is not smooth at all, but this is not a surprise. By construction, due to the rectangular kernel, data points drop out of the running mean computation abruptly, and hence we have the jumps.

2.2.2 Gaussian Kernel Smoothing

We can fix the above problem by using a kernel with infinite support, i.e. none of the weights should be exactly zero. An obvious choice for a weighting scheme that puts emphasis on nearby data points, down weighs distant observations and is never zero is the probability density function of the Gaussian distribution. The definition is:

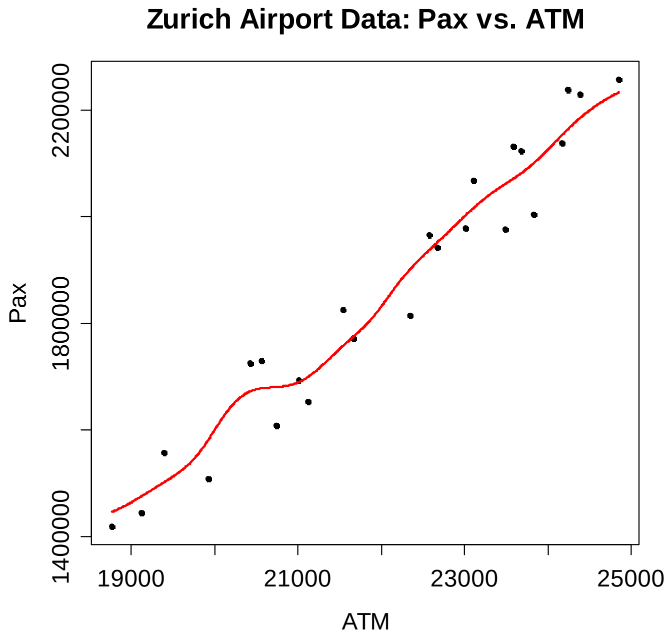
$$\hat{f}_\lambda(x) = \frac{\sum_{i=1}^{n} w_i y_i}{\sum_{i=1}^{n} w_i} \text{ with weights } w_i = \exp\left(-\frac{(x-x_i)^2}{\lambda} \right).$$

Thus, there is no longer a window that determines which data points take part in the running mean computation. But we use a Gaussian bell curve that determines the weights for the observations – no matter where, always all of them are used to compute the estimate. As we can easily imagine, this solves the issue with the data points that are lost abruptly, and the result is a smooth function



Above, computing a Gaussian Kernel Smoother is illustrated. At $x = 21'000$, a weighted average over all data points' y-values is taken. The weights come from the grey Gaussian bell curve. Its width is such that it corresponds to `bandwidth=1000` in R, which means that the 25%-quantile of the distribution is at $-0.25 \cdot 1'000 = -250$ and the 75%-quantile is at 250. Fitting in R is convenient, i.e.:

```
> fit <- ksmooth(unique2010$ATM, unique2010$Pax,
                 kernel="normal", n.points=1000,
                 bandwidth=1000)
```



While visually, the solution may look more or less reasonable here, a closer inspection suggests that it is rather sensitive to outliers. Moreover, there is a severe boundary effect associated with both the running mean and the Gaussian kernel estimator. Because near the boundaries, we do not observe a full window, we have a bias. At the lower end of the x-range, the smoother overestimates, while at the upper end of the range, it underestimates.

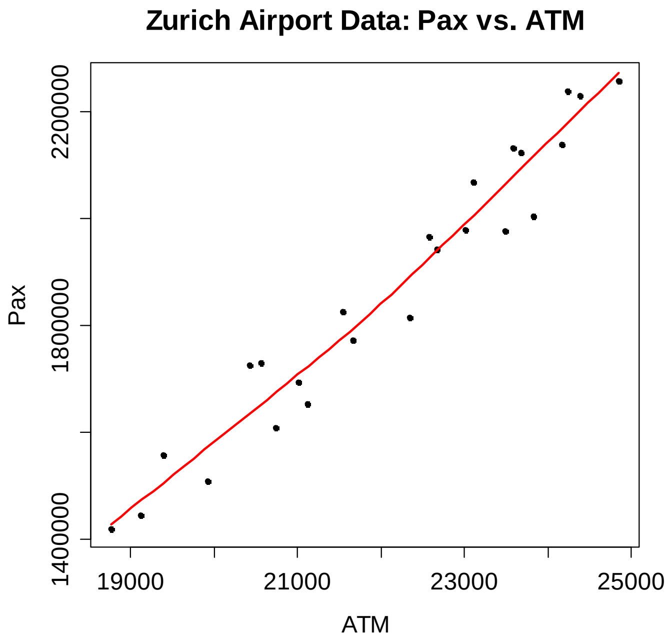
2.2.3 The LOESS Smoother

There is a wealth of literature that suggests improvements on kernel smoothing. However, with this scriptum, we will not further embark in that topic. But we present the *LOESS smoother*: it is a robust procedure that has nicer mathematical properties than the kernel smoothers, and that should be preferred in practice. LOESS is based on local parametric regressions: for obtaining the estimate at x, linear or polynomial models are fitted using data points in a neighborhood of x, weighted by their distance from x. The type of models used (linear or polynomial), the size of the neighborhood and also the type of fitting algorithm (least squares or robust) can be controlled in R. We do here without giving any theoretical details about the LOESS estimator. This is beyond the scope of our course, and it also requires intimate knowledge of linear modeling, which we do not yet have. However, as we will encounter LOESS smoothers throughout our studies in linear modeling, and it is a handy tool for visualizing the relation between two variables, we provide the necessary R commands:

```
> smoo <- loess.smooth(unique2010$ATM, unique2010$Pax)
```

For the `loess.smooth()` function, we need to specify the x and y variables. There are some further adjustments that can be made, but this is rarely necessary, because the default settings usually yield good results. Argument `span` controls the amount of smoothing and is set to `2/3`. Per default, we have `degree=1` which means local linear fitting, setting this to 2 means more flexibility through local polynomial fitting. Finally, argument `family` is set to `"symmetric"`, thus robust fitting is applied. A least squares fitting routine can be invoked by using `"gaussian"`. Lastly, we can control the number of points at which the smoother is evaluated. Mostly, the default of `evaluation=50` is fine, though it may sometimes be required to increase that number for relations with high curvature. We leave it to the reader to experiment with those settings and focus on displaying the result.

```
> plot(Pax ~ ATM, data=unique2010, main="...")
> lines(smoo, col="red", lwd=2)
```



We observe that the LOESS fit is almost, but not exactly a straight line, as it shows some progressive increase. Surely, when comparing to the Running Mean and the Gaussian Kernel Smoother, this is the most trustworthy result so far.

2.3 Simple Linear Regression

Instead of the non-parametric smoothing approaches, we will now turn our attention to linear modeling in the case where there is a response variable y and only one single predictor x. This problem is known as *simple linear regression*.

2.3.1 The Model

In our example, it seems logical that the more air traffic movements we have, the more passengers there are – at least on average. Also, it seems plausible that the systematic relation is well represented by a straight line. It is of the form:

$$Pax = \beta_0 + \beta_1 \cdot ATM \text{ , respectively } f(x) = \beta_o + \beta_1 x$$

While this is the mathematically simplest way of describing the relation, it proves itself as very useful in many applications. And as we will see later, just some slight modifications to this concept render it to a very powerful tool when it comes to describing predictor-response relations. The two parameters β_0, β_1 are called *intercept* and *slope*. The former is the expected value of y when $x = 0$, and the latter describes the increase in y when x increases by 1 unit.

We now bring the data into play. It is obvious from the scatterplot that there is no straight line that runs through all the data points. It may describe the systematic relation well, but there is scatter around it, due to various reasons. We attribute these to randomness, and thus enhance the model equation by the error term:

$$y_i = \beta_0 + \beta_1 x_i + E_i \text{, for all } i = 1, ..., n .$$

The index i stands for the observations, of which there are n in total. In our example, we have $n = 24$. The interpretation of the above equation is as follows:

y_i is the response or target variable of the i^{th} observation. In our example, this is the passenger number in the i^{th} month. Note that the response is a random variable, as it is the sum of a systematic and a random part.

x_i is the explanatory or predictor variable, i.e. the number of air traffic movements in the i^{th} month. The predictor is treated as a fixed, deterministic value and has no randomness.

β_0, β_1 are unknown parameters, and are called *regression coefficients*. These are to be estimated by using the data points which are available. β_0 is called *intercept*, whereas β_1 is the *slope*. The latter indicates by how much the response changes, if the x-value is increased by 1 unit.

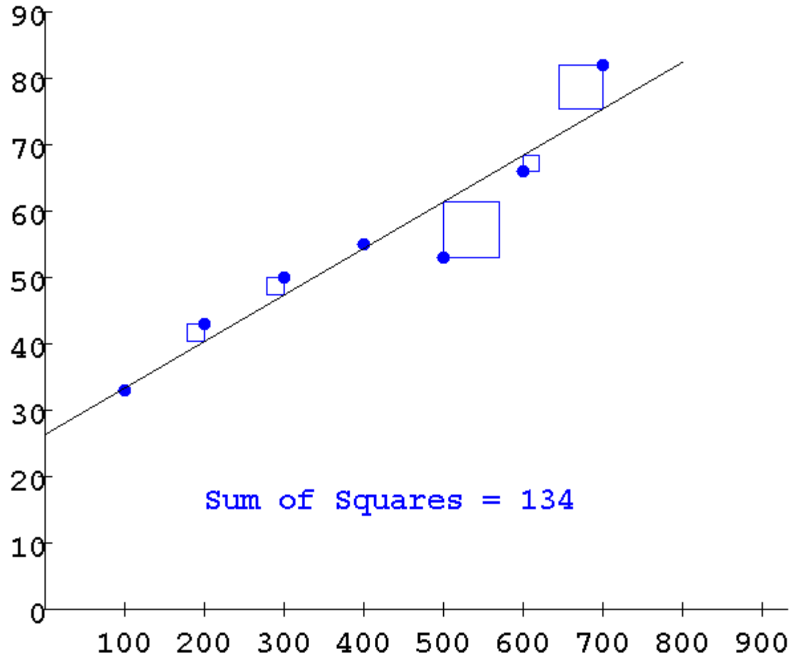
E_i is the *error term*. It is a random variable, or more precisely, the random difference between the observed value y_i (which is seen as the realization of a random variable) and the model value fitted by the regression.

2.3.2 The Least Squares Algorithm

The goal in simple linear regression is to lay a straight line through the data points. If we did this by eyeballing, the solution between different persons would perhaps be similar, but not identical. It is clear that we cannot leave any arbitrariness for the regression line. Thus, we need a clear definition for the *best fitting line*, as well as an algorithm that unveils it.

> *Our paradigm for linear modeling is to determine the regression line such that the sum of squared residuals is minimal!*

There are a number of reasons for this paradigm which are explained below. We illustrate the least squares idea with the help of a very nice Java applet found at http://sambaker.com/courses/J716/demos/LeastSquares/LeastSquaresDemo.html:



The applet allows interactive search of the solution by positioning the regression line according to the users wish. The squared residuals and their total sum can be displayed. While experimentation by hand will eventually lead to the minimum, it is cumbersome and laborious. Is there a mathematical procedure that finds the solution? The answer is yes, it is the *ordinary least squares* (OLS) algorithm.

Picking up the above paradigm, the goal is to fit the regression line such that the sum of squared differences r_i between the observed values y_i and the regression line is minimal, given a fixed set of data points $(x_i, y_i)_{i=1,\ldots,n}$. We can thus define the following function that measures the quality of the fit:

$$Q(\beta_0, \beta_1) = \sum_{i=1}^{n} r_i^2 = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 = \sum_{i=1}^{n} (y_i - (\beta_0 + \beta x_i))^2 = \min!$$

The goal is to minimize $Q(\cdot,\cdot)$. Since the data are fixed, this has to be done with respect to the two regression coefficients β_0, β_1. Or in other words, the parameters need to be found such that the sum of squared residuals is minimal. The idea for the solution is to set the partial derivatives to zero:

$$\frac{\partial Q}{\partial \beta_0} = 0 \text{ and } \frac{\partial Q}{\partial \beta_1} = 0 \,.$$

We leave the calculus as an exercise, but the result is a linear equation system with two equations and the two unknowns β_0, β_1. In linear algebra, these are known as the normal equations. Under some mild conditions (in simple linear regression this is: we have at least two data points with different values for x_i), the solution exists, is unique and can be written explicitly:

$$\hat{\beta}_1 = \frac{\sum_{i=1}^{n}(x_i - \overline{x})(y_i - \overline{y})}{\sum_{i=1}^{n}(x_i - \overline{x})^2} \text{ and } \hat{\beta}_0 = \overline{y} - \hat{\beta}_1 \overline{x} \,.$$

We put a hat symbol (“^”) on the optimal solutions. This is to indicate that they are estimates, i.e. determined from a data sample. Given the data pairs $(x_i, y_i)_{i=1,\ldots,n}$ they could now be computed with a pocket calculator. Or better, and more conveniently, with R:

```
> lm(Pax ~ ATM, data=unique2010)

Call:
lm(formula = Pax ~ ATM, data = unique2010)

Coefficients:
(Intercept)          ATM
 -1197682.1        138.8
```

The `lm()` command (from *linear modeling*) is based on the formula interface. The relation has to be provided in the form $y \sim x$, and with argument `data`, it is specified in which data frame these variables can be found. The output repeats the function call and provides the estimates $\hat{\beta}_0$ and $\hat{\beta}_1$.

The interpretation of this solution is straightforward: every additional air traffic movement on average provides $\hat{\beta}_1 = 138.8$ additional passengers. And if there were no air traffic movements, we would have $\hat{\beta}_0 = -1'197'682$ passengers. While the solution for $\hat{\beta}_1$ is plausible, this is not the case for $\hat{\beta}_0$. How can this happen?

It is because the observed set of data points is very far to the right of $x = 0$. It tells us that the linear relation we identified does not hold for very small numbers of air traffic movements. From a practical viewpoint, this is well acceptable. If the demand was that much smaller at Zurich Airport, it would be serviced by smaller airplanes. Or in other words: the regression line (at best) holds for the data we observed, and not for hypothetical values far beyond the range of observed

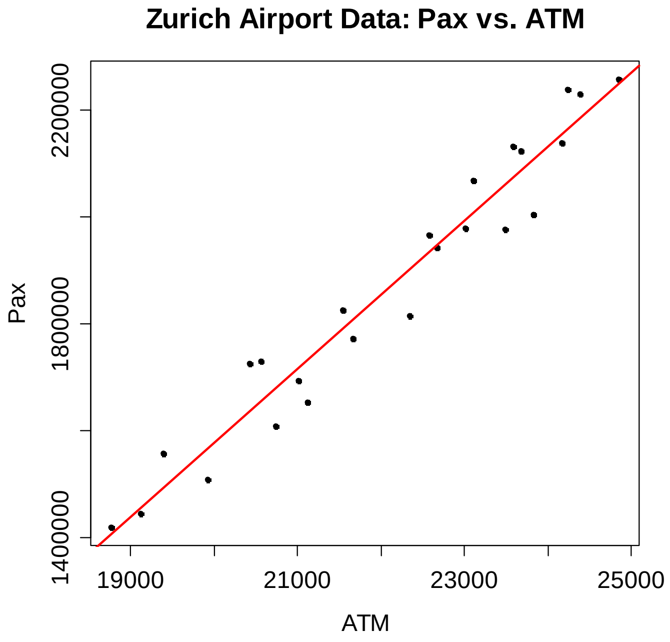
x-values. Thus, we do not need to worry much about the negative value for $\hat{\beta}_0$. Some further explanations on this as well as a potential remedy are provided later in this script. Using the estimated parameters, we obtain the *fitted values*, defined as:

$$\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i \text{ for all } i = 1,...,n.$$

These can of course be interconnected by the regression line. We here address the issue how the fitted values are accessed in R, and how the regression line is visualized:

```
> fit <- lm(Pax ~ ATM, data=unique2010)
> fitted(fit)
      1       2       3       4       5       6       7
1654841 1808312 2165068 2156465 2184911 2250545 2108731
      8       9      10      11      12      13      14
2062107 1493184 1902115 1456135 1679680 1637219 1718394
     15      16      17      18      19      20      21
2008267 1994391 2088333 2074873 1947490 1935418 1791799
     22      23      24
1733381 1406597 1566867

> plot(Pax ~ ATM, data=unique2010, pch=20)
> title("Zurich Airport Data: Pax vs. ATM")
> abline(fit, col="red", lwd=2)
```



The next issue that needs to be addressed is the quality of the solution. The OLS algorithm could be applied to any set of data points, even if the relation is curved instead of linear. In that case, it would not provide a good solution. The next section digs deeper and goes beyond the obvious.

2.3.3 Assumptions for OLS Estimation

The negative value for the estimated intercept had raised some doubts as to whether the OLS solution is trustworthy. We argued that $x = 0$ is far beyond the range of observed data, and that there is no guarantee that the regression line holds there. We can generalize this: on any dataset we perform regression, it remains (at best) unclear whether we can extrapolate the straight line, but most likely it is not the case. Within the range of observed data, we can make more statements. The OLS estimates are trustworthy, if:

$$E[E_i] = 0$$

The expectation (we could also say the best guess if we need to predict) for the errors is zero. This means that the relation between predictor and response is a linear function, or in our example: a straight line is the correct fit, there is no systematic deviation. Next, we require constant scatter for the error term, i.e.

$$Var(E_i) = \sigma_E^2 .$$

Finally, there must not be any correlation among the errors for different instances, which boils down to the fact that the observations do not influence each other, and that there are no latent variables (e.g. time) that do so. In particular,

$$Cov(E_i, E_j) = 0 \text{ for all } i \neq j .$$

Last, we require that the errors are (at least approximately) normally distributed:

$$E_i \sim N(0, \sigma_E^2)$$

The OLS algorithm will not yield a good solution under the presence of severe outliers or with a skewed error distribution. Moreover, all significance tests and confidence intervals that are presented later strictly rely on the Gaussian assumption.

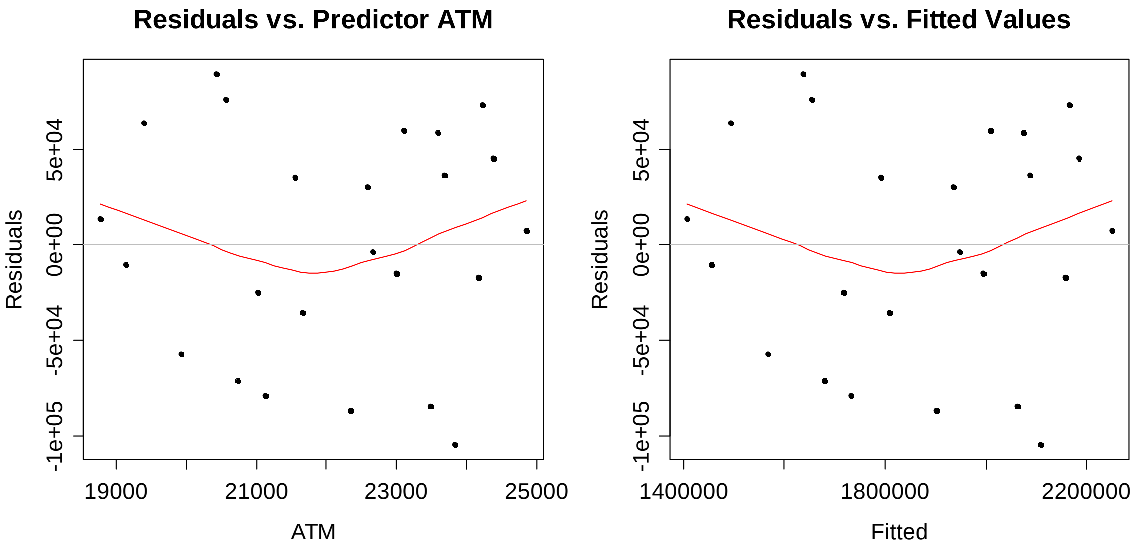
2.3.4 Residual Plots

Before the regression line is used, we need to check if the assumptions from section 2.3.3 are met. Some investigations on expectation, variance and distribution of the errors can be performed with the usual y vs. x scatterplot. However, it has proven more powerful to inspect residual plots that are directed towards identifying potential violations. As it turns out, the human eye is easily deceived when it needs to judge if some data points follow an inclined straight line. However, it is much better in detecting deviations from the horizon. This is utilized in the first residual plot, where the effect of the regression line is subtracted. This means that the *residuals are plotted against the predictor*. The visualization can be enhanced by adding a horizontal line and a scatterplot smoother (we choose a LOESS).

```
> ## Residuals vs. Predictor
> xx <- unique2010$ATM
> yy <- residuals(fit)
> plot(xx, yy, xlab="ATM", ylab="Residuals", pch=20)
> title("Residuals vs. Predictor ATM")
> lines(loess.smooth(xx,yy),col="red")
> abline(h=0, col="grey")
```

Another option is to plot the residuals versus the fitted values. This is known as the *Tukey-Anscombe plot*, according to the researchers who made it popular. As can be seen below, the two plots are one and the same except for the different x-axis. This is no surprise, because the fitted value $\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x$ stems from a linear transformation of x. While plotting *residuals vs. predictor* is perhaps the more natural way of doing it in simple regression, the Tukey-Anscombe plot provides a simple and intuitive summary in multiple regression, where several predictors exists. Thus, it is often also applied for simple regression.

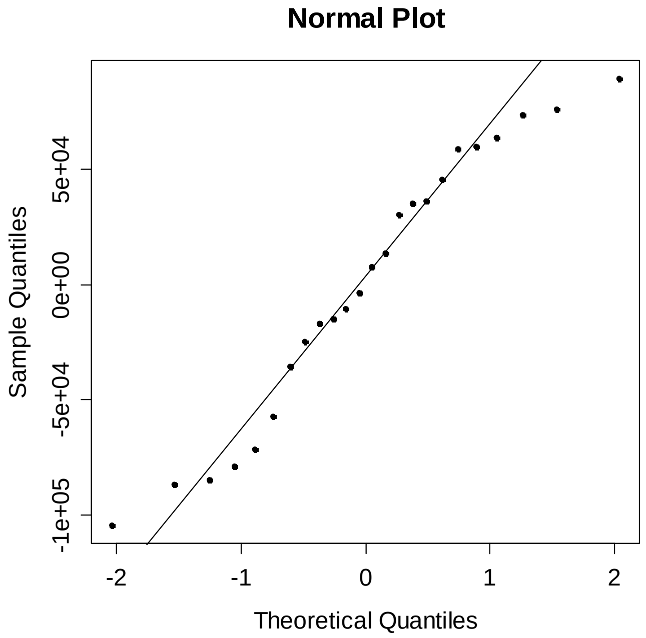
```
> ## Tukey-Anscombe Plot
> uu <- fitted(fit)
> plot(uu, yy, xlab="Fitted", ylab="Residuals", pch=20)
> title("Residuals vs. Fitted Values")
> lines(loess.smooth(uu,yy),col="red")
> abline(h=0, col="grey")
```



The smoother deviates from the horizon, and there is quite a clear kink in the relation. It seems as if the residuals for low and high *ATM* (resp. fitted) values are systematically positive, and negative for medium *ATM* values. If that is the case, it is a violation of the $E[E_i] = 0$ assumption; a straight line is not the correct fit and improving the model is mandatory. For the moment however, we keep in mind that some doubts are raised by this residual plot, but continue with developing theory. The constant variance assumption can also be judged from the above plot. It seems as if the scatter is more or less constant for the entire range of ATM values. Or maybe better: there is no obvious violation.

We proceed to checking if the residuals follow a Gaussian distribution. This can be done with a so-called *Normal Plot*, sometimes also named *QQ-Plot*, where the ordered residuals are shown versus quantiles of the Gaussian distribution. The data must more or less follow a straight line. This is sufficiently met here in our case; the residuals are even slightly short-tailed with respect to the Gaussian. An in-depth discussion about what still fits within the assumption and what does not is again postponed to later.

```
> qqnorm(residuals(fit))
> qqline(residuals(fit))
```



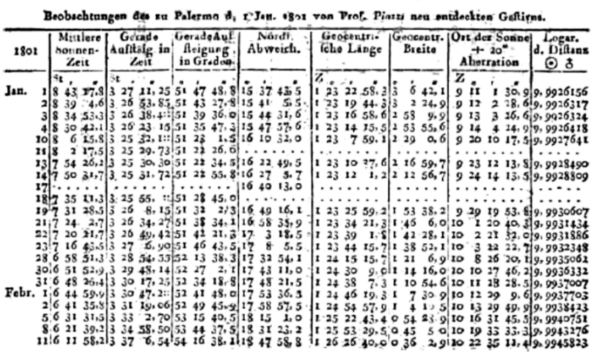
One last assumption has not been verified yet, namely the one whether the errors are uncorrelated. In many regression problems, this is the most difficult to verify. Also here, we could ask ourselves whether events such as the 9/11 terror attacks, or the SARS lung disease might have unduly influence. They could have led to back-to-back months with lower seat load factors, thus less passengers than expected by the air traffic movements during normal periods, and by this induce correlated errors. Because none of these events falls within our period of observation, we do not pursue the issue here. It will be addressed in detail when we talk about multiple linear regression.

2.3.5 History of Least Squares

You may find it somewhat arbitrary that we chose the sum of squares residuals as the criterion to minimize. We might as well optimize the absolute values' sum of the residuals, the so-called L_1 *-regression*. There are a number of reasons to prefer the former. The first one lies in history, least squares was simply the first such algorithm that was used in practice. The English Wikipedia site on the term least squares holds the following information:

On January 1, 1801, the Italian astronomer Giuseppe Piazzi discovered the dwarf planet Ceres and was able to track its path for 40 days before it was lost in the glare of the sun. Based on these data, astronomers desired to determine the location of Ceres after it emerged from behind the sun without solving the complicated Kepler's nonlinear equations of planetary motion. The only predictions that successfully allowed relocating Ceres were those performed by the 24-year-old Carl Friedrich Gauss using the least squares algorithm.

Gauss did not publish the method until 1809, when it appeared in volume two of his work on celestial mechanics, together with a mathematical optimality result, the Gauss-Markov theorem (see below). In the meantime, the OLS algorithm was independently formulated by Adrian Marie Legendre, who was the first to publish it in 1806 as an appendix to his book on the paths of comets. Below, see a table of Piazzi's observations, and portraits of Gauss (left) and Legendre (right).



Beobachtungen des zu Palermo d. 1. Jan. 1801 von Prof. Piazzi neu entdeckten Geſtirns.

1801		Mittlere Sonnen-Zeit	Gerade Aufſteig. in Zeit	Gerade Aufſteigung in Graden	Nördl. Abweich.	Geocentriſche Länge	Geocentr. Breite	Ort der Sonne + 20″ Aberration	Logar. d. Diſtanz ⊙ ♁
		St ′ ″	St ′ ″	° ′ ″	° ′ ″	Z ° ′ ″	° ′ ″	Z ° ′ ″	
Jan.	1	8 43 27,8	3 27 11,25	51 47 48,8	15 37 43,5	1 23 22 58,3	3 6 42,1	9 11 1 30,9	9,9926156
	2	8 39 4,6	3 26 53,85	51 43 27,8	15 41 5,5	1 23 19 44,3	3 2 24,9	9 12 2 28,6	9,9926317
	3	8 34 53,3	3 26 38,4	51 39 36,0	15 44 31,6	1 23 16 58,6	2 58 9,9	9 13 3 26,6	9,9926324
	4	8 30 42,1	3 26 23,15	51 35 47,3	15 47 57,6	1 23 14 15,5	2 53 55,6	9 14 4 24,9	9,9926418
	10	8 6 15,8	3 25 32,1	51 23 1,5	16 10 32,0	1 23 7 59,1	2 29 0,6	9 20 10 17,5	9,9927641
	11	8 2 17,5	3 25 29,73	51 22 26,6	. . . . . .	. . . . . .	. . . . . .	. . . . . .	. . . . . .
	13	7 54 26,2	3 25 30,30	51 22 34,5	16 22 49,5	1 23 10 27,6	2 16 59,7	9 23 12 13,8	9,9928490
	14	7 50 31,7	3 25 31,72	51 22 55,8	16 27 5,7	1 23 12 1,2	2 12 56,7	9 24 14 13,5	9,9928809
	17	. . . . . .	. . . . . .	. . . . . .	16 40 13,0	. . . . . .	. . . . . .	. . . . . .	. . . . . .
	18	7 35 11,3	3 25 55, ::	51 28 45,0	. . . . . .	. . . . . .	. . . . . .	. . . . . .	. . . . . .
	19	7 31 28,5	3 26 8,15	51 32 2,3	16 49 16,1	1 23 25 59,2	1 53 38,2	9 29 19 53,8	9,9930607
	21	7 24 2,7	3 26 34,27	51 38 34,1	16 58 35,9	1 23 34 21,3	1 46 6,0	10 1 20 40,3	9,9931434
	22	7 20 21,7	3 26 49,42	51 42 21,3	17 3 18,5	1 23 39 1,8	1 42 28,1	10 2 21 32,0	9,9931886
	23	7 16 43,5	3 27 6,90	51 46 43,5	17 8 5,5	1 23 44 15,7	1 38 52,1	10 3 22 22,7	9,9932348
	28	6 58 51,3	3 28 54,33	52 13 38,3	17 32 54,1	1 24 15 15,7	1 21 6,9	10 8 26 20,1	9,9935062
	30	6 51 52,9	3 29 48,14	52 27 2,1	17 43 11,0	1 24 30 9,0	1 14 16,0	10 10 27 46,2	9,9936332
	31	6 48 26,4	3 30 17,25	52 34 18,8	17 48 21,5	1 24 38 7,3	1 10 54,6	10 11 28 28,5	9,9937007
Febr.	1	6 44 59,9	3 30 47,2 ::	52 41 48,0	17 53 36,3	1 24 46 19,3	1 7 30,9	10 12 29 9,6	9,9937703
	2	6 41 35,8	3 31 19,06	52 49 45,9	17 58 57,5	1 24 54 57,9	1 4 15,5	10 13 29 49,9	9,9938423
	5	6 31 31,5	3 33 2,70	53 15 40,5	18 15 1,0	1 25 22 43,4	0 54 23,9	10 16 31 45,5	9,9940751
	8	6 21 39,2	3 34 58,50	53 44 37,5	18 31 23,2	1 25 53 29,5	0 45 5,0	10 19 33 33,3	9,9943276
	11	6 11 58,2	3 37 6,54	54 16 38,1	18 47 58,8	1 26 26 40,0	0 36 2,9	10 22 35 11,4	9,9945823

Was it by coincidence that OLS was invented first? The answer is no: the quality function $Q(\cdot,\cdot)$ is differentiable, so that a unique solution can be found and written in explicit form. This is not possible with L_1-regression, because the absolute value function is not continuously differentiable. While this problem can nowadays be circumvented with numerical methods, this was not yet feasible at the beginning of the 19^{th} century. The reason why OLS is still popular today is because there are mathematical optimality results, and because under Gaussian errors, the exact distribution of the estimated coefficients and a number of test statistics is known.

2.3.6 Mathematical Optimality of OLS

The main result is the *Gauss-Markov theorem* (GMT) that dates back to 1809:

> Under the model assumptions from section 2.3.3 (*zero expected value, constant variance and uncorrelatedness for the errors*), the OLS estimates $\hat{\beta}_0, \hat{\beta}_1$ are unbiased (i.e. $E[\hat{\beta}_0] = \beta_0$ and $E[\hat{\beta}_1] = \beta_1$). Moreover, they have minimal variance among all unbiased, linear estimators, meaning that they are most precise. Please note that Gaussian errors are not required.

This theorem does not tell us to use OLS all the time, but it strongly suggests doing so if the assumptions are met. In cases where the errors are correlated or have unequal variance, we will do better with other algorithms than OLS. Also, note that even though normality is not required for the GMT, there will be non-linear or biased estimates that do better than OLS under non-Gaussian errors.

As we have seen just before, the regression coefficients are unbiased if the assumptions from section 2.3.3 are met. It is also very instructive to study the variance of the estimates. It can be shown that:

$$Var(\hat{\beta}_0) = \sigma_E^2 \cdot \left(\frac{1}{n} + \frac{\overline{x}}{\sum_{i=1}^{n} (x_i - \overline{x})^2} \right), \text{ and}$$

$$Var(\hat{\beta}_1) = \frac{\sigma_E^2}{\sum_{i=1}^{n} (x_i - \overline{x})^2} .$$

These results also show how a good experimental design can help to improve the quality of the estimates, or in other words, how we can obtain a more precisely determined regression line. Namely:

- we can increase the number of observations n.
- we have to make sure that the predictors x_i scatter well.
- by using a suitably-chosen predictor, we can keep σ_E^2 small.
- for $\hat{\beta}_0$ it helps, if the average predictor value $\overline{x}$ is close to zero.

If the errors are Gaussian, then $\hat{\beta}_0, \hat{\beta}_1$ are normally distributed, too. With their expectation and variance specified as above, the distribution is fully known. Additionally, the OLS solution is also the maximum likelihood estimator under Gaussian errors. Some further useful properties of the OLS solution (that are independent of the error distribution) are:

- the regression line runs through the center of gravity $(\overline{x}, \overline{y})$.
- the sum of residuals adds up to zero: $\sum r_i = 0$.

The last property also implies that the mean value of the residuals is always zero.

2.3.7 Estimating the Error Variance

Besides the regression coefficients, we also need to estimate the error variance. It is a necessary ingredient for all tests and confidence intervals. The estimate is based on the *residual sum of squares* (abbreviation: RSS).

$$\hat{\sigma}_E^2 = \frac{1}{n-2} \cdot \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

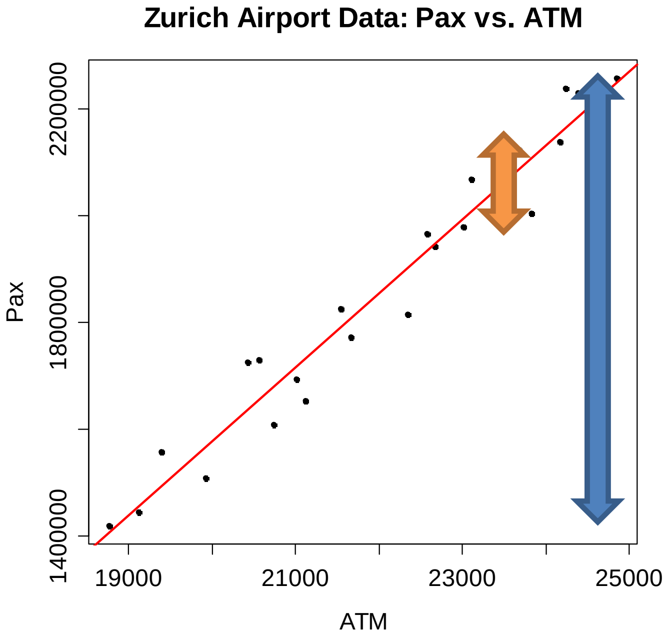
In the R summary, an estimate for the error's standard deviation $\hat{\sigma}_E$ is given as the `Residual standard error`.

2.4 Inference

The goal in this section is to infer the response-predictor relation with performance indicators and statistical tests. Note that except for 2.4.1, the assumption of *independent, identically distributed Gaussian errors* is central to derive the results.

2.4.1 The Coefficient of Determination

An intuitive way of measuring the goodness-of-fit of a simple linear regression model is with the *coefficient of determination* R^2, also called *multiple R-squared*. It measures which portion of the total variation is accounted for by the regression.



If we needed to predict the *Pax* number without any knowledge of the *ATM* value, the best guess is the average number of passengers over the last two years. The scatter around that prediction is visualized by the blue arrow. However, since we know *ATM* and the regression line, we can come up with a more accurate forecast. The then remaining scatter is indicated by the orange arrow. It is obvious that the regression line is more useful, the smaller the orange arrow is compared to the blue. This can be measured by taking one minus the quotient of the two:

$$R^2 = 1 - \frac{\sum_{i=1}^{n} (\hat{y}_i - y_i)^2}{\sum_{i=1}^{n} (y_i - \bar{y})^2} \in [0,1]$$

In the numerator, the orange arrow is represented by the scatter of the data points around the fitted values, i.e. the *RSS*. The denominator has the scatter of the data points around their mean. This is the *total sum of squares* (*TSS*).

The maximum value is $R^2 = 1$. It is attained if all data points are on the regression line. The other extreme case is $R^2 = 0$ and means that the blue and orange arrows have the same size. Then, the regression line is flat ($\hat{\beta}_1 = 0$) and does not have any explanatory power. The actual value can be read from the R summary:

```
> summary(fit)
Coefficients: Estimate Std. Error t value Pr(>|t|)
(Intercept) -1.198e+06  1.524e+05  -7.858 7.94e-08 ***
ATM          1.388e+02  6.878e+00  20.176 1.11e-15 ***
---
Residual standard error: 59700 on 22 degrees of freedom
Multiple R-squared: 0.9487,  Adjusted R-squared: 0.9464
F-statistic: 407.1 on 1 and 22 DF, p-value: 1.11e-15
```

The result here is $R^2 = 0.9487$, thus most of the variation in the *Pax* variable is explained by *ATM*. It is important to note that for simple linear regression, R^2 is equal to the *squared Pearson correlation coefficient* between predictor and response. Moreover, the summary reports the adjusted R-squared. Its value is always smaller but usually close to R^2, because:

$$aR^2 = R^2 - \frac{1-R^2}{n-2}.$$

An important question is now: what is a good value for R^2? Unfortunately, it remains without an answer. There are no general guidelines as to which value needs to be met for a regression to be useful, and there are no formal tests for R^2. And please note that a high value for R^2 does not automatically mean that we have a good fit that we can rely on – often, further improvement by alternative models (i.e. by using transformations) is still possible.

2.4.2 Confidence Interval for the Slope

The estimated slope $\hat{\beta}_1$ is a random variable and has variability. If the assumptions for the OLS algorithm are met, we have the Gauss-Markov theorem telling us its value will be close to the truth β_1, but not right there. Also, the value $\hat{\beta}_1$ was computed from a sample. Had we had a different one, or would we just omit one single data point from our current one, $\hat{\beta}_1$ would turn out different. The goal is to reflect that uncertainty with a *95% confidence interval* (CI). The formula is:

$$\hat{\beta}_1 \pm qt_{0.975;n-2} \cdot \hat{\sigma}_{\hat{\beta}_1} \text{, resp. } \hat{\beta}_1 \pm qt_{0.975;n-2} \cdot \sqrt{\hat{\sigma}_E^2 \Big/ \sum_{i=1}^{n} (x_i - \overline{x})^2} \text{,}$$

where $qt_{0.975;n-2}$ is the 97.5% quantile of Student's t-distribution with $n-2$ degrees of freedom. The colloquial interpretation is that the interval holds all values which, besides the point estimate $\hat{\beta}_1$, are plausible for β_1. In R, one types:

```
> confint(fit, "ATM")
       2.5 %  97.5 %
ATM 124.4983 153.025
```

We estimated the increase in passengers per additional air traffic movement as $\hat{\beta}_1 = 138.8$. That is the best guess given the data, but values between 124.5 and 153.0 are also plausible. This reflects the uncertainty and variability in our regression analysis. If the 95%-CI seems unacceptably wide, all we can do is trying to bring $\hat{\sigma}_{\hat{\beta}_1}$ down, i.e. have more or better data, see section 2.3.6.

2.4.3 Testing the Slope

For finding out whether an arbitrary value b is plausible for the slope, we can check whether it is contained in the 95%-CI from above. Alternatively, there is a test for the *null hypothesis* $H_0 : \beta_1 = b$. The most popular variant is $H_0 : \beta_1 = 0$: this is asking if the slope could be zero, which would mean that the regression line runs horizontally and the predictor x has no influence on the response y. The natural goal is to reject the null for gaining evidence that the relation between y and x exists. One usually tests two-sided on the 95% level, i.e. the alternative is $H_A : \beta_1 \neq b$. The *test statistic* and its *distribution* are as follows:

$$T_{H_0:\beta_1=b} = \frac{\hat{\beta}_1 - b}{\hat{\sigma}_{\hat{\beta}_1}} \sim t_{n-2}.$$

Student's t-distribution with $n-2$ degrees of freedom can be used to determine acceptance and rejection regions, as well as the *p-value*. In fact, both the *test statistic* (`t value`) and the *p-value* (`Pr(>|t|)`) for $H_0 : \beta_1 = 0$ are routinely given in the R summary output:

```
> summary(fit)

Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept) -1.198e+06  1.524e+05  -7.858 7.94e-08 ***
ATM          1.388e+02  6.878e+00  20.176 1.11e-15 ***
---
Residual standard error: 59700 on 22 degrees of freedom
Multiple R-squared: 0.9487,  Adjusted R-squared: 0.9464
F-statistic: 407.1 on 1 and 22 DF, p-value: 1.11e-15
```

We have very strong evidence for $\beta_1 \neq 0$ here, and thus the null hypothesis is rejected with a p-value of $1.1 \cdot 10^{-15}$. The fact of rejection was already clear from the 95%-CI which contains all null hypotheses that are not rejected – and zero was not therein – with a huge margin, that is, and hence the extreme p-value.

It is very important to stress again, that all confidence intervals and test results are only to be trusted if the assumptions for OLS fitting (i.e. zero expectation, constant variance, Gaussian distribution and uncorrelatedness of the errors) are closely met. If any clear deficiencies were found from the residuals plots, it is mandatory to improve the model before these results are reassessed!

2.4.4 Testing the Intercept

In many simple linear regression problems, theory dictates that we have a response of $y=0$ whenever $x=0$. That is the case with the Zurich Airport Data, too. If there were no air traffic movements, we would not see any passengers. However, it is hardly ever a good idea to fit a model without an intercept term. This forces the regression line to go through the origin which is a very strong restriction, that in most cases leads to a poor fit.

Commonly, the reason for the poor fit is because the data points are far off $x=0$. This leads to very high leverage with respect to β_0, and just some slight non-linearity between response and predictor results in an intercept that is markedly different from zero. This happens in our example where $\hat{\beta}_0 = -1'197'682$. In analogy to sections 2.4.2 and 2.4.3, tests and confidence intervals for β_0 exist. For the Zurich Airport data, the null hypothesis $H_0 : \beta_0 = 0$ is strongly rejected with a p-value of $7.9 \cdot 10^{-8}$, and the confidence interval is:

```
> confint(fit, "(Intercept)")
                2.5 %    97.5 %
(Intercept) -1513786 -881578.2
```

However, both test and confidence interval for β_0 are of relatively low practical importance. As a *general rule*, we should *not fit regression models without an intercept term*. If the null is not rejected and thus zero is a plausible value, it is still better and safer to keep it in the model. If it turns out to be significantly different from zero, take it as evidence for either some non-linearity or calibration errors in the data. In these latter cases, the results will be clearly worse (i.e. strongly biased) without the intercept. We close here with the remark that for many regression problems which need to run through the origin, using the log-log-model displayed in section 2.6.4 is the best choice.

2.5 Prediction

One of the primary goals with linear regression is to generate a prediction for y, given the value of x. The result is the conditional expectation for y given x, i.e. what we expect for y if the predictor value x is known:

$$E[y \mid x] = \hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x$$

For 24‘000 air traffic movements, we expect $-1'197'682 + 24'000 \cdot 138.8 = 2'133'518$ passengers. Please note that only a prediction within the range of x-values that were present for fitting is sensible. This is called *interpolation*. On the other hand, *extrapolation*, i.e. a prediction beyond the boundaries of the x-values previously observed, has to be treated with great care: there is no guarantee that the regression line holds in non-observed regions of the predictor space. Thus, we must not predict the Pax figure for ATM values such as 50’000, 5’000 or 0.

In R, we can obtain the fitted values for the training data points by just typing `predict(fit)`. If we want to use the regression line for forecasting with new x-values, they have to be provided in a data frame, where the column(s) are named equally to the predictor(s):

```
> fit <- lm(Pax ~ ATM, data=unique2010)
> dat <- data.frame(ATM=c(24000))
> predict(fit, newdata=dat)
1 2132598
```

2.5.1 Confidence Interval for the Regression Line

As we had seen above in section 2.4.2, the regression coefficients are random variables. Thus, also the regression line is a random variable, and might have turned out to be different with another sample (even if from the same population). Thus, it is important to understand, quantify and visualize the variability of the fitted value. This is done on the basis of a *95%-CI for the conditional expectation*. The formula is:

$$\text{95\%-CI for } E[y\,|\,x]:\ \hat{\beta}_0+\hat{\beta}_1 x \pm qt_{0.975;n-2}\cdot\hat{\sigma}_E\cdot\sqrt{\frac{1}{n}+\frac{(x-\overline{x})^2}{\sum_{i=1}^{n}(x_i-\overline{x})^2}}$$

The formula itself is of relatively little importance for the practitioner, because that functionality is pre-existing in R. The syntax is:

```
> predict(fit, newdata=dat, interval="confidence")
           fit     lwr     upr
     1 2132598 2095450 2169746
```

The meaning of this output is as follows: for an ATM value of $24'000$, we expect $2'132'598$ passengers. A 95%-CI for that conditional expectation ranges from $2'095'450$ to $2'169'746$.

2.5.2 Prediction Interval for Future Data Points

While the above 95%-CI tells characterizes the variability in the fitted value, it does not tell us where the (future) y-value will be, i.e. what number of passengers we will observe for a given ATM value. The reason is that (also within the training data), the observed y-values scatter around the regression line (i.e. their conditional expectation). Taking this into account, we can derive a *95% prediction interval* (PI) for y. The formula is:

$$\text{95\%-PI for } y:\ \hat{\beta}_0+\hat{\beta}_1 x \pm qt_{0.975;n-2}\cdot\hat{\sigma}_E\cdot\sqrt{1+\frac{1}{n}+\frac{(x-\overline{x})^2}{\sum_{i=1}^{n}(x_i-\overline{x})^2}}$$

The difference in the formula is that another unit of $\hat{\sigma}_E$ is included to account for the scatter of the data points around the regression line. Again, the formula is implemented in R:

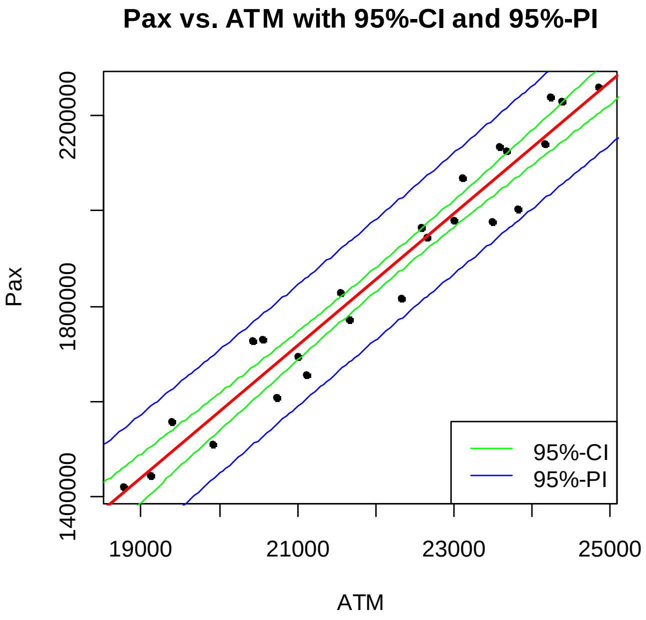
```
> predict(fit, newdata=dat, interval="prediction")
           fit     lwr     upr
     1 2132598 2003343 2261853
```

Because we are still predicting for an ATM value of $24'000$, we the conditional expectation remains at $2'132'598$ passengers. A 95% prediction interval for a future observation when there are $24'000$ air traffic movements ranges from $2'003'343$ to $2'261'853$.

2.5.3 Visualizing Confidence and Prediction Intervals

It is very instructive to compute point-wise CIs and PIs and to display them in the xy-scatterplot, along with the regression line. There is no straightforward procedure in R to do so, but some rather tedious handwork is required. A possible solution is as follows:

```
> dat  <- data.frame(ATM=seq(18000, 26000, length=200))
> ci   <- predict(fit, newdata=dat, interval="confidence")
> pi   <- predict(fit, newdata=dat, interval="prediction")
> plot(Pax ~ ATM, data=unique2010, pch=20)
> title("Pax vs. ATM with 95%-CI and 95%-PI")
> lines(dat$ATM, ci[,2], col="green")
> lines(dat$ATM, ci[,3], col="green")
> lines(dat$ATM, pi[,2], col="blue")
> lines(dat$ATM, pi[,3], col="blue")
> abline(fit, col="red", lwd=2)
```



The result is a confidence region for the regression line, and a prediction region for future observations. The interpretation is that the former contains all plausible regression lines. The latter indicates how precisely we can forecast future observations. While the 95%-CI turns out to be rather small here, reflecting a high confidence in the estimated regression line, the 95%-PI is bigger an reflects the non-understood scatter of the observations due to reasons such as differing seat loads factors, cargo flights, et cetera.

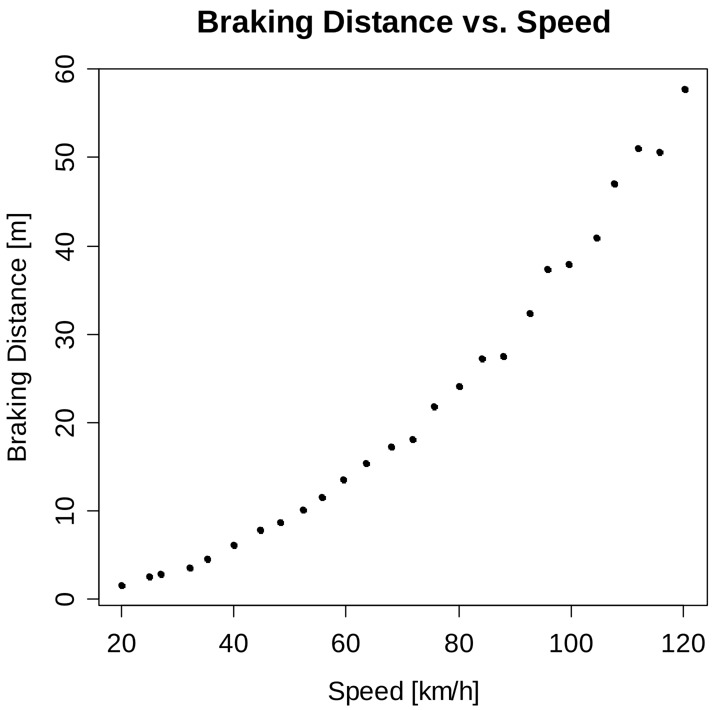
2.6 Model Extensions

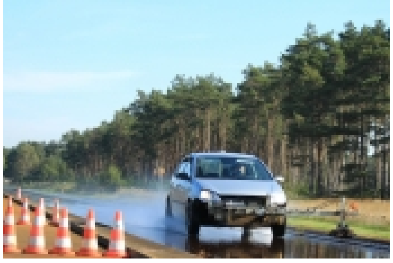
So far, linear regression was synonym to fitting a straight line in an xy-scatterplot. However, it has to offer much more: we can also fit curves, as long as we can describe them with a relation that is linear in the regression coefficients. The following example motivates why fitting curves can be a necessity.

2.6.1 Example: Automobile Braking Distance

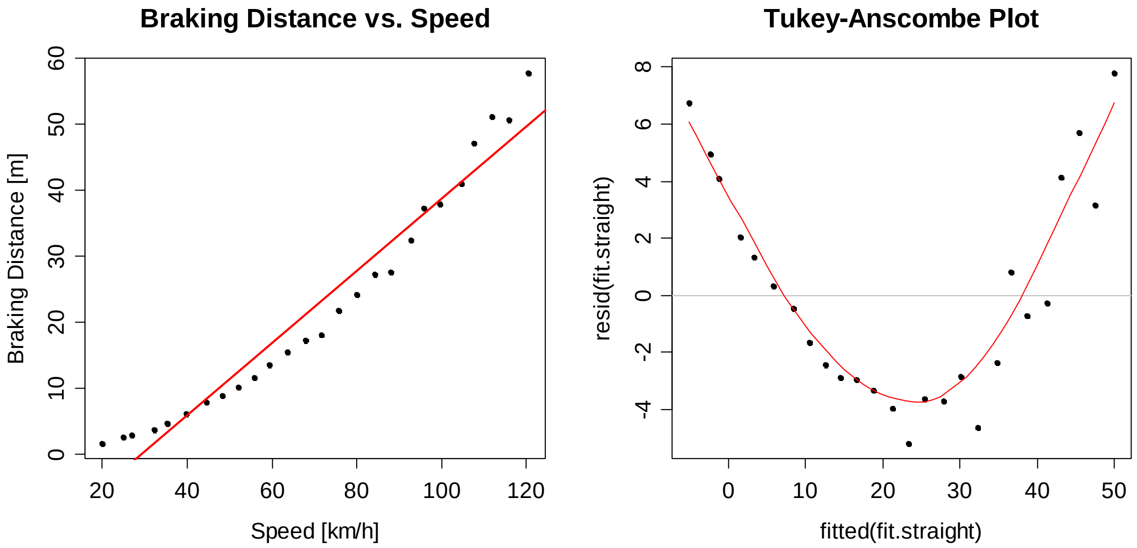
An automobile magazine tests summer tires with respect to the braking performance that is achieved. For acquiring data, a set of 26 test drives are made, where at various speeds the stopping distance is measured after a “pedal-to-the metal” braking procedure. The goal is to estimate the deceleration parameter.

obs	speed	brdist
1	19.96	1.60
2	24.97	2.54
3	26.97	2.81
4	32.14	3.58
5	35.24	4.59
6	39.87	6.11
7	44.62	7.91
8	48.32	8.76
9	52.18	10.12
10	55.72	11.62
11	59.44	13.57
12	63.56	15.45
...	...	...
24	111.97	51.09
25	115.88	50.69
26	120.35	57.77





Apparently, the relation between braking distance and speed is not a straight line, but seems to have a parabolic form. This is not surprising, as it is well known from physics that the energy and thus the braking distance go with the square of the speed, i.e. at double speed it takes four times as long to standstill. Moreover, there is some variability in the data. It is due to factors that have not been taken into account, mostly the surface conditions, tire and brake temperature, head- and tailwind, etc.



Fitting a plain linear function, i.e. laying a straight line through the data points results in a poor and incorrect fit. We have a strong systematic deviation from the regression line, and the Tukey-Anscombe plot shows a strong violation of the zero error assumption. As a way out, we better fit a quadratic function:

$$BrDist_i = \beta_0 + \beta_1 \cdot Speed_i^2 + E_i \text{, respectively}$$

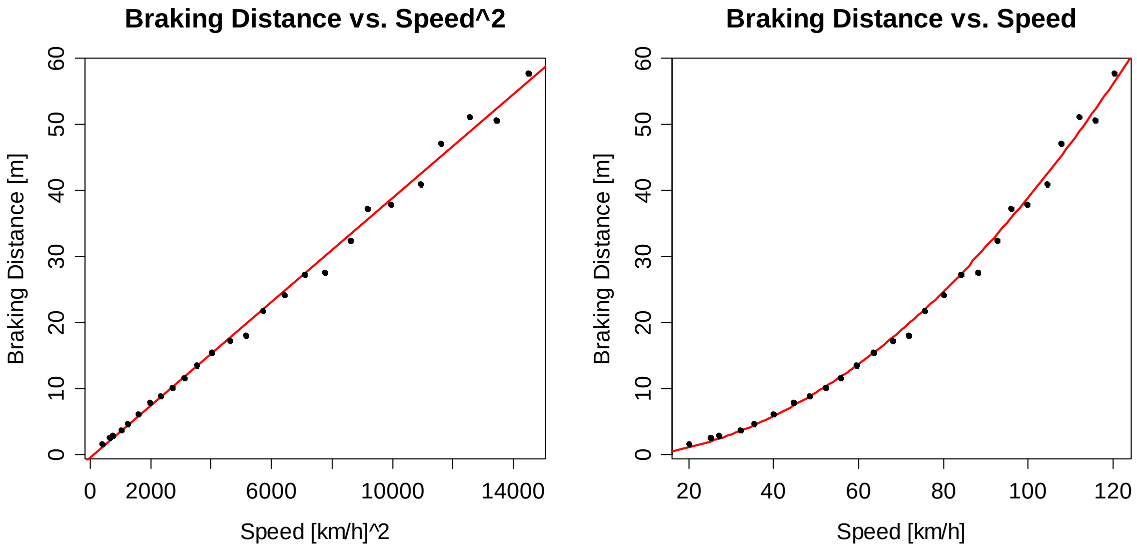
$$y_i = \beta_0 + \beta_1 \cdot x_i' + E_i \text{, where } x_i' = x_i^2 = Speed_i^2$$

The above model still is a simple linear regression problem. There is only one single predictor, the coefficients β_0, β_1 enter linearly and can be estimated with the OLS algorithm. Owing to the linearity, taking partial derivatives still works as usual here, and an explicit solution for $\hat{\beta}_0, \hat{\beta}_1$ will be found from the normal equations. In R, the syntax for fitting the quadratic function is as follows:

```
> fit.q <- lm(brdist ~ I(speed^2), data=abd)
```

When using powers as predictors, we should always use function `I()`. It prevents that the power is interpreted as a formula operator, when it in fact is an arithmetic operation that needs to be performed on the predictor values. It is important to note that the quadratic relation can either be interpreted as a straight line in a y vs. x^2 plot, or as a parabola in a regular y vs. x scatterplot. The following code can be used for visualizing the result:

```
> ## Braking Distance vs. Speed^2
> plot(brdist~speed^2, data=abd, main="...")
> abline(fit.q, col="red", lwd=2)
>
> ## Braking Distance vs. Speed
> yy <- predict(fit.q, newdata=data.frame(speed=10:130))
> plot(brdist ~ speed, data=abd, main="...")
> lines(10:130, yy, col="red", lwd=2)
```



As it seems at first impression, the parabola yields a good fit to the braking distance data. The regression coefficients can be used to estimate the deceleration which turns out to be roughly $-10m/s$. Some drawbacks of this model will be pointed out below.

2.6.2 Curvilinear Regression

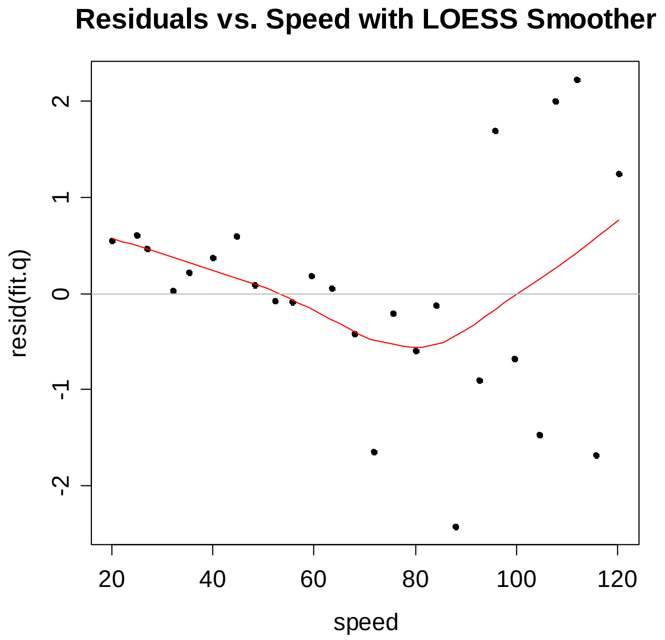
From the automobile example, we conclude that simple linear regression is more than just fitting straight lines. In fact, any curvilinear relation can be fitted, e.g.:

- $y = \beta_0 + \beta_1 \cdot \ln(x) + E$
- $y = \beta_0 + \beta_1 \cdot \sqrt{x} + E$
- $y = \beta_0 + \beta_1 \cdot x^{-1} + E$,

All these models, and many more, can be rewritten in the form $y = \beta_0 + \beta_1 x' + E$, where the predictor is either $x' = \ln(x)$, $x' = \sqrt{x}$ or $x' = x^{-1}$. Thus, estimating the parameters β_0, β_1 can be reduced to the well-known simple linear regression problem, for which the OLS algorithm can be used. While this may sound like the ideal solution to many regression problems, it is not, for a number of reasons.

First, when the residuals from the quadratic model are plotted versus predictor speed, it turns out that the situation is far less than optimal. Clearly apparent is a violation of the constant error-variance assumption. That is not so surprising, even without looking at the data; we might have expected that the scatter in braking distances becomes bigger as the speed increases. This is problematic because the high speed observations so (implicitly) obtain more weight in determining the regression coefficients. Consequently, we observe a bias for the low speed braking distances, because OLS focuses on the data points with large residuals on the right hand side, but puts less emphasis on what is going on at lower speeds.

```
> plot(speed, resid(fit.q))
> title("Residuals vs. Speed with LOESS Smoother")
> smoo <- loess.smooth(speed, resid(fit.q))
> lines(smoo, col="red")
> abline(h=0, col="grey")
```



Thus, while at first the parabola seemed to fit well to the data, closer inspection shows that we have not found a very good solution yet. Unfortunately, that is often the case when just single power terms are used as predictors.

2.6.3 Example: Infant Mortality

Our next goal is to study how infant mortality in a country depends on its wealth. We have observations from 105 countries; the data were first published in the New York Times in 1975. The infant mortality is measured as the (average) number of 1000 live born babies that do not reach the age of 5 years. The living standard is given as per-capita income in US$. They data are accessible in R's `library(car)` as `data(Leinhardt)`. For clarity, we remove four countries with partly missing values and two outliers: Saudi Arabia and Lybia, both oil-exporting countries with an inhomogeneous population consisting of a few very rich leaders and mostly poor population. The data can be displayed in a scatterplot:

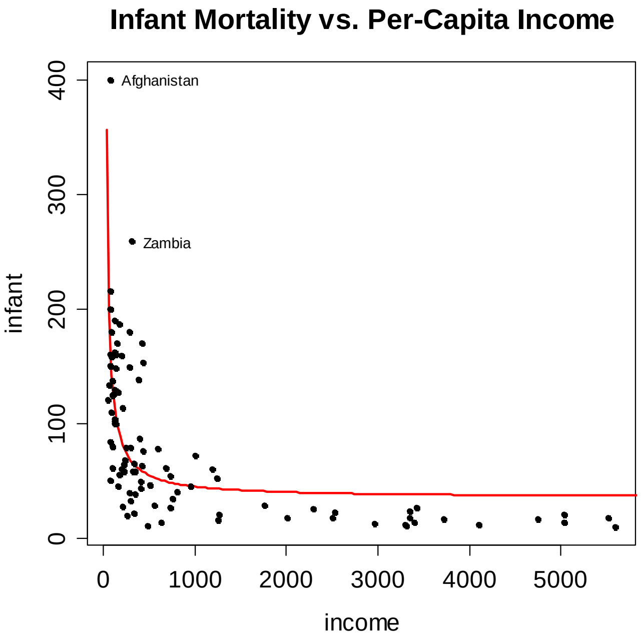
```
> plot(infant ~ income, data=im, pch=20)
> title("Infant Mortality vs. Per-Capita Income")
```

Since the relation between mortality and income seems to be inversely proportional, we might try a curvilinear regression model of the form:

$$infant \sim \beta_0 + \beta_1 \cdot (income)^{-1} + E$$

As explained in 2.6.2, this is a simple linear regression problem where we can estimate the coefficients with OLS. The result is added to the scatterplot.

```
> fit <- lm(infant ~ I(income^-1), data=im)
> xx  <- data.frame(income=seq(0, 6000, length=200))
> yy  <- predict(fit, newdata=xx, interval="prediction")
> lines(xx$income, yy[,1], col="red", lwd=2)
> points(infant ~ income, data=im, pch=20)
```



The resulting fit is poor, as the infant mortality is strongly overestimated in all rich countries. One might conclude that this is because we failed to identify the correct exponent for the *income* variable. Rather than just trying a few different powers, we might be tempted to estimate it from data, with a model such as:

$$y = \beta_0 + \beta_1 \cdot x^{\beta_2} + E$$

That however, is no longer a relation that is linear in the parameters. Least squares fitting, i.e. taking partial derivatives in the quality function will not lead to a linear equation system, because the result is of more complicated form.

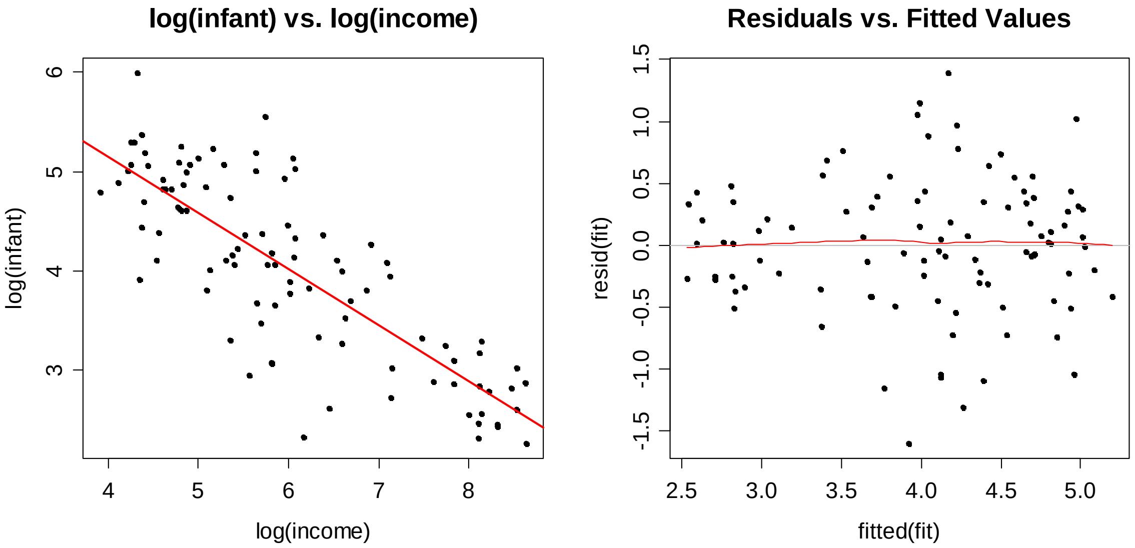
2.6.4 The log-log Model

In the above example, we are looking for a viable alternative to solve the regression problem. We could (and potentially would) resort to a numerical solution for minimizing the RSS, if there was not a much better analytical solution that is based on a simple, yet very powerful trick. The transformation

$$y' = \log(y), \;\; x' = \log(x)$$

is of great help, as we can see with a scatterplot in the log-log scale:

```
> plot(log(infant) ~ log(income), data=im, pch=20)
> title("log(infant) vs. log(income)")
> fit <- lm(log(infant) ~ log(income), data=im)
> abline(fit, col="red", lwd=2)
> plot(fitted(fit), resid(fit), pch=20)
> abline(h=0, col="grey")
> smoo <- loess.smooth(fitted(fit), resid(fit))
> lines(smoo, col="red")
> title("Residuals vs. Fitted Values")
```



After the variable transformations, the relation seems to be a straight line. The OLS regression line fits the data well, and the Tukey-Anscombe plot does not show strongly violated assumptions, except for a maybe slightly non-constant variance (that we accept here). What has happened? If a straight line is fitted on the log-log-scale, i.e.:

$$y' = \beta_0' + \beta_1' \cdot x' + E' \text{ where } y' = \log(y), \;\; x_i' = \log(x)$$

we can derive the relation on the original scale by taking the exponential function on both sides. The result is as follows:

$$y = \exp(\beta_0') \cdot x^{\beta_1'} \cdot \exp(E') = \beta_0 \cdot x^{\beta_1} \cdot E \text{ , with } \beta_0 = \exp(\beta_0') \text{ and } \beta_1 = \beta_1' .$$

The slope from the log-log-scale is the exponent to x on the original scale. Moreover, we have a multiplicative rather than an additive model, where the error term follows a log-normal distribution. Hence, the errors will scatter more the bigger x is, and are skewed towards the right, i.e. bigger values. While this model may seem arbitrary, it fits well in many cases, even more often than the canonical, transformation-free approach. The coefficients are:

```
> lm(log(infant) ~ log(income), data=im)
Coefficients:
(Intercept)  log(income)
     7.4134      -0.5661
```

The interesting part is the interpretation of the model equation. It is relative, in the following way: if x, i.e. the income increases by 1%, then y, i.e. the mortality decreases by $\hat{\beta}_1 = 0.56\%$. In other words, β_1 characterizes the relative change in the response y per unit of relative change in x.

For obtaining predictions of the infant mortality, we can use the regression model on the transformed scale, and then just re-exponentiate to invert the log-transformation:

$$\hat{y} = \exp(\hat{y}')$$

However, some care is required: due to the skewness in the lognormal distribution, the above is an estimate for the median of the conditional distribution $y \mid x$, but not for its mean $E[y \mid x]$. Often, the difference is small and can be neglected. However, in cases where we unbiased estimation is key, we can use a correction factor.

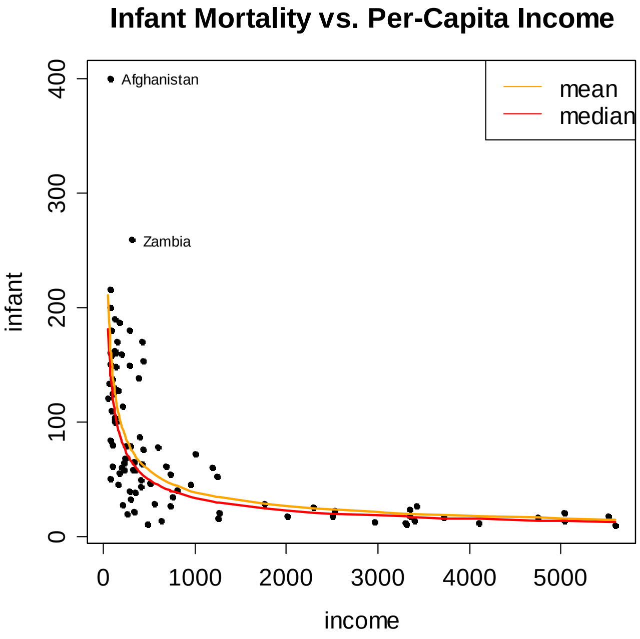
$$\hat{y} = \exp(\hat{y}' + \hat{\sigma}_E^2 / 2)$$

Owing to the exponential back-transformation, the fit on the original scale cannot take negative values. This is another aspect that here strongly speaks for fitting on the log-log-scale. A model that predicts negative values for infant mortality would not be plausible in practice.

For the confidence and prediction intervals, we can simply compute these as usual on the transformed scale. Simple re-exponentiating brings them back to the original scale. There is no need for a correction factor as we are dealing with quantiles of the respective distributions:

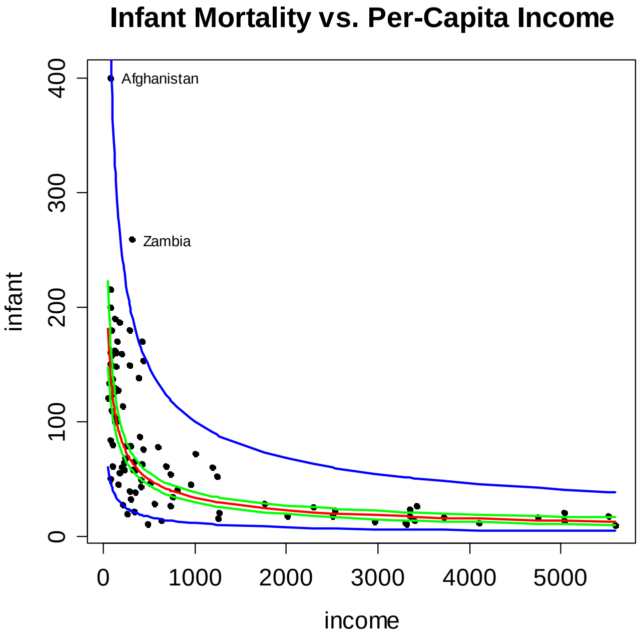
$$[l,u] \rightarrow [\exp(l), \exp(u)]$$

```
> ## Predictions
> po  <- exp(predict(fit))
> poc <- exp(predict(fit)+(summary(fit)$sigma^2)/2)
>
> ## Scatterplot with Fitted Curves
> plot(infant ~ income, data=im, pch=20)
> lines(sort(im$income), po[order(im$income)], col="red")
> lines(sort(im$income), poc[order(im$income)], col="orange")
```



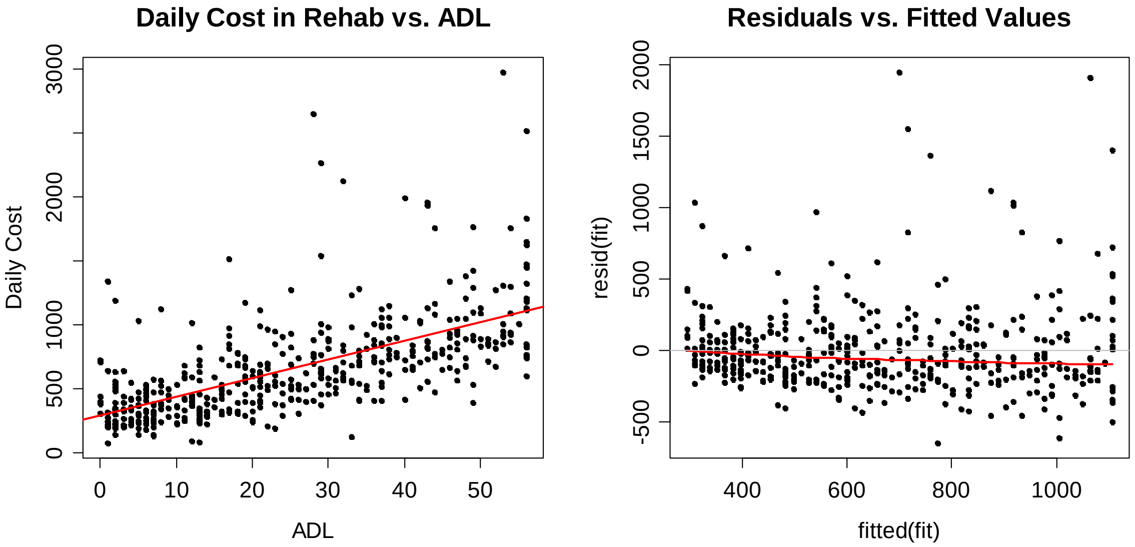
Again, an important advantage of the log-log-model is that neither of these intervals does take negative values on the original scale. Moreover, they are no longer symmetric, reflecting the fact that there is more room for error towards bigger values, and less towards smaller errors.

```
> poci  <- exp(predict(fit, interval="confidence"))
> popi  <- exp(predict(fit, interval="prediction"))
```



2.6.5 The Logged Response Model

This far, we considered log-transformations for both variables, as well as for the predictor only. If one sees this as a trick, rather than having a specific model formulation in mind, we might try to work with a logged response but the original predictor. As it turns out, also this model is widely used and accepted in practice. We illustrate it with the following example:



The data originate from a research project of the author. The goal was to study the *daily cost in neurological rehabilitation*. In seven hospitals, a random sample of 473 patients was studied, most of whom were originally suffering from *craniocerebral injuries* or *apoplectic strokes*. The total (time) effort for care, therapy and medical examinations was measured, expressed as CHF/day and serves as the response variable. Also, for each patient an ADL assessment was taken. It is based on about 20 items that quantify the autonomy of a patient in the *activities of daily life*, i.e. personal hygiene, feeding, etc..

Above, the data are visualized in a scatterplot. A simple linear regression model had been fitted, along with a Tukey-Anscombe plot for judging the quality of the fit. At first impression, the straight line does not fit too badly, but a closer inspection shows that there is a bias (i.e. *non-zero expectation for the error*), and a *right-skewed error distribution*. These are strong model violations, and thus, the simple linear model yields a poor explanation of the daily rehabilitation cost. As a way out, we suggest to log-transform the response variable, but to leave the predictor as is:

$$y' = \log(y),\ x' = x$$

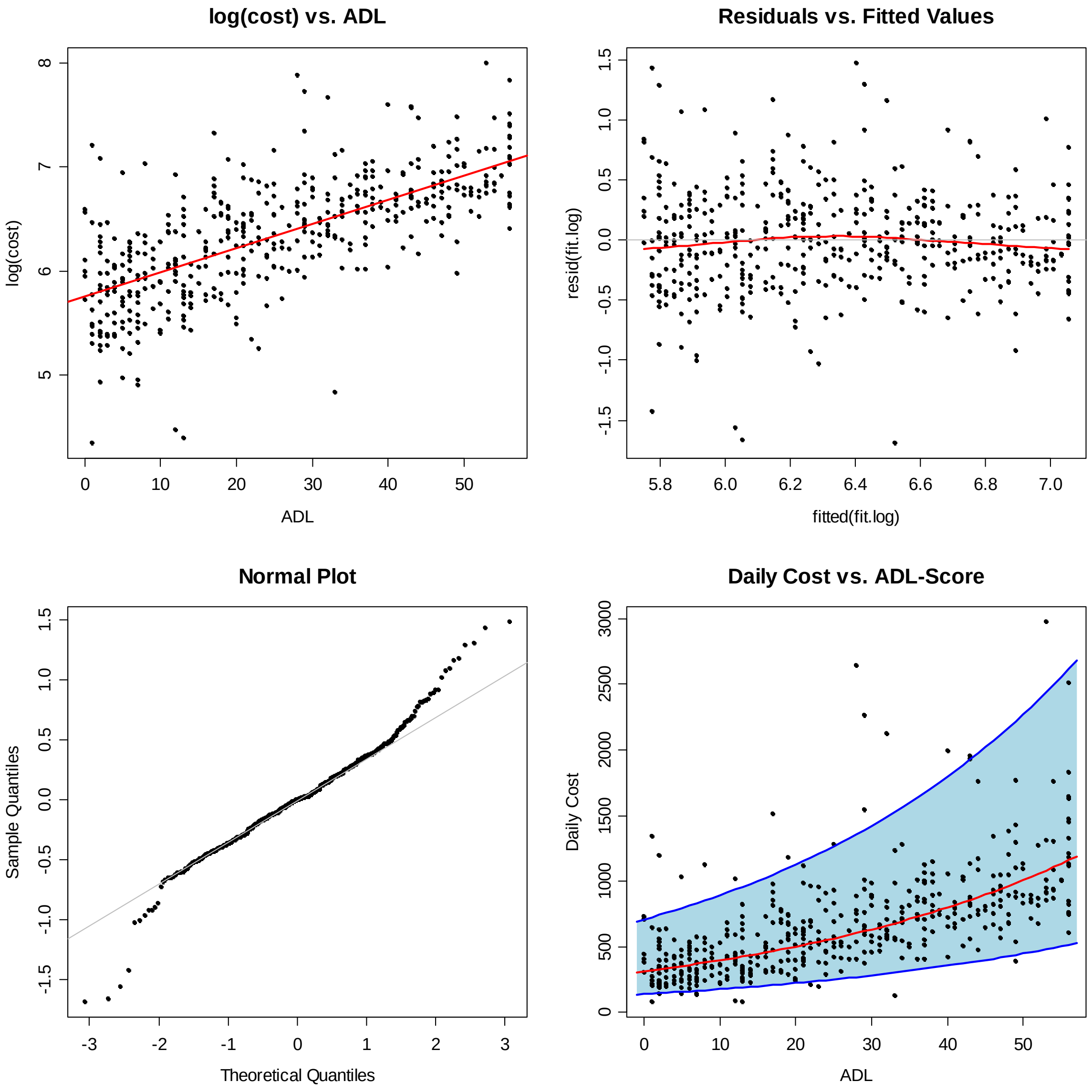
This simple trick yields a good fit, see below. Also, we will soon outline that the log-transformation is indicated for any right-skewed variable such as cost, whereas the uniformly distributed ADL predictor does not require action. The model is:

$y' = \log(y) = \beta_0 + \beta_1 x + E$, respectively, if we back-transform such that the response is on the original scale:

$$y = \exp(\beta_0) \cdot \exp(\beta_1 x) \cdot \exp(E) .$$

This is a multiplicative model. In contrast to the log-log model, β_1 is not an exponent controlling the curvature, but only a scale parameter to the predictor. The usual assumption for the error is $E \sim N(0, \sigma_E^2)$, and thus, we again have a multiplicative lognormal error term on the original scale. This results in right-skewed scatter that increases with increasing daily cost, matching what we observe in the data. The interpretation is as follows: *an increase by one unit in the predictor x multiplies the fitted value by* $\exp(\beta_1)$. In our case, one additional ADL point, meaning less autonomy of the patient, increases the cost on average by 2.36%. We then display fit, diagnostics and prediction interval:

```
> lm(log(cost) ~ adl, data=rehabilitation)
 (Intercept)          adl
    5.75106      0.02331
```



It turns out that after the transformation, a straight line provides a reasonable fit. Still, the Tukey-Anscombe plot exhibits a slight bias. The residuals follow a symmetric, but prominently long-tailed distribution. Hence, not all assumptions for OLS fitting are 100% fulfilled, but the situation is already much, much better than previously, with $daily\ cost\ vs.\ ADL$. Moreover, there are no more simple tricks or transformations with which we could improve the model further.

As a side note, we remark that further model improvement is possible here by using advanced methods such as Box-Cox transformations, or a generalized linear model based on the Gamma distribution. These topics are (far) beyond the scope of this introductory section on simple linear regression and thus not discussed here. It is also important to mention that while they are beneficial to the quality of the prognosis interval and the parameter tests, they do not improve the precisions of the point forecasts much.

2.6.6 When and How to Log-Transform

From the above examples, it is evident that variable transformations lead to novel predictor-response relations, often strongly improve the fit and are of tremendous importance to many applied regression problems. Thus, when and how to transform? Long-time practical experience has led to a few simple guidelines. A log-transformation of a variable, i.e. $x' = \log(x)$ and/or $y' = \log(y)$ is indicated and often very beneficial for the model fit if:

- Practice dictates that the regression line must run through $(0/0)$.
- Generally if a variable is on a scale that is left-closed with zero as the smallest possible value, but open to the right so that it can theoretically take arbitrarily large values.
- If the marginal distribution of a variable, as we can observe it from a histogram, is clearly skewed to the right. This is often the case for the above-mentioned variables that only take positive values.
- If a variable is “on a relative scale”, i.e. a change from 1 to 2 does not mean the same or have the same impact as from 100 to 101, but we rather need to care about the relative/percentage increase.

In summary, I dare to say that using the log-transformation is almost the norm rather than the exception when we talk about linear modeling. On the other hand, there are also variables where a transformation would be wrong, or is not possible at all. The latter concerns all variables that take negative values and even when there are zero values, we may run into problems, because the logarithm is defined for strictly positive values $x, y > 0$ only. In summary:

- For predictor/response variables that take negative values, the log-transformation, and hence the log-log model is typically not suitable.

- If either $y = 0$ or $x = 0$ appears, the log-transformation is still not possible. Do not exclude these data points from the analysis, this leads to a systematic error. One can though additively shift the variable: $x \leftarrow x + c$
- The usual choice for the constant is $c = 1$. However, this makes the regression model no longer invariant versus scale transformations. Thus, it is better (and recommended) to set c to the smallest value > 0.

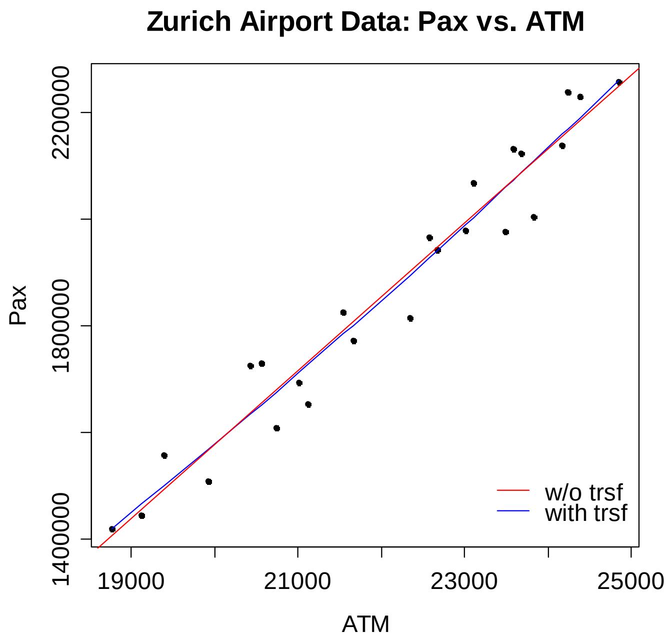
2.6.7 Final Considerations

By reflecting the previous examples, we notice that in the Leinhardt data both *infant mortality* and *income* are right-skewed variables which only take positive values. Thus, a log-transformation needs to be considered for both, and as the results from section 2.6.4 show, yields good results. Moreover, the *daily cost in neurological rehabilitation* is right-skewed and positive, while the predictor *ADL* is not. Hence only the response was log-transformed, again with good outcome. Finally, we turn our attention back to the Zurich Airport example. One aspect is that the residual plots in section 2.3.4 raised some doubts whether the straight line is a trustworthy result. And then, both *Pax* and *ATM* are positive variables what makes them candidates for a transformation.

$$ATM' = \log(ATM),\ Pax' = \log(Pax)$$

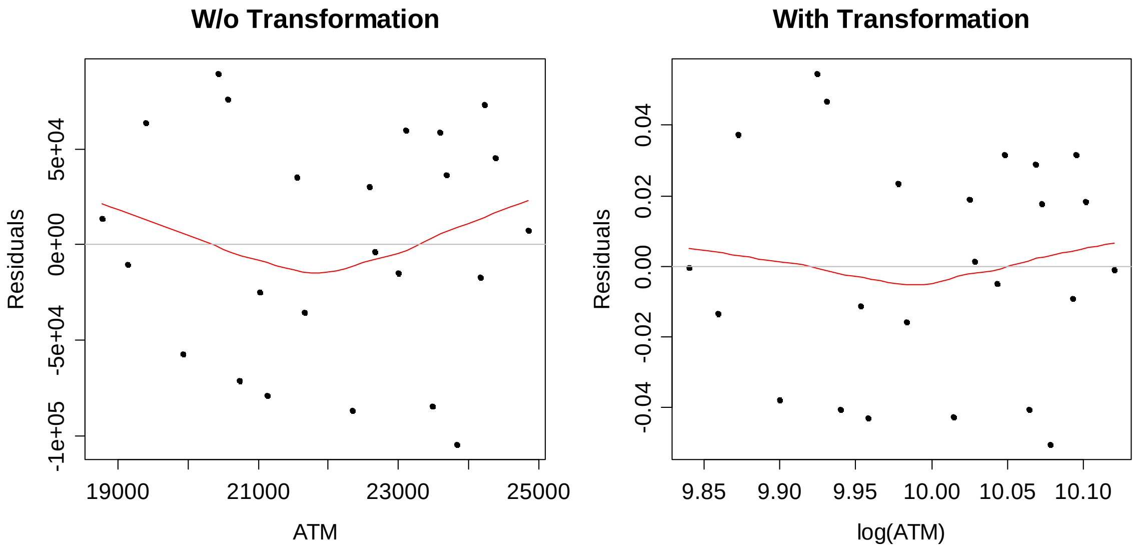
The code for fitting the model and producing a scatterplot is:

```
> fit        <- lm(Pax ~ ATM, data=unique2010)
> fit.log    <- lm(log(Pax) ~ log(ATM), data=unique2010)
> fit.y.orig <- exp(fitted(fit.log)[order(unique2010$ATM)])
> plot(Pax ~ ATM, data=unique2010, main="...")
> lines(sort(unique2010$ATM), fit.y.orig, col="blue")
> abline(fit, col="red")
```



The result no longer corresponds to a straight line into the scatterplot, but a curve. Additionally, the increase in *Pax* is no longer linear with *ATM*, but relative. The difference between the two solutions seems to be minimal. Still, the variable transformations improve, as we can see from the residual plots:

```
> xx <- unique2010$ATM
> yy <- residuals(fit)
> plot(xx, yy, xlab="ATM", ylab="Residuals", main="...")
> lines(loess.smooth(xx,yy),col="red")
> abline(h=0, col="grey")
> xx <- log(unique2010$ATM)
> yy <- residuals(fit.log)
> plot(xx, yy, xlab="log(ATM)", ylab="Residuals", main="...")
> lines(loess.smooth(xx,yy),col="red")
> abline(h=0, col="grey")
```



The log-log-model manages to reduce the bias of the plain linear one, although there is still some kink in the residuals. But the log-log-model has another attractive point: it does no longer predict negative *Pax* values - though that does not mean it is safe for extrapolation! The coefficients are:

```
> lm(log(Pax) ~ log(ATM), data=unique2010)
Coefficients:
(Intercept)     log(ATM)
     -2.116        1.655
```

Thus, the fitted relation corresponds to:

$y = \exp(-2.116) \cdot x^{1.655}$, resp. $Pax = 0.120 \cdot ATM^{1.655}$

So, if *ATM* increases by 1%, then *Pax* increases by 1.655%. That is at least as plausible as an increase of 138.8 passengers per additional flight, because it is well known that the seat load factor is higher and bigger airplanes are used in busy times with more air traffic movements.

3 Multiple Linear Regression

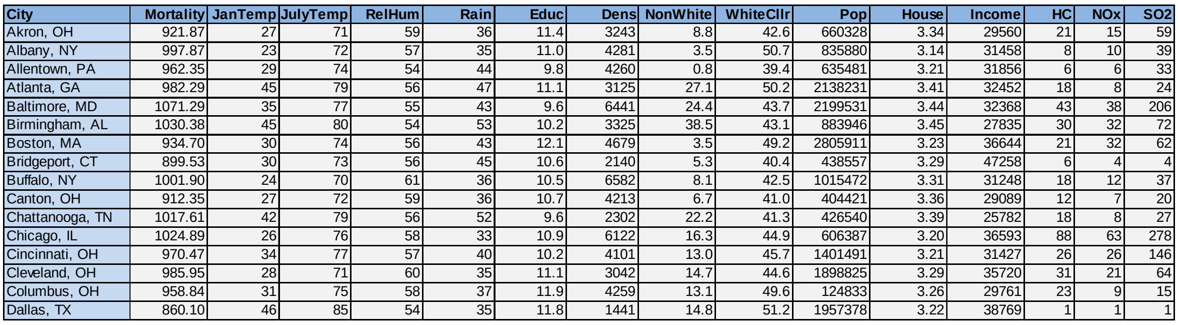
It is very rare that the variation in a response variable y is due to one single predictor only. Even for the relatively trivial *Pax* vs. *ATM* example, the seat load factor and the amount of cargo that is handled may play an important role, too. For the other examples that were considered in section 1.1, the dependency on several input variables was clearly pointed out. We will now address the methodology for estimating multiple linear regression models where:

$$y = \beta_0 + \beta_1 x_1 + ... + \beta_p x_p + E \, .$$

We will continue using OLS for estimating the coefficients $\beta_0, ..., \beta_p$. However, a number of new issues arise here; the most important perhaps being the fact that visualizing the relation is no longer easily possible. Thus, understanding the input and output becomes an important and challenging task.

3.1 Example: Air Pollution and Mortality

Since the beginning of the environmental movement, attention has focused on the protection of human health. Soon, air pollution was identified as a major threat to well-being. Therefore, researchers at General Motors collected data on 59 US Standard Metropolitan Statistical Areas for a study whether air pollution contributes to the age-adjusted mortality of the population. The *apm* dataset includes predictors measuring demographic characteristics of the cities, variables measuring climate parameters and finally three records for the air pollution in the ambient air: concentrations of hydrocarbons (HC), nitrous oxide (NO_x) and sulfur dioxide (SO_2). An excerpt of the data is as follows:



City	Mortality	JanTemp	JulyTemp	RelHum	Rain	Educ	Dens	NonWhite	WhiteCllr	Pop	House	Income	HC	NOx	SO2
Akron, OH	921.87	27	71	59	36	11.4	3243	8.8	42.6	660328	3.34	29560	21	15	59
Albany, NY	997.87	23	72	57	35	11.0	4281	3.5	50.7	835880	3.14	31458	8	10	39
Allentown, PA	962.35	29	74	54	44	9.8	4260	0.8	39.4	635481	3.21	31856	6	6	33
Atlanta, GA	982.29	45	79	56	47	11.1	3125	27.1	50.2	2138231	3.41	32452	18	8	24
Baltimore, MD	1071.29	35	77	55	43	9.6	6441	24.4	43.7	2199531	3.44	32368	43	38	206
Birmingham, AL	1030.38	45	80	54	53	10.2	3325	38.5	43.1	883946	3.45	27835	30	32	72
Boston, MA	934.70	30	74	56	43	12.1	4679	3.5	49.2	2805911	3.23	36644	21	32	62
Bridgeport, CT	899.53	30	73	56	45	10.6	2140	5.3	40.4	438557	3.29	47258	6	4	4
Buffalo, NY	1001.90	24	70	61	36	10.5	6582	8.1	42.5	1015472	3.31	31248	18	12	37
Canton, OH	912.35	27	72	59	36	10.7	4213	6.7	41.0	404421	3.36	29089	12	7	20
Chattanooga, TN	1017.61	42	79	56	52	9.6	2302	22.2	41.3	426540	3.39	25782	18	8	27
Chicago, IL	1024.89	26	76	58	33	10.9	6122	16.3	44.9	606387	3.20	36593	88	63	278
Cincinnati, OH	970.47	34	77	57	40	10.2	4101	13.0	45.7	1401491	3.21	31427	26	26	146
Cleveland, OH	985.95	28	71	60	35	11.1	3042	14.7	44.6	1898825	3.29	35720	31	21	64
Columbus, OH	958.84	31	75	58	37	11.9	4259	13.1	49.6	124833	3.26	29761	23	9	15
Dallas, TX	860.10	46	85	54	35	11.8	1441	14.8	51.2	1957378	3.22	38769	1	1	1

Most of the variables are self-explanatory: the temperatures are averages in degrees Fahrenheit, humidity is a percentage, the rainfall is given as annual sum in inches, education is the median number of years in the population, which itself is given as an absolute number, as well as a density per area and housing unit. Moreover, we have the percentages of non-white inhabitants and white collar workers, the median per-capita income and finally the concentrations of the pollutants.

The task is to study how *air pollution contributes to mortality*. Thus, the influence of the three pollution variables is of primary interest. The remaining ones can be seen as potentially confounding factors, for which we try to correct. Since we know that mortality is affected by other causes than just the pollution alone, we have to correct for the effect of these covariates. Just studying the relation between mortality and pollution would lead to flawed results. Fortunately, with multiple linear regression we can incorporate all covariates and derive sound conclusions.

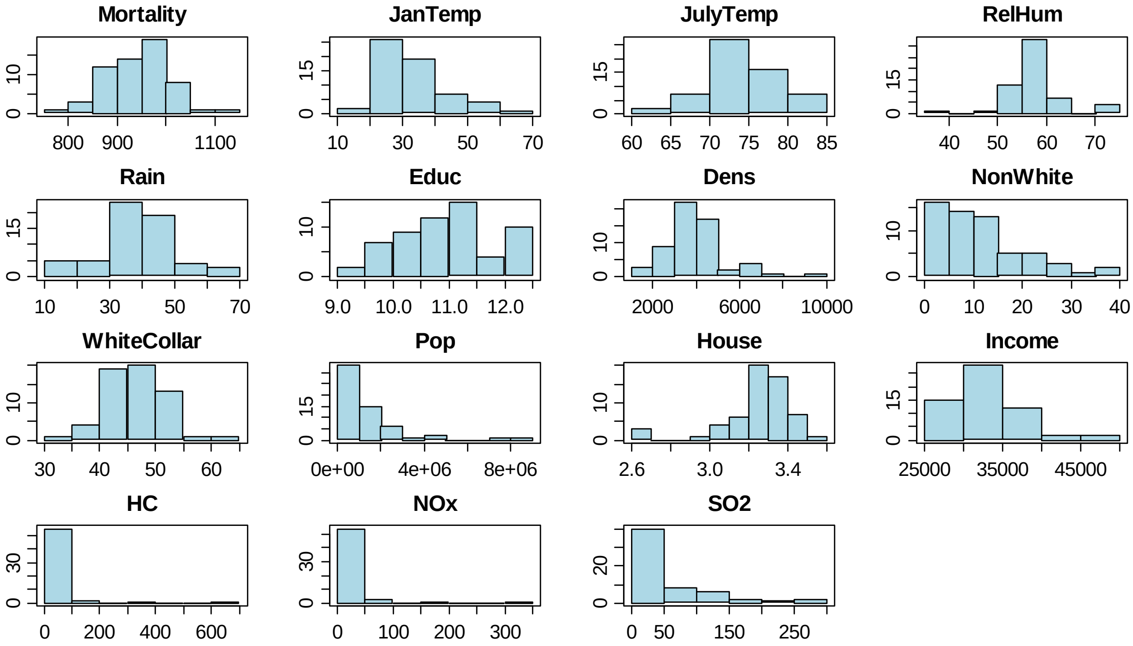
3.2 Preparing the Data

For simple regressions, we were able to visualize the data in an xy-scatterplot. This was beneficial for identifying the correct response-predictor relation, making variable transformations, detecting outliers and some further potential problems. In the present example, the data live in a 15-dimensional space, and there is no plot that can show them in full generality. Still, gaining an impression of the data and preparing them well for regression analysis is absolutely essential.

3.2.1 Marginal Plots

As a way out, we can visualize the univariate distribution of response and predictors with histograms (or barplots, should there be categorical predictors). As mentioned above, this does not give the full multivariate picture, but it still allows for detecting skewness in the variables, the presence of outliers and perhaps other important specialties such as missing values that are coded with numerical values.

```
> par(mfrow=c(4,4))
> for (i in 1:15) hist(apm[,i], title=”...”)
```



What immediately catches the attention is the extreme skewness of the pollution variables. This needs to be addressed with variable transformations; else the results from a multiple linear regression will be poor. Furthermore, also the population is right-skewed. Apart from this, there do not seem to be too many peculiarities in the *apm* data. An analysis using the R command

```
> any(is.na(apm))
[1] FALSE
```

shows that there are no missing values coded by `NA`. Neither do we have any suspicions that they might be coded by some numerical value. If that was the case, we urgently need to clarify the issue, and set the respective values to `NA`. Besides the histograms, one could also do scatterplots of the response variable vs. each of the predictors (or boxplots, in case of categorical predictors). Again, this does not visualize the multivariate setting in full depth, and is mostly less useful than the histograms shown above.

3.2.2 Variable Transformations

Regression results will be much easier to understand if the data are in units that we are well familiar with. In the context of the mortality example that means converting the temperatures to degrees Celsius rather than Fahrenheit, and rainfall in $cm / year$ rather than $inches / year$. We copy the original data frame, generate the new variables and drop the old ones:

```
> apm$JanTemp  <- (5/9)*(apm$JanTemp-32)
> apm$JulyTemp <- (5/9)*(apm$JulyTemp-32)
> apm$Rain     <- (2.54)*apm$Rain
```

All of the above are linear variable transformations of the form $x' = ax + b$. It is very important to notice that these do not change the regression output: all fitted values, tests and the prediction interval will remain identical. The only thing that changes is the coefficient β_j and its standard error, but only to account for transformation that was made.

This is clearly not the fact for non-linear transformations such as the log (or also the square root, the inverse, etc.): they ultimately change the regression relation and all results (fitted values, tests, confidence intervals, ...) will be different. The change is not necessarily for the bad, and thus we carry out the transformations that are indicated on the *apm* data. That includes taking the $\log(\cdot)$ for the three pollution variables plus the population. Most other predictors are annual sums or averages, show sufficiently symmetrical distribution and are left alone.

Implementation-wise, we do not carry out these transformations in the data frame, but choose the convenient option of writing the `log(Pop)`, `log(HC)`, `log(NOx)` and `log(SO2)` terms directly into the model equation, see below.

3.3 Model and Estimation

What to do with such cases, where multiple predictor variables are available? The poor man's approach would be to do many simple linear regressions on each of the predictors separately. This has the somewhat doubtful advantage that the relation between each predictor and the response can be displayed in a two-dimensional scatterplot. However, it is very important to note that *doing many simple linear regressions is not equivalent to a multiple linear regression*. The findings, i.e. the regression coefficients and their p-values, will generally be different. The only case when they are identical is if the predictors are exactly orthogonal; and this is almost never the case with data from observational studies.

As indicated above, the appropriate tool for simultaneously including the effects of several predictors at a time is *multiple linear regression*. Geometrically speaking, one tries to fit the least squares hyperplane in the $(p+1)$-dimensional space (p is the number of predictors). Generally, this fit cannot be visualized if $p > 2$. We start our discussion with a simple example that illustrates some of the peculiarities of multiple linear regression.

Example

In this artificial example, there are only 2 predictors and 8 observations. Because the optimal solution is obvious, we do not need to estimate the regression coefficients but can guess them. The data are as follows:

Observation	x1	x2	yy
1	0	-1	1
2	1	0	2
3	2	1	3
4	3	2	4
5	0	1	-1
6	1	2	0
7	2	3	1
8	3	4	2

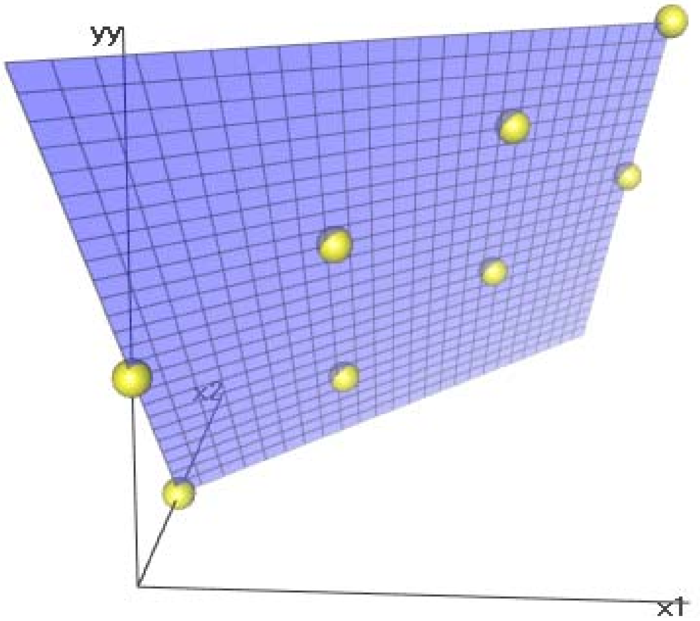
The optimal solution of the multiple regression problem for the above data is

$$y_i = 2x_{i1} - x_{i2} \text{ for all } i = 1,...,8$$

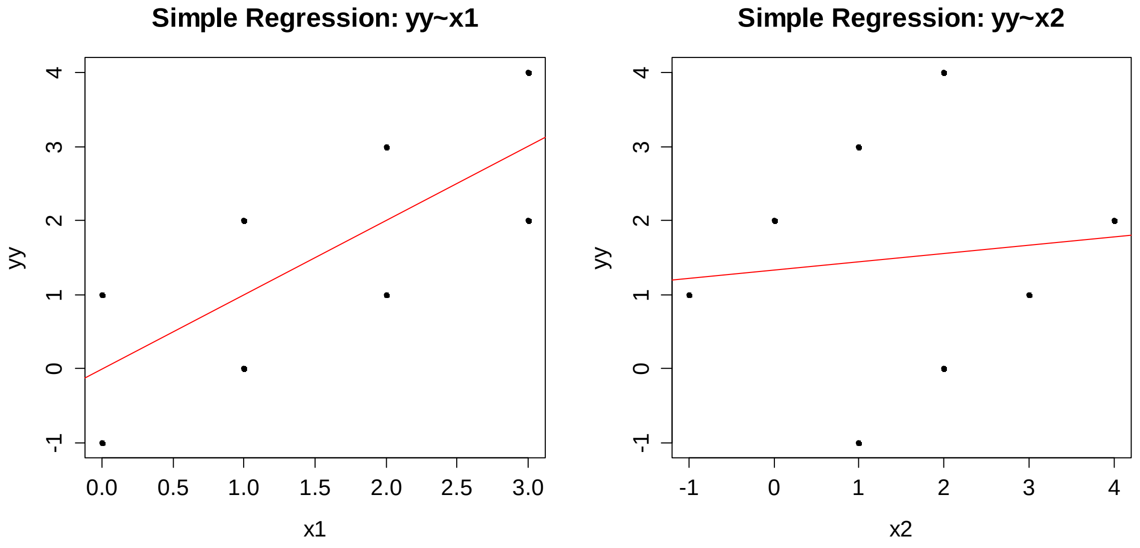
We are in a very special situation and have a perfect fit, thus there are no errors.

Because there are only two predictors plus the response, we can visualize the fit in a 3d-scatterplot. As we observe below, the data points lie in a plane, the regression plane.

```
> toy.ex <- data.frame(x1=c( 0,1,2,3, 0,1,2,3),
                       x2=c(-1,0,1,2, 1,2,3,4),
                       yy=c( 1,2,3,4,-1,0,1,2))
> library(Rcmdr)
> attach(toy.ex)
> scatter3d(yy ~ x1 + x2, axis.scales=FALSE)
> detach(toy.ex)
```



To convince ourselves that single and multiple linear regression is not one and the same thing, we regress $y \sim x_1$ and $y \sim x_2$. We can visualize these fits in two-dimensional scatterplots.



The slope estimates from the simple regressions turn out to be 1.00 and 0.11, respectively. Hence they are both different than the coefficients for x_1 and x_2 in the (perfect) solution from multiple linear regression. Moreover, we do not achieve a perfect fit in neither of the two simple models. Hence, for describing the variation in y, we need to build on both variables x_1 and x_2 simultaneously.

3.3.1 Notation

We turn our attention back to the mortality example in dataset *apm*. In colloquial formulation, the multiple linear regression model is as follows:

$$Mortality_i = \beta_0 + \beta_1 \cdot JanTemp_i + \beta_2 \cdot JulyTemp_i + ... + \beta_{14} \cdot \log(SO_2)_i + E$$

More generally and technically, the multiple linear regression model specifies the relation between response y_i and predictors $x_{i1},...,x_{ip}$ for observations $i = 1,...,n$, including a random error term E_i. The double index notation is defined as:

$$y_i = \beta_0 + \beta_1 x_{i1} + ... + \beta_p x_{ip} + E_i \text{, for } i = 1,...n\,.$$

The term β_0 is still called *intercept* and corresponds to the (theoretical) mortality value when all predictors $x_{i1} = x_{i2} = ... = x_{ip} = 0$. The remaining parameters $\beta_1,...,\beta_p$ are, in contrast to simple regression, no longer called slope(s), but just *regression coefficients*. The interpretation is as follows:

> *The regression coefficient β_j is the increase in the response y when predictor x_j increases by 1 unit, but all other predictors remain unchanged.*

A more convenient way of writing down a multiple linear regression model is with the so-called matrix notation. It is simply:

$$y = X\beta + E \text{, with } y = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix},\ X = \begin{pmatrix} 1 & x_{11} & x_{12} & ... & x_{1p} \\ 1 & x_{21} & x_{22} & ... & x_{2p} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{n1} & x_{n2} & ... & x_{np} \end{pmatrix},\ \beta = \begin{pmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{pmatrix},\ E = \begin{pmatrix} E_1 \\ E_2 \\ \vdots \\ E_n \end{pmatrix}.$$

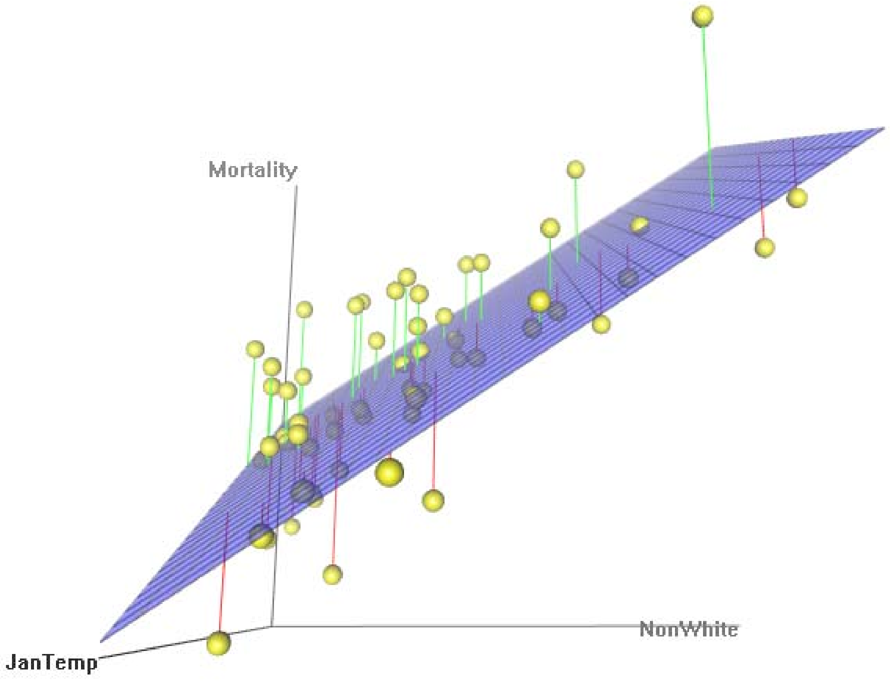
The terms in this equation are called the *response vector*, the *design matrix*, the *coefficient vector* and the *error vector*. If a matrix multiplication is carried out and the result is written down, we are back with the double index notation. This also illustrates the role of the particular first column of the design matrix: it is the intercept, which is also part of multiple linear regression.

Our next goal is to fit a multiple linear regression model. The task which needs to be done is to estimate the coefficient vector β from the data; in a way that the solution is optimal. The criterion is still to minimize the sum of squared residuals. The next section illustrates the concept with an example and then focuses on the solution plus some technical aspects.

3.3.2 OLS: Method & Identifiability

For illustrating the concept of least squares regression, we consider the mortality data with two predictors only: *NonWhite* and *JanTemp*. The regression coefficients are estimated such that the sum of squared residuals is minimal. The fitted regression plane with the residuals looks as follows:

```
> scatter3d(Mortality~NonWhite+JanTemp, axis.scale=FALSE)
```



We observe that the mortality decreases with higher winter temperatures, and increases in urban regions with more non-white population. The basis for finding this solution lies in the residuals, which are:

$$r_i = y_i - (\beta_0 + \beta_1 x_{i1} + ... + \beta_p x_{ip}) .$$

Then, we choose the parameters $\beta_0,...,\beta_p$ such that the sum of squared residuals is minimal. We again formulate the quality function.

$$Q(\beta_0,\beta_1,...,\beta_p) = \sum_{i=1}^{n} r_i^2 = \sum_{i=1}^{n} (y_i - (\beta_0 + \beta_1 x_{i1} + ... + \beta_p x_{ip}))^2$$

We need to minimize this function, which can be tackled by taking partial derivatives and setting them to zero. This results in the so-called *normal equations*. We do now take full advantage of the matrix notation that was introduced above and can write the normal equations as

$$(X^T X)\beta = X^T y .$$

If $X^T X$ is *invertible* (or *regular*), we can obtain the least squares estimates of the regression coefficients by some simple matrix calculus as $\hat{\beta} = (X^T X)^{-1} \cdot X^T y$.

If the regularity condition for $X^T X$ is fulfilled, there is a unique and explicit solution for the regression coefficients $\hat{\beta}$, and thus no numerical optimization is needed. A side remark: in software packages, the inverse of $X^T X$ is usually not computed for numerical reasons, but the computations will be based on a QR-decomposition or similar methods of simplifying $X^T X$. In R, multiple linear least squares regression is carried out with command `lm()`. The syntax is as follows:

```
fit <- lm(Mortality ~ JanTemp + JulyTemp + RelHum + Rain +
                      Educ + Dens + NonWhite + WhiteCollar +
                      log(Pop) + House + Income + log(HC) +
                      log(NOx) + log(SO2), data=apm)
```

As in simple linear regression, we have the response variable on the left hand side. It is related to the predictors on the right hand side, which are joined by '+' signs. Note that potential log-transformations of predictors and/or response can directly be written into the formula, and that we need to specify the data frame from which the variables need to be taken.

It is worth noting that there is a simple variant of specifying regression problems with many predictors in R. The notation `lm(Mortality ~ ., data=apm)` means that mortality is explained by all the other variables that exist in data frame *apm*. However, in our example these two commands will not yield identical results, because of the log-transformations that are missing in the short notation. Once the model is fitted, we can extract the regression coefficients, here rounded to two digits, by:

```
> round(coef(fit),2)
(Intercept)     JanTemp    JulyTemp       RelHum         Rain
    1297.38       -2.37       -1.75         0.34         1.49
       Educ        Dens    NonWhite  WhiteCollar     log(Pop)
     -10.00        0.00        5.15        -1.88         4.39
      House      Income     log(HC)     log(NOx)     log(SO2)
     -45.74        0.00      -22.04        33.97        -3.69
```

We claimed above that the normal equations have a unique solution if and only if $X^T X$ is regular and thus invertible. This is the case if X has full rank, i.e. all columns of the design matrix, or in other words, all predictor variables are linearly independent. This is often the case in practice, and whenever the full rank condition for X is fulfilled, we are fine.

On the other hand, there will also be cases where X does not have full rank and $X^T X$ is singular. Then, there are usually infinitely many solutions. Is this a problem? And how does it occur? The answer to the first question is "yes". When the design matrix X does not have full rank, the model is "poorly formulated", such that the regression coefficients β are at least partially unidentifiable. It is mandatory to improve the design, in order to obtain a unique solution, and regression coefficients with a clear meaning. Below, we list some typical mistakes that lead to a singular design.

1) **Duplicated variables**

   It could be that we use a person's height both in meters and centimeters as a predictor. This information is redundant, and the two variables are linearly dependent. One thus has to remove one of the two.

2) **Circular variables**

   Another example is when the number of years of pre-university education, the number of years of university education and also the total number of years of education are recorded and included in the model. These predictors will be linearly dependent, thus X does not have full rank.

3) **More predictors than cases**

   Note that a necessary (but not sufficient) condition for the regularity of $X^T X$ is $p < n$. Thus, we need more observations than we have predictors! This makes sense, because the regression is over-parameterized (or super-saturated) else and will not have a (unique) solution.

What does R do in non-identifiable problems?

Generally, statistics packages handle non-identifiability differently. Some may return error messages; some may even fit models because rounding errors kill the exact linear dependence. R handles this a bit different: it recognizes unidentifiable models and fits the largest identifiable one by removing the excess predictors in reverse order of appearance in the model formula. The removed predictors will still appear in the summary, but all their values are `NA`, and a message also says "`Coefficients: k not defined because of singularities`"). While this still results in a fit, it is generally better in such cases to rethink the formulation of the regression problem, and remove the non-needed predictors manually.

Estimation of the Error Variance

An additional quantity that is a necessary ingredient for all tests and confidence intervals needs to be estimated from the data: it is the error variance σ_E^2. The estimate can be obtained by standardizing the sum of squared residuals with the appropriate degrees of freedom, which is the number of observations n minus the number of estimated parameters. With p predictor variables and an intercept, this amounts to $p+1$, and the error variance estimate is:

$$\hat{\sigma}_E^2 = \frac{1}{n-(p+1)} \sum_{i=1}^{n} r_i^2 \,.$$

In the next section, we will discuss if and when the OLS results are a good solution. The assumptions are identical to the ones we had in simple linear regression, as is the main result, the Gauss-Markov theorem. By assuming a Gaussian distribution for the errors, we can show even more and lay the basis for inference in multiple linear regression.

3.3.3 Properties of the Estimates

The use of the least squares procedure is attractive due to its simplicity and the explicit solution that can be found without any numerical optimization. Additionally, there are some mathematical optimality results that further justify its application. However, we require some conditions for being able to derive them, namely:

$$E[E_i] = 0 .$$

Again this means that there is no systematic error, i.e. the true relation between predictors and response is the linear function that we imposed. Or in other words: the hyper plane is the correct fit. Additionally, we require constant variance of the error term, i.e.

$$Var(E_i) = \sigma_E^2 .$$

Finally, there must not be any correlation among the errors for different instances, which boils down to the fact that the observations, respectively their errors, do not influence each other, and that there are no latent variables (e.g. time/sequence of the measurements) that do so. In particular,

$$Cov(E_i, E_j) = 0 \text{ for all } i \neq j .$$

Under these three conditions, we can derive that the coefficient estimates are unbiased and find their covariance matrix. The *Gauss-Markov theorem* states that there is *no other linear, unbiased estimator that is more efficient*.

$$E[\hat{\beta}] = \beta \text{ and } Cov(\beta) = \sigma_E^2 \cdot (X^T X)^{-1},$$

As in simple linear regression, the precision of the regression coefficients depends on the design and the number of observations which are present. While the Gauss-Markov theorem does not require the assumption of normally distributed errors E_i, be careful in case of clearly non-Gaussian distribution. On one hand, there may be non-linear estimators that are clearly more efficient than OLS, and even more importantly, all inference results (i.e. *tests, confidence intervals, prediction interval*) to be discussed below ultimately require independent Gaussian errors. Hence it is standard to also require

$$E_i \textit{ i.i.d.} \sim N(0, \sigma_E^2)$$

for OLS regression. Then, and only then, the estimators for the regression coefficients will follow an exact Gaussian distribution, as will the distribution of the fitted values. The specifications are as follows:

$$\hat{\beta} \sim N\left(\beta, \sigma_E^2 (X^T X)^{-1}\right) \text{ and } \hat{y} \sim N(X\beta, \sigma_E^2 X (X^T X)^{-1} X^T)$$

For error distributions that deviate from the Gaussian, we can rely on the central limit theorem. It tells us that asymptotically (i.e. for large samples) the normal distribution of the estimates will still hold. Thus, small deviations from Gaussian errors may be tolerable in practice. It is generally an expert call what is alarming and what is acceptable, but the bigger the dataset and the less extreme the error distribution deviates, the more tolerable one can be. Also, deviations from normal errors are usually less worrying if the task is prediction, but more so if one is after inference with exact p-value reporting.

As mentioned above, both $\hat{\beta}$ and $\hat{y}$ are unbiased estimates and since their covariance matrices and distribution is known, confidence intervals and tests can be determined. Another important result from mathematical statistics is also that under Gaussian distribution, OLS is the *maximum likelihood estimator* (MLE). Hence there cannot be any other unbiased estimator that is asymptotically more efficient than OLS. Please note that this statement is stronger than the Gauss-Markov theorem, but it requires more, namely normal errors.

In summary, there are very good reasons to prefer OLS over other methods to estimate the linear regression coefficients. However, we require that the four assumptions made are at least roughly fulfilled. This needs to be verified by a number of model diagnostic plots, as shown in section 3.7 of this scriptum. In case of clear violations, one usually tries to improve the model with variable transformations, which rightly done serves to achieve better behaved errors. Alternatively, more complicated estimation procedures that require fewer assumptions can sometimes be used instead.

Hat Matrix

For the mathematically interested, we will now take further advantage of the matrix notation and study the solution of the OLS algorithm. We can write the fitted values $\hat{y}$ very simply as

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

We now do some further calculus and plug-in the solution for $\hat{\beta}$ from above. We then observe that the fitted values $\hat{y}$ are obtained by a matrix product, namely the *hat matrix* H, with the observed response values y :

$$\hat{y} = X\hat{\beta} = X(X^TX)^{-1}X^Ty = Hy$$

The matrix H is called hat matrix, because "it puts a hat on the y's", i.e. transforms the observed values into fitted values. This clarifies that the OLS estimator is linear and opens the door to a geometrical interpretation of the procedure: the hat matrix H is the *orthogonal projection* of the response y onto the space spanned by the columns of the design matrix X. Please note that (except for some rare cases with perfect fit), we cannot linearly combine the columns of the design matrix to generate the response y. The OLS solution then is the best approximation, in the sense of an orthogonal projection.

Disclaimer: do not worry if this geometric notion of OLS regression is hard to grasp. It is a nice interpretation for those with imagination and the necessary background in linear algebra , but it is of little practical importance.

3.4 Inference

Here, we will discuss some methods for inferring the relation between response and predictor. While a few topics are a repetition to the inference topics in simple linear regression, quite a number of novel aspects pop up, too. Please note that except for the coefficient of determination, the assumption of *independent, identically distributed Gaussian errors* is central to derive the results.

3.4.1 The Coefficient of Determination

In simple linear regression, we had presented the coefficient of determination R^2 as an intuitive goodness-of-fit measure that compares the scatter in y-direction with and without knowing the regression line. Though visualization is no longer possible with multiple linear regression, the idea (and formula) behind is identical: R^2 expresses which portion of the total variation in the response y is accounted for by the regression hyperplane. The definition is as follows:

$$R^2 = 1 - \frac{\sum_{i=1}^{n} (y_i - \hat{y}_i)^2}{\sum_{i=1}^{n} (y_i - \overline{y})^2} \in [0,1]$$

In the numerator, we measure the scatter of the data points around the fitted values, i.e. the *RSS*. The denominator has the scatter of the data points around their mean. This is the *total sum of squares* (*TSS*). Again, the maximum value is $R^2 = 1$. It is attained if all data points are on the regression hyperplane. The other extreme case is $R^2 = 0$ and means that there is no explanatory power in the regression fit, and $\hat{\beta}_1 = \hat{\beta}_2 = ... = \hat{\beta}_p = 0$. The actual value is provided in the R summary in the second to last row:

```
> summary(fit)

Call:
lm(formula = Mortality ~ JanTemp + JulyTemp + RelHum + Rain +
    Educ + Dens + NonWhite + WhiteCollar + log(Pop) + House +
    Income + log(HC) + log(NOx) + log(SO2), data = apm)

Coefficients:
               Estimate Std. Error t value Pr(>|t|)
(Intercept)  1.297e+03  2.934e+02   4.422 6.32e-05 ***
JanTemp     -2.368e+00  8.851e-01  -2.676   0.0104 *
JulyTemp    -1.752e+00  2.031e+00  -0.863   0.3931
[output partly ommitted...]
log(SO2)    -3.687e+00  7.359e+00  -0.501   0.6189
---
Residual standard error: 34.48 on 44 degrees of freedom
Multiple R-squared: 0.7685,  Adjusted R-squared: 0.6949
F-statistic: 10.43 on 14 and 44 DF,  p-value: 8.793e-10
```

The result is $R^2 = 0.7685$, hence a good portion of the response variation is explained by the predictors. However, the raw R^2 should be interpreted with care: the more predictors that are added to a multiple linear regression model, the smaller its residual sum of squares becomes, and the higher R^2 is. This improvement may be bigger or smaller according to the predictive power of the added predictor, but the goodness-of-fit never gets worse. This makes the multiple R-squared a cumbersome tool for comparing models with different number of predictors. However, one can overcome this by using the *adjusted R-squared*. The definition is:

$$adjR^2 = 1 - \frac{n-1}{n-(p+1)} \cdot (1-R^2) \in [0,1]$$

As we can see, there is a penalty term for more complex models, i.e. models where the number of predictors p is higher. Consequently, the *adjusted R-squared* is always smaller than the *multiple R-squared*. The difference is most pronounced when there are few observations, many predictors and a poor signal. Vice versa, it becomes almost nil if we have lots of observations, just few predictors and strong signal. Final advice in this topic: for not privileging models with excess predictors, we recommend the use of the adjusted R-squared only.

3.4.2 Confidence Intervals for the Coefficients

The confidence intervals for the regression coefficients β_j, $j = 0,...,p$ provide a way of expressing the uncertainty in these estimates. They contain all the null hypotheses $\beta_j = b$ which the corresponding individual hypothesis test fails to reject and hence all values which are plausible for β_j. A quick but approximate way of computing these confidence intervals is:

$$Coefficient\ Estimate \pm 2 \cdot Standard\ Error$$

The necessary information can be found in the R summary and it is valuable to know about his ad-hoc method for quickly assessing the precision of the estimated coefficients. The actual, precise formula for computing a 95% confidence interval for the regression coefficient β_j is:

$$\hat{\beta}_j \pm qt_{0.975;n-(p+1)} \cdot \hat{\sigma}_{\hat{\beta}_j} = \hat{\beta}_j \pm qt_{0.975;n-(p+1)} \cdot \hat{\sigma}_E \cdot \sqrt{(X^T X)^{-1}_{ii}}$$

Knowing this exact formula by heart is somewhat less important for the practitioner. However, it is important to be familiar with the command `confint()` that computes the exact confidence intervals in R:

```
> round(confint(fit),2)
              2.5 %  97.5 %
(Intercept)  706.15 1888.61
JanTemp       -4.15   -0.58
JulyTemp      -5.84    2.34
```

```
...
[output partially omitted]
...
log(NOx)       5.26   62.68
log(SO2)     -18.52   11.14
```

As it has been mentioned above, the confidence intervals contain all values which can be seen as plausible for the regression coefficients. If in particular zero lies within the intervals, it is a plausible value, too. Hence it might be that the predictor in question does not contribute to the variation in the response and thus it is non-significant. This leads us to the individual hypothesis tests that will be discussed in the next section.

3.4.3 Individual Hypothesis Test

For finding out whether an arbitrary value b is plausible for the regression coefficient β_j, we can check whether it is contained in the 95%-CI from above. Alternatively, there is a test for the *null hypothesis* $H_0 : \beta_j = b$. The most popular variant is $H_0 : \beta_1 = 0$: this is asking if the coefficient could be zero, which would mean that the predictor x_j has no influence on the response y. The natural goal is to reject the null for gaining evidence that the relation between y and the predictor exists. One usually tests two-sided on the 95% level, i.e. the alternative is $H_A : \beta_1 \neq b$. The *test statistic* and its *distribution* are as follows:

$$T_{H_0:\beta_j=b} = \frac{\hat{\beta}_j - b}{\hat{\sigma}_{\hat{\beta}_j}} \sim t_{n-(p+1)} .$$

On this basis, it is straightforward to determine acceptance and rejection regions, as well as *p-values*. All the necessary ingredients together with the *test statistic* (`t value`) and the *p-value* (`Pr(>|t|)`) for $H_0 : \beta_j = 0$ are routinely given in the R summary output:

```
> summary(fit)
Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept)  1.297e+03  2.934e+02   4.422 6.32e-05 ***
JanTemp     -2.368e+00  8.851e-01  -2.676   0.0104 *
JulyTemp    -1.752e+00  2.031e+00  -0.863   0.3931
...
[output partially omitted]
...
log(NOx)     3.397e+01  1.425e+01   2.384   0.0215 *
log(SO2)    -3.687e+00  7.359e+00  -0.501   0.6189
```

As an additional example, we test $\beta_1 = -5$. The value of the test statistic is $(-2.368 + 5) / 0.8851 = 2.973675$. The acceptance region is easily computed from R:

```
> qt(0.975,df=44)
```

```
[1] 2.015368
```

Hence, we reject the null hypothesis, if the observed value of the test statistic exceeds 2.015 in absolute value. This is the case, and hence $H_0: \beta_1 = -5$ is rejected. The p-value with which this happens is computed by:

```
> 2*pt(-abs((-2.368+5)/0.8851),df=44)
[1] 0.004760858
```

We conclude that our null hypothesis is quite clearly rejected. While these tests are simply carried out and are useful in practice, their interpretation is a bit tricky and has a few traps that one must not fall victim to, namely:

1) The *multiple testing problem*: if we repeatedly do hypothesis testing on the α =5% significance level, our total type I error increases. In particular, for p hypothesis tests, it is $1-(1-\alpha)^p$. Note that for example with 30 predictors, the chance of making at least one false rejection in the individual hypothesis tests is already 0.785, a pretty high value!

2) It can happen that all individual hypothesis tests fail to reject the null hypothesis (say at the 5% significance level), although it is in fact true that some predictor variables have a known effect on the response. This does often occur due to correlation among the predictor variables, so that the predictive power is distributed and none seems too important in the presence of the others.

Another important point is the interpretation of the individual hypothesis test: it verifies the effect of predictor x_j on the response in the presence of all the other predictors. As a consequence, any change in the predictor set leads to (sometimes drastically) different test results. This is especially important because decisions about the omitting of variables are often based on the individual hypothesis tests. Due to the above, *one must not drop more than one non-significant variable at a time* – this need be done step-by-step.

3.4.4 Comparing Hierarchical Models

The idea behind the test presented in this section is a correct comparison of two multiple linear regression models when the smaller has more than one predictor less than the bigger. This can be useful in practice, i.e. for evaluating whether *air pollution* (which appears as 3 predictors) has an effect on *mortality*. Moreover, the test will also be required for correct handling of categorical predictors, the so-called factor variables (see in section 3.6). We assume that there are two models.

Big model: $y = \beta_0 + \beta_1 x_1 + ... + \beta_q x_q + \beta_{q+1} x_{q+1} + ... + \beta_p x_p$
Small model: $y = \beta_0 + \beta_1 x_1 + ... + \beta_q x_q$

The big model must contain all the predictors that are in the small model, else the models cannot be considered as being hierarchical and the test which is presented below does not apply. The null hypothesis is that the excess predictors in the big model do not bring any benefit, hence:

$$H_0 : \beta_{q+1} = \beta_{q+2} = ... = \beta_p = 0$$

We test against the alternative that at least one of the excess predictors has an effect, i.e. $\beta_j \neq 0,\ j = q+1,...p$. The comparison of the two models will be based on the residual sum of squares (*RSS*). This quantity will always be smaller for the big model; the question is just by how much. If the difference is small, then one might not accept the additional variables, if it is big, then one should. The method for quantifying this is as follows:

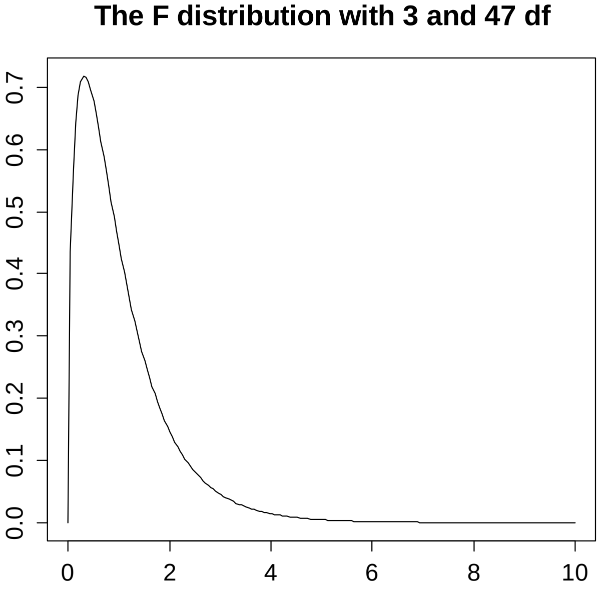
$$F = \frac{n-(p+1)}{p-q} \cdot \frac{RSS_{Small} - RSS_{Big}}{RSS_{Big}} \sim F_{p-q,n-(p+1)}$$

Apparently, we have a relative comparison of the model adequacy, and also the number of observations, the total number of predictors and the difference in the number of predictors are taken into account. Under the null hypothesis, i.e. if the excess predictors do not contribute, the test statistic has an F-distribution with $p-q$ and $n-(p+1)$ degrees of freedom. Using that distribution, we can decide if the difference between the models is of significance or not. As an example, we consider the mortality data. Here, we want to test if the three predictors that are linked to air pollution can be omitted from the multiple linear regression model without any loss. We do this in R:

```
> fit.small <- update(fit, .~.-log(HC)-log(NOx)-log(SO2))
> anova(fit, fit.small)
Analysis of Variance Table

Model 1: Mortality ~ JanTemp + JulyTemp + RelHum + Rain +
                     Educ + Dens + NonWhite + WhiteCollar +
                     log(Pop) + House + Income + log(HC) +
                     log(NOx) + log(SO2)
Model 2: Mortality ~ JanTemp + JulyTemp + RelHum + Rain +
                     Educ + Dens + NonWhite + WhiteCollar +
                     log(Pop) + House + Income
  Res.Df   RSS Df Sum of Sq      F  Pr(>F)
1     44 52312
2     47 61142 -3   -8829.3 2.4755 0.07388 .
```

Note that the small model was defined with an update from the big model. It is not required to do so, we could also write it explicitly using the `lm()` command. The R function for the hierarchical model comparison is `anova()`. As input, it takes the big and small model. In the output, the two model formulas are repeated, before the quantitative result is presented. We recognize the RSS for the two models, also the degrees of freedom and the value of the test statistic are given. This is gauged against the F distribution, which in this particular case looks as follows:



If the excess predictors (i.e. the air pollution) do not have an effect and hence under the null hypothesis, we expect the test statistic to be smaller than:

```
> qf(0.95,3,47)
[1] 2.802355
```

This is the case, hence we are in the acceptance region and the null hypothesis cannot be rejected. The p-value is provided in the R output, it is 0.074. In conclusion, it might be that the air pollution, in the way it was measured here, does not affect mortality. At least we failed to reject the null that it does not have influence on the outcome with the current data and model. We finish this section by remarking that if a hierarchical model comparison is done for two models where the difference is only one single predictor, it coincides with the individual hypothesis test.

3.5 Prediction

Besides inference, the other very important application of the multiple regression fit is prediction. As soon as we are given the predictor values $x_{\bullet 1},...,x_{\bullet p}$ for a new observation that was not part of the fitting and where the response is potentially unknown, we can provide its predicted value, i.e. the conditional expectation:

$$E[y_{\bullet} \mid x_{\bullet 1},...,x_{\bullet p}] = \hat{y}_{\bullet} = \hat{\beta}_0 + \hat{\beta}_1 x_{\bullet 1} + ...\hat{\beta}_p x_{\bullet p}$$

In simple regression, we had explained that a prediction within the range of observed x-values is safe if the regression line does not have a systematic error. The very same can be said about multiple regression, however here it is much more difficult to say what is within the range of observed x-values, and what is beyond. For understanding this, it is important to keep in mind that (usually, except some very few special cases) cannot overlook and visualize the p-dimensional predictor space. Moreover, even when all individual values in the new observations' predictors $x_{\bullet j}$ lie within the values of the observed $x_{1j},...,x_{nj}$ in that predictor, it is not guaranteed that we are still not extrapolating. This phenomenon is known as the *curse of dimensionality*: the p-dimensional predictor space is huge and even when staying within the hypercube defined by the observed predictor values, the new observation can be in a location where no data were present for the fitting process. However, as long as the fit is free of a systematic error, and when the new observation is within that hypercube, the predictions are usually safe.

Besides producing predictions, it is also very important to understand their precision. As in simple regression, we can provide both a 95% confidence interval for the conditional expectation $E[y_\bullet \mid x_{\bullet 1},...,x_{\bullet p}]$, as well as the 95% prediction interval for the future observation. The meaning of these two intervals is exactly the same as in simple regression. The formulae are best written in matrix notation, in particular:

95% confidence interval: $\hat{y}_\bullet \pm t_{0.975;n-(p+1)} \cdot \hat{\sigma}_E \cdot \sqrt{x_\bullet^T \left(X^T X\right)^{-1} x_\bullet}$

95% prediction interval: $\hat{y}_\bullet \pm t_{0.975;n-(p+1)} \cdot \hat{\sigma}_E \cdot \sqrt{1 + x_\bullet^T \left(X^T X\right)^{-1} x_\bullet}$

In this notation, $x_\bullet^T = (1, x_{\bullet 1},...,x_{\bullet p})$ is the predictor vector for the new observation, including the intercept term. The computation of these intervals is implemented in R's `predict()` function. As input for this routine, we need to provide the regression fit, the new predictor values $x_{\bullet 1},...,x_{\bullet p}$ in form of a data frame with column names that are identical to the ones that were used for the fit. We illustrate with the following example, where we predict the mortality in a fictional city:

```
> new.x <- data.frame(JanTemp=32, JulyTemp=75, RelHum=55,
           Rain=51, Educ=10, Dens=3500, NonWhite=8.7,
           WhiteCollar=42, Pop=1200000, House=3,
           Income=41000, HC=22, NOx=18, SO2=38)
>
> predict(fit, newdata=new.x, interval="confidence")
       fit      lwr     upr
1 979.4028 936.9754 1021.83
>
> predict(fit, newdata=new.x, interval="prediction")
       fit      lwr      upr
1 979.4028 897.9834 1060.822
```

We observe that the predicted mortality is 979.4, with a 95% confidence interval ranging from 937.0 to 1021.8. The 95% prediction interval is (as always) wider and marks the range where we would expect a new observation. The numerical value of this interval is 898.0 to 1060.8.

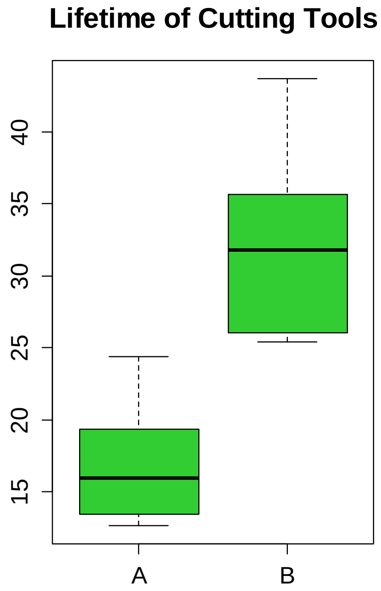
3.6 Categorical Predictors

The variables we considered so far were all continuous, i.e. temperature, distance, pressure, et cetera. While the response must be continuous, it is perfectly valid to use *categorical predictors*, such as e.g. *sex* (male or female), *status variables* (employed or unemployed), *shifts* (day, evening, night). In general, these categorical variables have no natural scale of measurement. Thus, we must assign a set of levels to a categorical variable to account for the effect that the variable may have on the response. This is done through the use of indicator variables. In the regression context, they are better known as *dummy variables*. In the following sections, we will study the use of categorical predictors.

3.6.1 Example with 1 Categorical Predictor

The simplest case is a model where we have a continuous response y and one single categorical predictor $\tilde{x}$. The example that we consider is from a lathe (in German: "Drehbank"), where y is the lifetime of the cutting tool and the categorical predictor $\tilde{x}$ refers to two different tool types A and B. A typical way of displaying observed lifetimes in relation to the two tool types is with boxplots:

```
> boxplot(hours ~ tool, data=lathe)
```



We observe that the lifetimes of tools of type B are considerably higher than the ones of type A. The usual question in this setting is to estimate the expected lifetimes for the two tool types and answering the question whether the two means are identical. The boxplots let us assume that this is not the case. We can quantitatively undermine this by performing a Student's t-Test for non-paired data. The R command is as follows:

```
> t.test(hours ~ tool, var.equal=TRUE, data=lathe)
Two Sample t-test
data:  hours by tool
t = -6.435, df = 18, p-value = 4.681e-06
alternative hypothesis: true diff in means is not equal to 0
95 percent confidence interval:
-19.655814  -9.980186
sample estimates:
mean in group A mean in group B
         17.110          31.928
```

What does this have to do with regression analysis? More than you think. We can achieve the very same quantitative results by fitting a regression of $y \sim \tilde{x}$. Because regression is a technique for numerical variables, we need to replace the categorical predictor $\tilde{x}$ by an indicator variable that takes values 0 and 1 to identify the tool types – this is a so-called dummy variable.

$$x = \begin{cases} 0 & tool\ \ type\ \ A \\ 1 & tool\ \ type\ \ B \end{cases}$$

The choice of 0 and 1 to identify the levels of this categorical predictor is arbitrary. In fact, any two distinct values for x would be satisfactory, although 0 and 1 are the normal choice. Then, if we consider the simple linear regression model

$$y_i = \beta_0 + \beta_1 x_i + E_i \,,$$

this becomes $y_i = \beta_0 + E_i$ for observations i with tool type A and hence $x_i = 0$. Then, for observations j with tool type B, $x_j = 1$ and the regression equates to $y_j = \beta_0 + \beta_1 + E_j$. Consequently, β_0 is the expected lifetime for tools of type A, and $\beta_0 + \beta_1$ the one for tools of type B. Or we can also say that β_1 is the difference in the two lifetime expectations. With R, fitting regression models with categorical predictors is straightforward. We do not even need to take care of the generating the dummy variable, but can just provide a factor variable, i.e. `class(lathe$tool)= "factor "`. The summary output is as follows:

```
> summary(lm(hours ~ tool, data=lathe))

Call: lm(formula = hours ~ tool, data = lathe)

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)   17.110      1.628  10.508 4.14e-09 ***
toolB         14.818      2.303   6.435 4.68e-06 ***
---
Residual standard error: 5.149 on 18 degrees of freedom
Multiple R-squared: 0.697, Adjusted R-squared: 0.6802
F-statistic: 41.41 on 1 and 18 DF, p-value: 4.681e-06
```

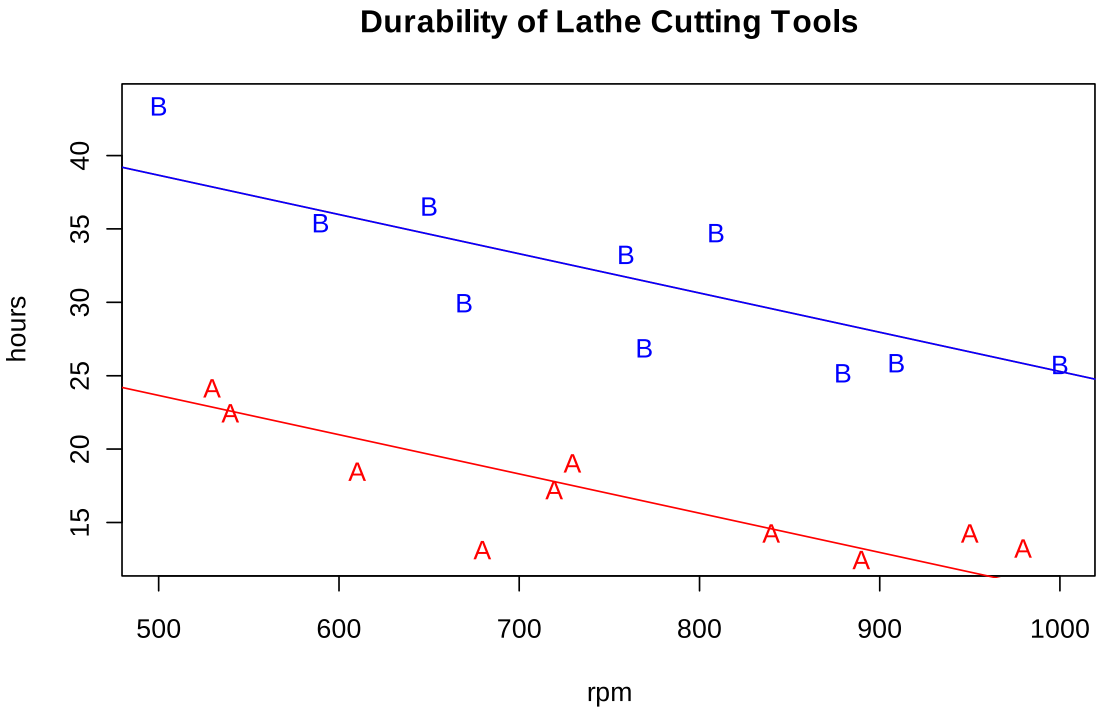
We observe that the regression coefficients are identical to the results from the testing procedure above, where arithmetic means were drawn. Furthermore, the test for the null hypothesis $\beta_1 = 0$ addresses exactly the same question as the t-test for non-paired data does. However, not only the question is identical, but also the answer (and the methodology behind). The p-values with both approaches are one and the same. Hence, if we can do regression, we could in fact retire the non-paired t-test altogether.

3.6.2 Mix of Categorical and Continuous Predictors

We now enhance our previous example and want to relate the lifetime y of a cutting tool on the speed of the machine in rpm (x_1) and the type of cutting tool used ($\tilde{x}_2$). The first predictor is continuous, while the second is categorical, again with levels A and B. As before, it will be replaced it by an indicator or dummy variable that takes values 0 and 1 to identify the tool types.

$$x_2 = \begin{cases} 0 & tool \;\; type \;\; A \\ 1 & tool \;\; type \;\; B \end{cases}$$

We can display the data in a scatter plot of *hours* vs. *rpm*, and distinguish the two tool types by different plotting characters.



The plot also shows parallel regression lines for tool types A and B. We will now explain how they are found. The regression model for the situation with one continuous and one categorical predictor is as follows:

$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + E$ or in R notation `hours ~ rpm + tool`.

The summary output for this regression model is:

```
> summary(lm(hours ~ rpm + tool, data = lathe))

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) 36.98560    3.51038  10.536 7.16e-09 ***
rpm         -0.02661    0.00452  -5.887 1.79e-05 ***
toolB       15.00425    1.35967  11.035 3.59e-09 ***
---
Residual standard error: 3.039 on 17 degrees of freedom
Multiple R-squared: 0.9003,  Adjusted R-squared: 0.8886
F-statistic: 76.75 on 2 and 17 DF,   p-value: 3.086e-09
```

We will now turn our attention to the interpretation of this regression model. We first consider an observation i where the tool is of type A. There, we have $x_{i2} = 0$ and thus the model simplifies to:

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 \cdot 0 + E_i = \beta_0 + \beta_1 x_{i1} + E_i \,.$$

Thus, the relation between tool life and lathe speed for tool type A is a straight line with intercept $\beta_0 = 36.99$ and slope $\beta_1 = -0.027$. Important: note that the slope is generally not equal to the one we would obtain from a simple linear regression for tools of type A only! Now conversely, for any observation j with tool type B, we have $x_{j2} = 1$, and thus:

$$y_j = \beta_0 + \beta_1 x_{j1} + \beta_2 \cdot 1 + E_j = (\beta_0 + \beta_2) + \beta_1 x_{j1} + E_j$$

That is, for tool type B the relation between tool durability and lathe speed is also a straight line with the same slope $\beta_1 = -0.027$, but different intercept $\beta_0 + \beta_2 = 51.99$. Thus, the model estimates a common, identical slope coefficient for the two tool types. The regression coefficient β_2 of the dummy variable x_2 accounts for the additive shift in durability of tool type B vs. tool type A, i.e. measures the difference in mean tool life when changing from tool type A to tool type B. Note that the two regression lines are parallel by definition. To make the analysis complete, we would need to check the diagnostic plots. We leave this as an exercise, because there are no peculiarities for this specific example. For the diagnostic plots, it is helpful to use different plotting symbols for tool types A and B.

3.6.3 Interaction Terms

Above, the regression line for tools A and B had different intercept, but identical slope. In this example, the fit seemed to be pretty well even under this restriction. However, we can easily imagine a situation where two parallel regression lines are not appropriate. The question this section deals with is whether and how a model with two different regression lines can be fitted. It is possible to model this situation with a single regression equation by using indicator variables. The model is:

$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2 + E$ or `hours ~ rpm + tool + rpm:tool`.

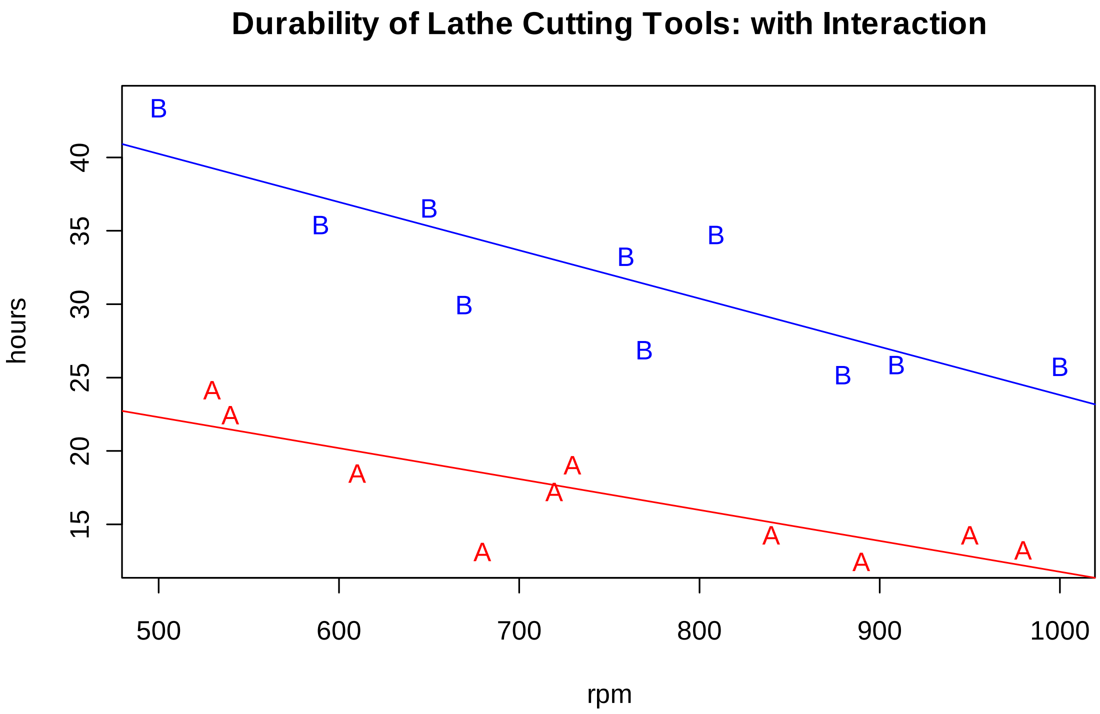
An interaction term or cross product x_1x_2 has been added to the model. To interpret the parameters in this model, we first consider an observation i with tool type A. Remember; this means that the dummy variable $x_{i2}=0$.

$$y_i=\beta_0+\beta_1x_{i1}+\beta_2\cdot 0+\beta_3\cdot 0+E_i=\beta_0+\beta_1x_{i1}+E_i$$

Thus, this is again a regression line with intercept β_0 and slope β_1. However, the slope β_1 will generally be different to the one found with the main effect model from section 3.6.2. For an observation j with tool type B, we have $x_{j2}=1$ for the dummy variable. Thus, the regression model becomes:

$$y_j=\beta_0+\beta_1x_{j1}+\beta_2\cdot 1+\beta_3x_{j1}\cdot 1+E_j=(\beta_0+\beta_2)+(\beta_1+\beta_3)x_{j1}+E_j$$

This is a straight-line model with intercept $\beta_0+\beta_2$ and slope $\beta_1+\beta_3$. Thus, the interaction model defines two regression lines with different intercepts and different slopes. Therefore the parameter β_2 reflects the change in the intercept associated with changing from tool type A to tool type B, and β_3 indicates the change in the slope associated with this change.



The scatterplot of `hours` vs. `rpm` is shown above, together with the two regression lines that are no longer parallel. There is a large vertical shift between the two regression lines. The slope however, only differs little. An obvious question is whether fitting two regression lines with different slopes is necessary, i.e. whether the difference is statistically significant or whether we could also do with the simpler model that has two parallel lines. This amounts to testing

$H_0:\beta_3=0$ against $H_A:\beta_3\neq 0$.

This is an individual parameter test for the interaction term, and the result can be directly read from the summary output.

```
> summary(lm(hours ~ rpm + tool + rpm:tool, data = lathe))
Coefficients:   Estimate Std. Error t value Pr(>|t|)
(Intercept)    32.774760   4.633472   7.073 2.63e-06 ***
rpm            -0.020970   0.006074  -3.452  0.00328 **
toolB          23.970593   6.768973   3.541  0.00272 **
rpm:toolB      -0.011944   0.008842  -1.351  0.19553
---
Residual standard error: 2.968 on 16 degrees of freedom
Multiple R-squared: 0.9105, Adjusted R-squared: 0.8937
F-statistic: 54.25 on 3 and 16 DF,  p-value: 1.319e-08
```

The p-value for our null hypothesis is 0.196, thus the interaction term is not statistically significant. This leads to the conjecture that if there are no further (practical) reasons strongly speaking for different slopes, we would (and could) fit parallel lines. Note that the (full) interaction model always yields the same result as two separate simple linear regressions on tools of type A, and tools of type B. Does that mean we should prefer simple regressions? The answer is definitely no, because with the common model we can formally test to which extent the two tools behave identically. From the above test, we can accept the hypothesis that the `rpm` variable has the same effect on lifetime for both tool types. Another, more general but equally interesting question is if there is any difference at all between the two tools with respect to lifetime. The associated null hypothesis is:

$$H_0 : \beta_2 = \beta_3 = 0 \text{ against } H_A : \beta_2 \neq 0 \ \ and/or \ \ \beta_3 \neq 0 .$$

Under the null, both the dummy and interaction coefficient are zero, meaning that there would be a common regression line for both tools. Our graphical display shows that this is implausible, but it is helpful to formally test the claim. Because we are testing two coefficients simultaneously, we require a partial F-test. The R-code and the output are as follows:

```
> fit1 <- lm(hours ~ rpm, data=lathe)
> fit2 <- lm(hours ~ rpm + tool + rpm:tool, data=lathe)
> anova(fit1, fit2)
Model 1: hours ~ rpm
Model 2: hours ~ rpm + tool + rpm:tool
  Res.Df     RSS Df Sum of Sq      F    Pr(>F)
1     18 1282.08
2     16  140.98  2    1141.1 64.755 2.137e-08 ***
```

We observe that the p-value is very small, and the partial F-test thus highly significant. While there is no evidence for different slopes in this example, there is strong evidence of a difference (in either slope or intercept). Regarding the scatterplot, with the pronounced vertical shift between tool types A and B, this does not surprise us.

Finally, we conclude this section by stating that the use of interaction models is not restricted to a combination of continuous and categorical predictors. In this case, they can be visualized most easily. However, we can have them between any types of predictors. They are appropriate whenever there is, or whenever we suspect a change in the effect of one predictor on the response, conditional on the level of another predictor.

3.6.4 Categorical Input with More than Two Levels

An obvious extension to the previous example with lathe cutting tools would be to consider three or more types of tools instead of only two. The tool variable then is still categorical, but no longer binary, and we need more dummy variables. For example, suppose that there are three tool type A, B and C. We then require two dummy variables to incorporate them into the model. The coding is as follows:

x_2	x_3	
0	0	*for observations of type A*
1	0	*for observations of type B*
0	1	*for observations of type C*

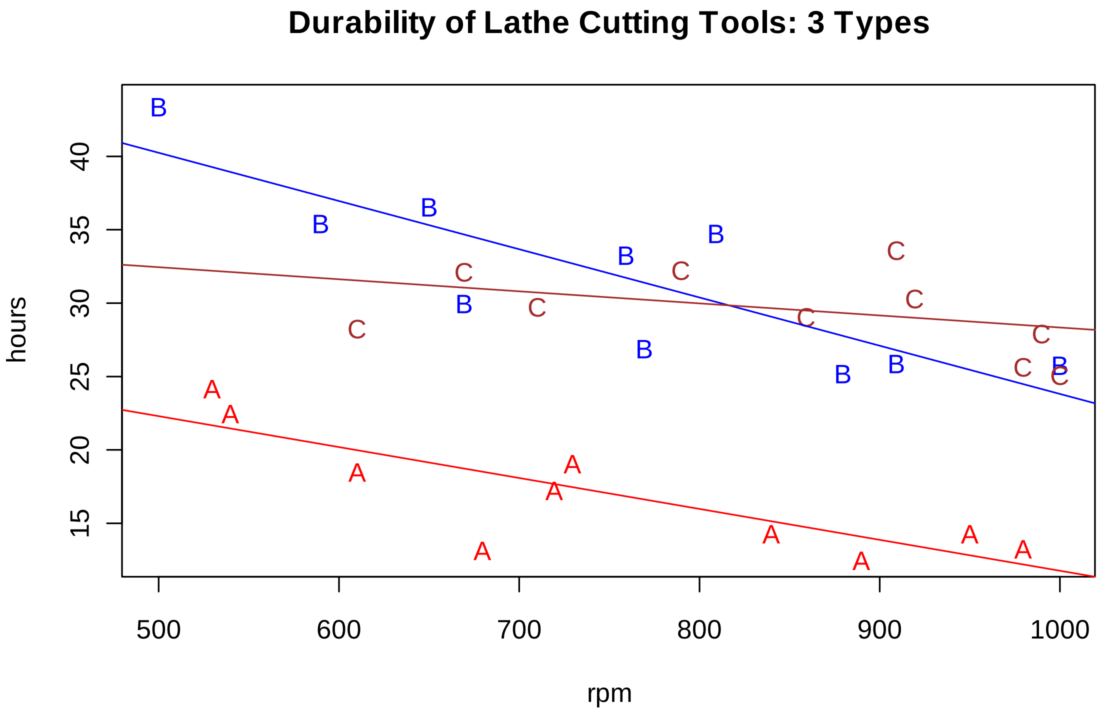
In general, a qualitative variable with ℓ levels is represented by $\ell-1$ dummy variables, each taking values 0 and 1. Be careful, categorical variables must be represented in this fashion, and generally cannot be numerically coded in one single variable with values $0,1,...,\ell-1$. Please also note that with the here presented dummy encoding, the first level (here: tool type A) is always the reference. This is also how R codes categorical input variables by default: the first factor level is the reference. There are, however, different options for coding, called contrasts. This is more of a topic in analysis of variance, thus we do not pursue that issue here. The main effects regression model with three types of tools and their respective dummy variables is now:

$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + E$, or in R simply `hours ~ rpm + tool`.

This will fit three parallel regression lines, where each has a different intercept. However, when we closely observe the scatter plot below, we gain the impression that the durability of tool type C seems to depend much less on `rpm` than the other two. While at slow speeds, its lifetime seems to be inferior to the type B tools, they seem to last longer at faster speeds. Because the main effects model cannot deal with the apparently different slopes, we fit the interaction model `hours ~ rpm + tool + rpm:tool`:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_1 x_2 + \beta_5 x_1 x_3 + E$$

The interpretation of this model is as before with binary categorical input. We leave it as an exercise to write down the cases for observations i, j and k of tool types A, B and C. The regression fit with R is again straightforward; we only need the `tool` variable to be a factor with multiple levels:



```
> summary(lm(hours ~ rpm + tool + rpm:tool, data = abc.lathe)

Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept) 32.774760   4.496024   7.290 1.57e-07 ***
rpm         -0.020970   0.005894  -3.558  0.00160 **
toolB       23.970593   6.568177   3.650  0.00127 **
toolC        3.803941   7.334477   0.519  0.60876
rpm:toolB   -0.011944   0.008579  -1.392  0.17664
rpm:toolC    0.012751   0.008984   1.419  0.16869
---
Residual standard error: 2.88 on 24 degrees of freedom
Multiple R-squared: 0.8906,   Adjusted R-squared: 0.8678
F-statistic: 39.08 on 5 and 24 DF,  p-value: 9.064e-11
```

The interpretation of this summary output now needs to be done with care. Individual parameter tests for dummy variable coefficients of categorical predictors with more than two levels are not meaningful! Thus, from the above output, we cannot conjecture that we can do without a different intercept for tool C, because the test for $H_0: \beta_3 = 0$ is not significant. Moreover, also the coefficients β_4 and β_5 for the interactions have p-values above 0.05. Does that mean that we can do without the interaction? No! We can only either exclude all the interaction terms at once, i.e. test the hypothesis

$$H_0: \beta_4 = 0 \; and \; \beta_5 = 0 \text{ against } H_A: \beta_4 \neq 0 \; and/or \; \beta_5 \neq 0.$$

This is again a partial F-test. Furthermore, we can also ask the question whether there is a difference between the regression lines of the three tool types altogether. Thus, we also test for the sub-model with only rpm as a predictor:

$$H_0: \beta_2 = \beta_3 = \beta_4 = \beta_5 = 0 \text{ against } H_A: \textit{any of } \beta_2, \beta_3, \beta_4, \beta_5 \neq 0 .$$

While many software packages have troubles with this, R is very convenient and very quick. We can just do anova(fit.abc) and obtain the following output:

```
> anova(fit.abc)

Analysis of Variance Table
          Df  Sum Sq Mean Sq F value    Pr(>F)
rpm        1  139.08  139.08 16.7641  0.000415 ***
tool       2 1422.47  711.23 85.7321 1.174e-11 ***
rpm:tool   2   59.69   29.84  3.5974  0.043009 *
Residuals 24  199.10    8.30
```

The command performs some hierarchical model evaluation. The bottom row entitled rpm:tool contains the partial F-test for the null $H_0: \beta_4 = 0 \textit{ and } \beta_5 = 0$ from above. It checks whether the interaction term with its two coefficients can be kicked out of the model. The consequence of this action is that all three tool types obtain the same slope. The result is weakly significant, thus there is some mild statistical evidence that there is a difference in life time diminishment caused by the speed for tool types A, B and C. In that case, testing further hypotheses with more parameters set to zero is obsolete.

For deeper understanding, we still explain the second row entitled with tool. It shows test statistic and p-value for the null $H_0: \beta_2 = \beta_3 = \beta_4 = \beta_5 = 0$, i.e. no difference among the tools at all. The p-value is way below 0.05, we thus have very strong evidence that there is a difference between the tools. That is not too surprising given the scatterplot. However, the test results is very useful indeed. Keep in mind that many (most!) regression problems cannot be visualized so easily, such that we have to rely on test results rather than visualization for being able to draw conclusions.

3.6.5 Categorizing Quantitative Predictors

A sometimes useful trick is to generate a categorical predictor out of a continuous one. In the lathe example from above, we could for example categorize the continuous predictor rpm into bins ranging from 400-600rpm, 600-800rpm, and 800-1000rpm. Does this make sense? At the first glance, there does not seem to be an advantage for doing so, and in this particular example, there is in fact none.

Also, the disadvantage of the categorization is that more parameters are required to represent the information of the continuous predictor. Thus, we increase the model complexity by this categorization. However, under the presence of enough data, this is sometimes desired, because it does not require the analyst to make any prior assumptions about the functional form of the relationship between the response and the predictor variable and enhances the flexibility.

Another advantage of the categorization approach is that it allows dealing with missing observations, without having to delete them. If they are numerous in a certain predictor, we could just categorize it, and assign all observations with missing information in that predictor the label “unknown”. Within the model, we would just estimate the effect of unknown status in that predictor. Such a categorization of continuous predictors is in some fields quite popular among data analysts. The approach is also known as “poor man’s GAM”.

3.7 Model Diagnostics

We need to check the assumptions we made for fitting a multiple linear regression model. Why? One reason is because we want to make sure that the estimates we produce and the inference we draw is valid. This seems quite technical and also somewhat fussy and boring. Still, it is absolutely essential to perform residual analysis before any findings from the summary output, confidence intervals or predictions are reported. If the model that was used is flawed, all these results might be dead wrong and presenting them unverified could bring you into a very uncomfortable situation.

However, there is a second, usually equally important reason to perform model diagnostics: any potential flaws that appear can help us to improve the model and enhance our understanding of the relation between response and predictors. In fact, we can go as far as saying “it is all in the residuals”, i.e. most of what we can learn about how to better shape a regression analysis is derived from some clever diagnostic plots. Such enhancements include response and/or predictor transformations, inclusion of further predictors or interaction terms among them, weighted regression analysis or in some situations also the use of more generally formulated or more robust models that are not based on OLS. This is explorative data analysis at its best – we fit a model, try some ideas, check the results and try to improve.

3.7.1 What Do We Need to Check For, and How?

We restate the assumptions we made for using the OLS procedure when fitting multiple linear regression model and drawing inference from them. One goal in model diagnostics is to detect potential deviations from them.

$$E[E_i]=0\,,$$

$$Var(E_i)=\sigma_E^2\,,$$

$$Cov(E_i,E_j)=0 \text{ for all } i\neq j\,,$$

$$E_i \sim N(0,\sigma_E^2 I),\ i.i.d\,.$$

While the first three conditions are necessary for performing least square estimation and the validity of the fitted values, the last condition is only required for any hypothesis tests, confidence intervals and prediction intervals. Since these are very important and the OLS estimator quickly becomes inefficient under non-Gaussian distribution, the normal assumptions shall also always be verified. While zero error, constant variance and the Gaussian property are relatively easy to check and will be addressed in the next subsection, uncorrelatedness or independence are more delicate matters that are postponed to a later chapter. Please also note that most of our diagnostic techniques are visual. This requires some expertise for their interpretation, but has the benefit of a very wide scope and good power for detecting what is important to be found.

3.7.2 Checking Error Assumptions

In this section, we present methods for checking the zero expectation, constant variance and normality assumptions of the errors E_i. These themselves are not observable, but we can examine the residuals r_i which are estimates of the errors. However, E_i and r_i are not the same, and to a certain extent, also have different properties. Even when the conditions on the errors are exactly met and hence $Var(E) = \sigma_E^2 I$, the residuals will be weakly correlated and heteroskedastic:

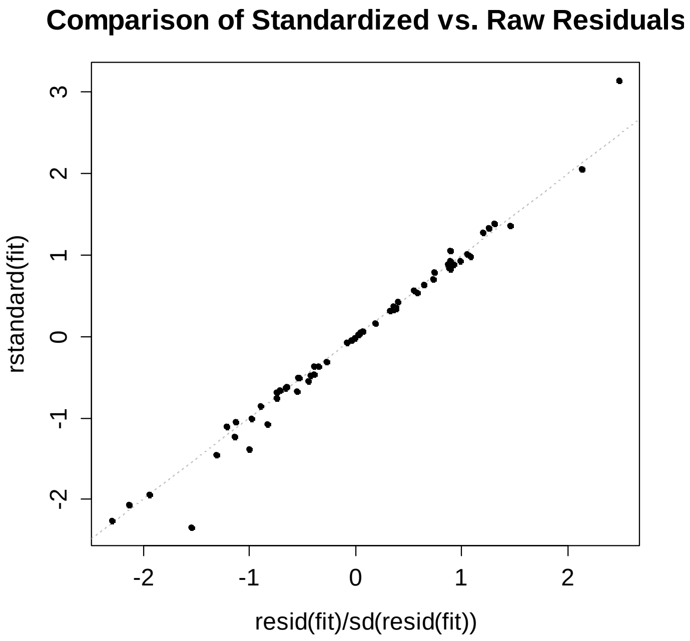
$$Var(r) = (I - H)\sigma_E^2 .$$

This is induced by the OLS estimation of r_i and the heteroskedasticity is relatively easy to understand. We already know that the confidence interval for $E[y \mid x]$ gets wider the further x lies from $\overline{x}$. Hence, there is more uncertainty in the fitted value for such observations and consequently, their residual has higher variance. This raises the question whether it is sensible to verify the error assumptions with the residuals. Fortunately, in well-posed regression problems where enough data are present, the effects of estimation-induced residual correlation and heteroskedasticity will be minor and can usually be neglected. Moreover, one can try to *standardize* or *studentize* the residuals for mitigating the heteroskedasticity. The two terms refer to a division of each residual by its estimated standard deviation to bring them on a scale with unit variance:

$$\tilde{r}_i = \frac{r_i}{\hat{\sigma}_E \sqrt{1 - h_{ii}}} .$$

Here, h_{ii} is the i^{th} diagonal element of the hat matrix and $\hat{\sigma}_E$ is an estimate of the residual standard error. Depending on whether $\hat{\sigma}_E$ comes from the full fit or from an alternate regression without the i^{th} data point, one speaks of standardized respectively studentized residuals. The distinction between the two types is mostly for academic purpose and not too relevant for practical application. Standardized and studentized residuals can be obtained in R through functions `rstandard()` and `rstudent()`, respectively. However, the difference between either of these and the raw residuals r_i can be pronounced for data points with extreme x values. We compare the rescaled raw and standardized residuals for the mortality data:

```
> plot(resid(fit)/sd(resid(fit)), rstandard(fit), pch=20)
```

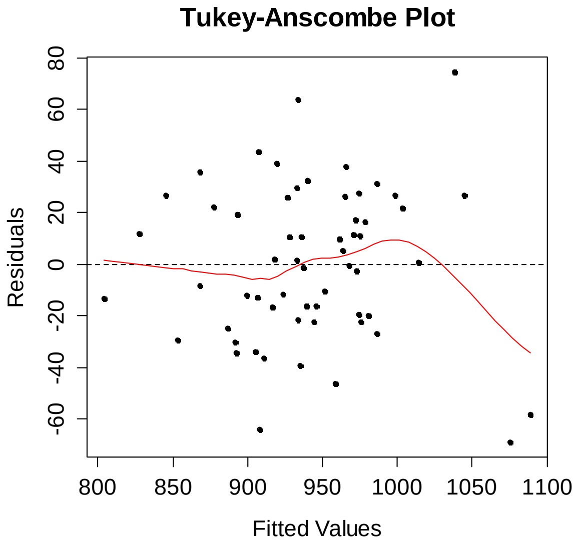


Except for the Tukey-Anscombe plot, the forthcoming residuals plots will be based on standardized residuals. This is how things are implemented in R and unless you know much better, it is recommended to stick to this.

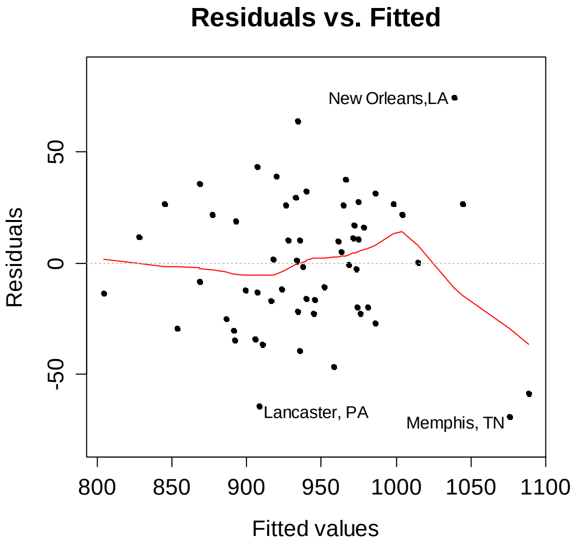
Tukey-Anscombe Plot

This plot of *residuals* r_i *vs. fitted values* $\hat{y}_i$ is named after the two researchers (who were brothers-in-law) that made it popular and is the most important diagnostic tool for any multiple linear regression fit. It is mainly aimed at verifying $E[E_i]=0$ and so evaluates whether the model is correct and makes unbiased predictions. However, please note that is not possible to check the assumption of zero expectation for each error individually – some residuals will be large and some will be small, but this proves nothing. What we need to check is whether the local mean of the residuals is related to some other quantity. This should not be the case, no matter what that quantity is. The easiest way to generate a Tukey-Anscombe plot in R is with the `plot.lm()` function, i.e. the command is simply `plot(fit, which=1)`. Because it is more instructive, we here show the code to self-generate the plot and display it along R's default version. As you can see, the two plots are nearly identical, except for some minor differences in the smoother which is due to the different algorithms that were used. Also, `plot.lm()` always annotates the name of the three data points with the biggest residuals which is very useful in practice.

```
> plot(fitted(fit), resid(fit), main="Tukey-Anscombe")
> lines(loess.smooth(fitted(fit), resid(fit)), col="red")
> abline(h=0, lty=2)
```

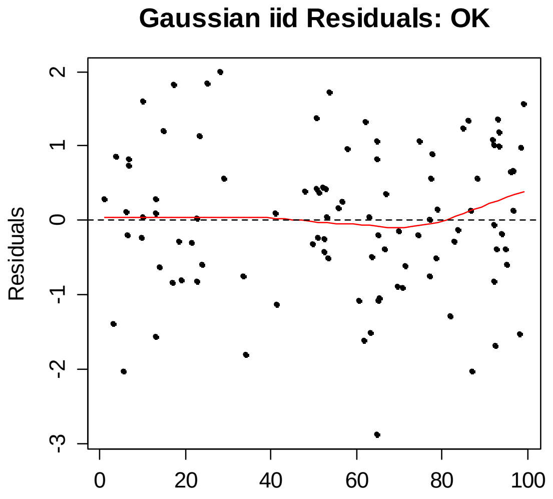


Tukey-Anscombe Plot

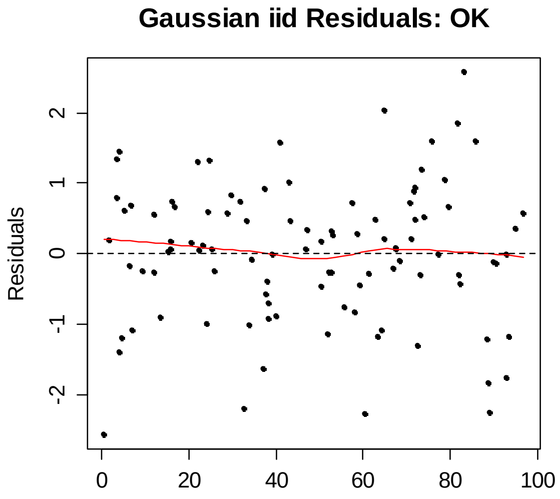


Residuals vs. Fitted

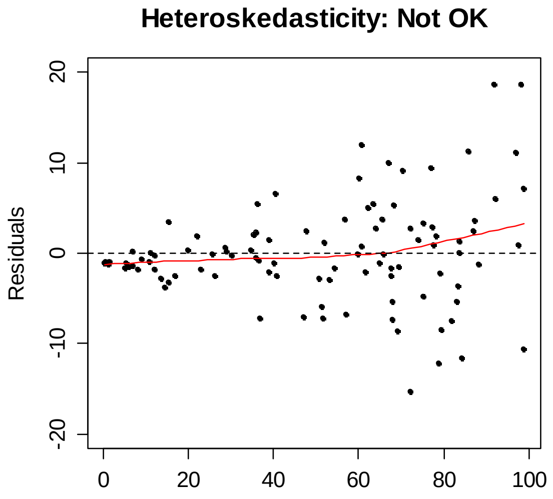
Producing a Tukey-Anscombe plot is one thing, drawing the correct conclusions from it the other. Some artificial examples illustrate the concept:



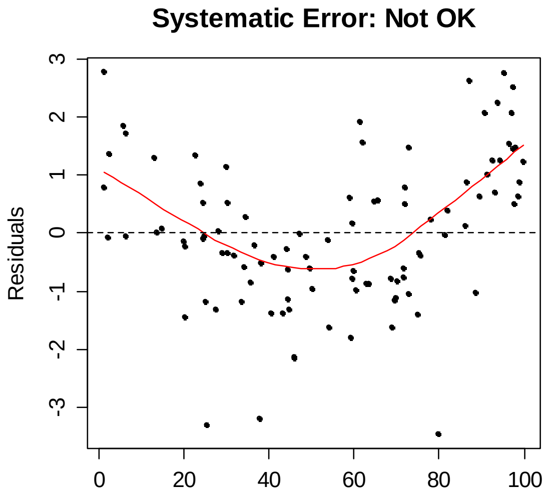
Gaussian iid Residuals: OK



Gaussian iid Residuals: OK



Heteroskedasticity: Not OK

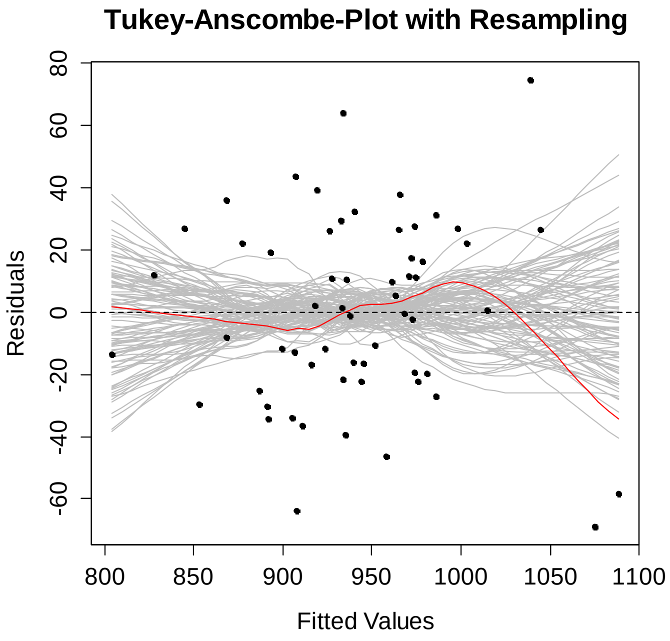


Systematic Error: Not OK

For the zero error expectation $E[E_i]=0$ assumption to hold, we require that the smoother does not systematically deviate from the x-axis. This is the case in the top two panels, because the "residuals" there originate from an iid Gaussian distribution. Hence, any deviation can be attributed to randomness alone. The situation is different in the bottom right panel: here, there is a systematic deviation of the smoother from the x-axis, and under no circumstances we could tolerate such a faulty model. The bottom left panel shows a situation where $E[E_i]$ does not systematically deviate from zero, but $Var(E_i)$ massively increases for large fitted values. Also this is a violation of the assumptions for OLS regression, although a less severe one.

So when does a smoother systematically deviate from the x-axis, and when is this just due to random variation? Generally, this is an expert call based on the magnitude of the deviation and the number of data points which are involved. An elegant way out of these (sometimes difficult) considerations is given by a resampling approach. It is based on keeping the fitted values $\hat{y}_i$ as they are, but for each data point a "new" residual r_i^* is assigned, obtained from sampling with replacement among the r_i. Then, with the new data pairs $(\hat{y}_i, r_i^*)$, a smoother is fitted and it is added to the Tukey-Anscombe plot as a grey line. The entire process is repeated for a number of times, e.g. 100x. Clearly, because the residuals were randomly assigned to the fitted values, there cannot be a systematic (but just a random) deviation of the smoother. Hence, these resampled smoothers illustrate the magnitude which a random deviation from the x-axis can take and help us to assess the true smoother.

```
> plot(fitted(fit), resid(fit), pch=20, main="...")
> for (i in 1:100) {
> +   sresid <- sample(resid(fit), replace=TRUE))
> +   lines (loess.smooth(fitted(fit), sresid), col="grey")}
> lines(loess.smooth(fitted(fit), resid(fit)), col="red")
```



The result on the previous page tells us that up to fitted values which are ≤ 1050, the original red smoother lies well within the grey scatter and thus just randomly deviates from the x-axis. At the right hand boundary, the situation remains fuzzy. The original smooth is at the edge of what can be generated by random sampling, but not clearly beyond. Also because it is only due two data points with strongly negative residuals, the author feels that we cannot reject the hypothesis $E[E_i] = 0$. Hence, we here attribute the deviation of the smoother to randomness.

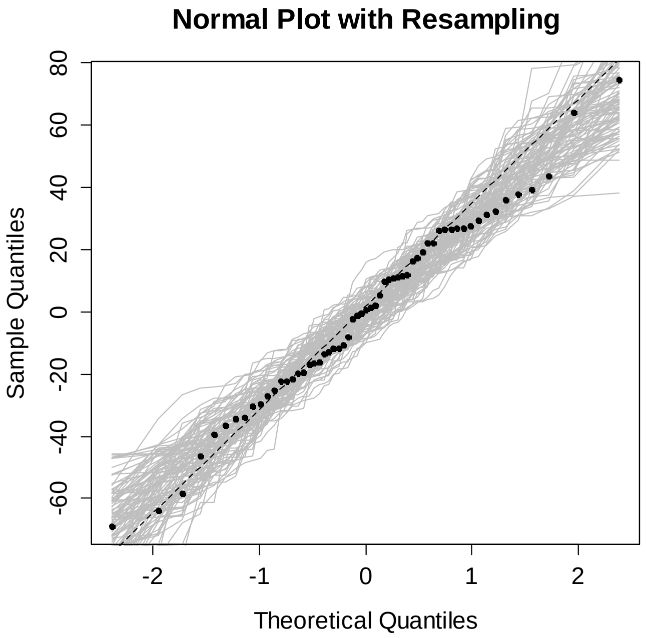
But what could we do in case of a systematic error? The answer is simple; we need to fit a better model. The difficult part is to find the correct way to improve the model. Often, (log-)transformations of the response and/or predictor variables help. In other cases, a systematic error may be cured by adding further predictors, higher order terms or interactions. In some (pretty rare) cases, we may also need to conclude that multiple linear regression modelling is not the correct way to approach the problem at hand. We conclude this section with a brief summary: if the smoother in the Tukey-Anscombe plot systematically deviates from the x-axis, the regression model has a systematic error. In this case, we should not generate predictions or report findings from the summary output, but need to improve the model. The most generic trick that helps in many situations is to consider log-transformations for the variables where this is sensible.

Normal Plot

The assumption of normally distributed errors can be checked with the *normal plot*, i.e. for $i = 1,...,n$ we plot the ordered residuals against the $i/(n+1)$ quantiles of the standard normal distribution. If the errors E_i are Gaussian, then this also holds for the residuals r_i. Thus, the data points in the normal plot should align, i.e. not show a systematic deviation of the line that is fitted through the 1st and 3rd quartiles of the two distributions. This may again raise some discussion as when a deviation is random or systematic. We can again support this decision by resampling, i.e. drawing 100 random samples of length n from a Gaussian distribution that shares mean and standard deviation with the residuals.

```
> qq <- qqnorm(resid(fit), pch=20, main="...")
> for (i in 1:100) {
> +   sresid <- rnorm(length(qq$y), mean(qq$y), sd(qq$y))
> +   lines(sort(qq$x), sort(sresid), col="grey")}
> points(qq$x, qq$y, pch=20); box()
> qqline(resid(fit), lty=2)
```

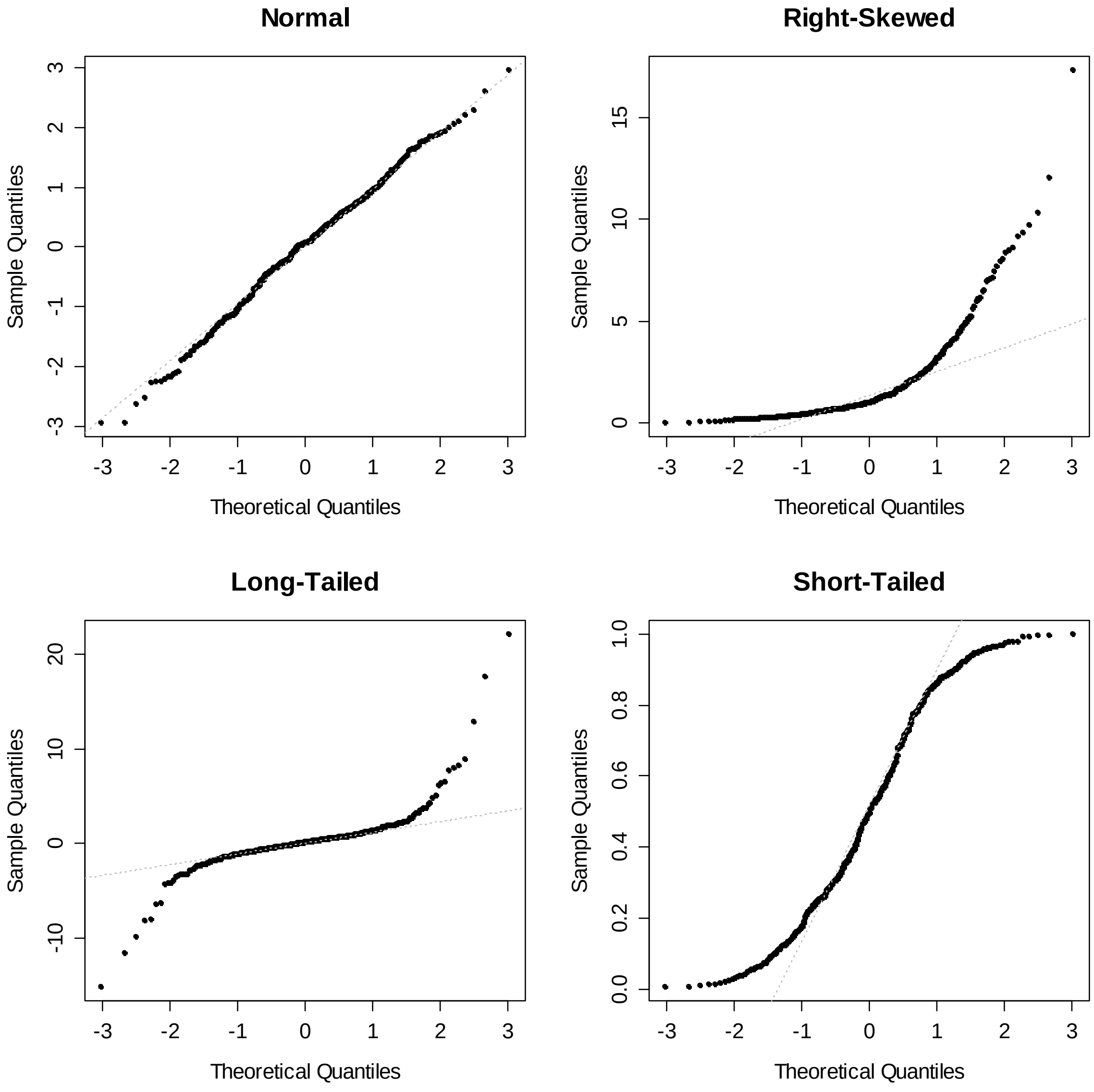
The result is displayed on the next page. We observe that all residuals from the mortality dataset fall within the resampling based confidence region, thus there is no systematic deviation from the normal distribution. The question which remains is what to do if there is a systematic deviation. This depends on the type of non-Gaussian residuals that are observed. The OLS estimator is not tolerant to skewed residuals, especially because they mostly coincide with a systematic error, i.e. a violation in the Tukey-Anscombe plot. Heavy- and especially short-tailed residual distributions are less worrying, as long as they are symmetrically distributed. In that case, they hardly have an adverse effect on the fitted values, which are still unbiased and trustworthy. In contrast, the accuracy in the levels of the confidence intervals that are computed and the precision of the tests suffers – an issue, which definitely has to be kept in mind. What also needs to be mentioned is that the efficiency of the OLS estimator degrades quickly for heavy-tailed distributions, meaning that there are other (i.e. robust) estimators that can estimate the regression coefficients with higher precision.

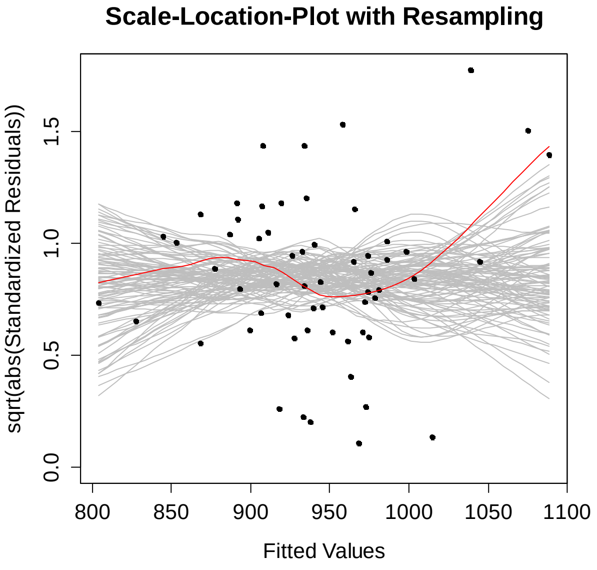


For illustrating some prototypical normal plots, see the next page. In clockwise order, starting from the top left, they show residuals from a normal distribution, then from the right-skewed lognormal distribution, the long-tailed Student's t_2-distribution and finally a short-tailed Uniform distribution.

Scale-Location Plot

This plot facilitates detecting non-constant variance, i.e. heteroskedasticity. We had argued above that one can also detect this by looking sharply at the Tukey-Anscombe plot, but the Scale-Location plot is more specific. It displays the square root of the absolute value of the standardized residuals $\sqrt{|\tilde{r}_i|}$ versus the fitted values. The crucial operation is the absolute value. It means that the bottom half of the Tukey-Anscombe plot is folded over, hence we can better detect a potential relation of the residuals' magnitude with the fitted value. Again, a smoother is added and if there is no heteroskedasticity, it will run horizontally. Also here, the task is to identify systematic deviations. We can again use the resampling idea of randomly drawing new data pairs $(\hat{y}_i, r_i^*)$ to produce a confidence region in the Scale-Location plot. The result is displayed on the next page. It seems as if the variance in the residuals grows with increasing fitted value. A popular cure for this is to apply a log-transformation to the response variable. If one tries (not displayed in this scriptum), there is a small benefit.


Normal
Right-Skewed
Long-Tailed
Short-Tailed
Sample Quantiles
Theoretical Quantiles
-3
-2
-1
0
1
2
3
5
10
15
-10
20
0.0
0.2
0.4
0.6
0.8
1.0

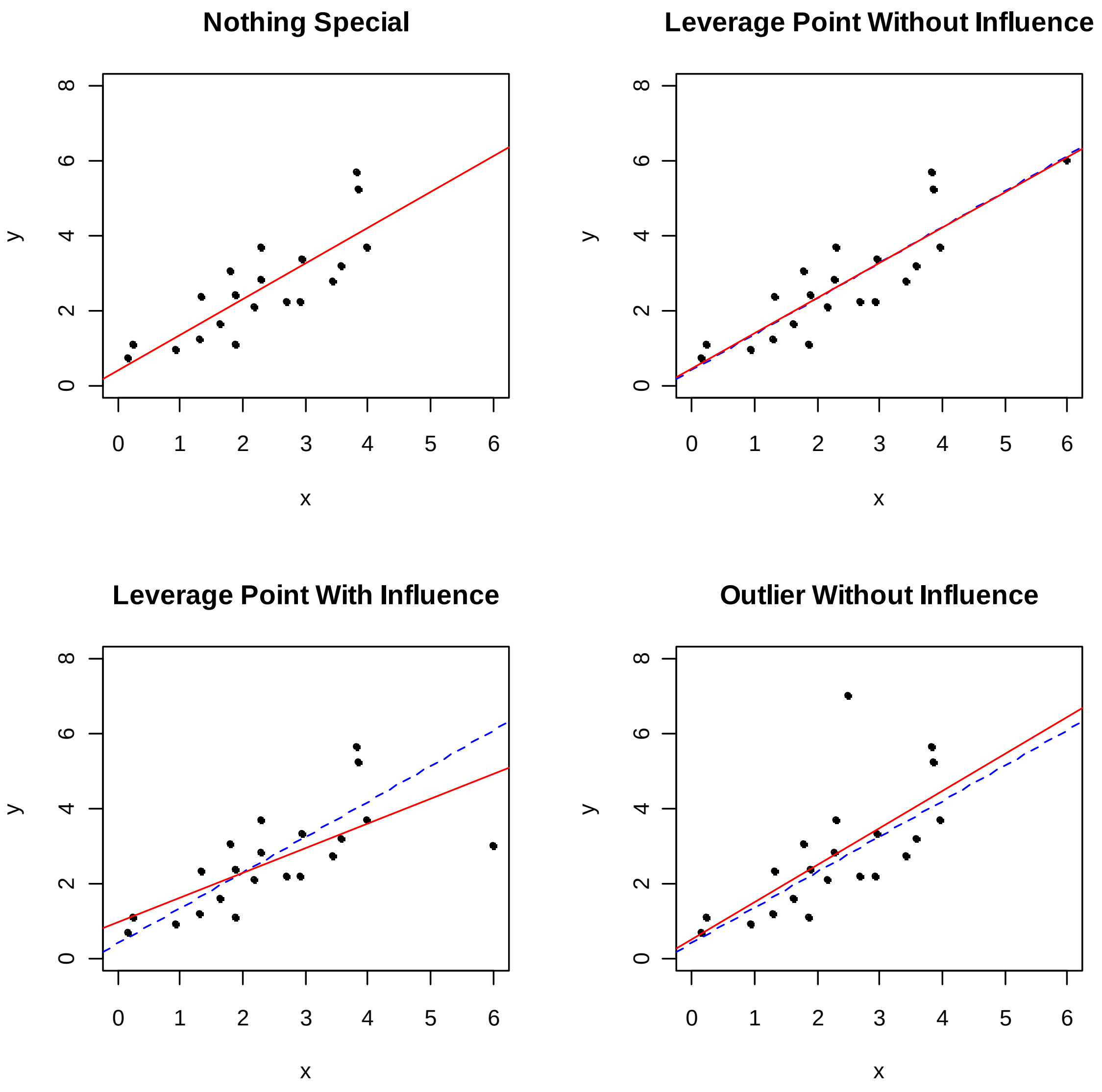

Scale-Location-Plot with Resampling
sqrt(abs(Standardized Residuals))
Fitted Values
0.0
0.5
1.0
1.5
800
850
900
950
1000
1050
1100

3.7.3 Leverage and Influential Data Points

There are situations where the regression coefficient estimates are strongly influenced by one single, or just a few data points. This is suboptimal; it is important to recognize such situations and to identify these data points. However, the previously discussed residual plots are not always very useful for this task.

Leverage

A *leverage point* is one with extreme x-values, i.e. lies “far” from the bulk of data. It is not necessarily influential, but has a high potential to be so. The plots below illustrate this: the top left shows a “normal” situation without leverage points. Top right, a leverage point was added, but it is not influential. This is different at the bottom left: the leverage point now has influence, i.e. the red regression line differs markedly from the blue one, which was computed by omitting the leverage point. Finally, the bottom right panel shows an outlier, which has only little influence on the regression line. This is because it has an x-value which is close to $\bar{x}$.



Nothing Special

Leverage Point Without Influence

Leverage Point With Influence

Outlier Without Influence

The leverage of a data point is relatively easy to determine. It simply corresponds to h_{ii}, the i^{th} diagonal element of the hat matrix H. This makes sense, as if the response y_i changes by Δy_i, then $h_{ii}\Delta y_i$ is the change in the fitted value $\hat{y}_i$. Thus, a high leverage for the i^{th} data point means that it has a strong potential to alter the regression line and force it to fit well to it. We have:

$$0 \le h_{ii} \le 1 \text{ for all } i \text{, and } \sum h_{ii} = p+1.$$

All data points with values exceeding $h_{ii} > 2(p+1)/n$ are regarded as leverage points. As we have seen above, observations that have high leverage and at the same time a large residual are most influential. We need to identify these!

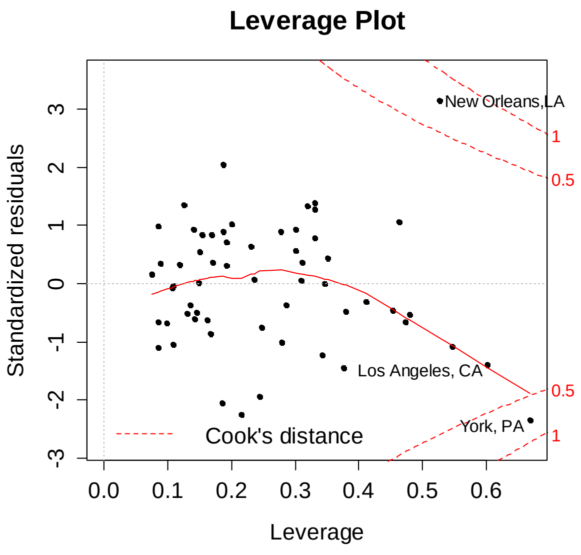
Cook's Distance

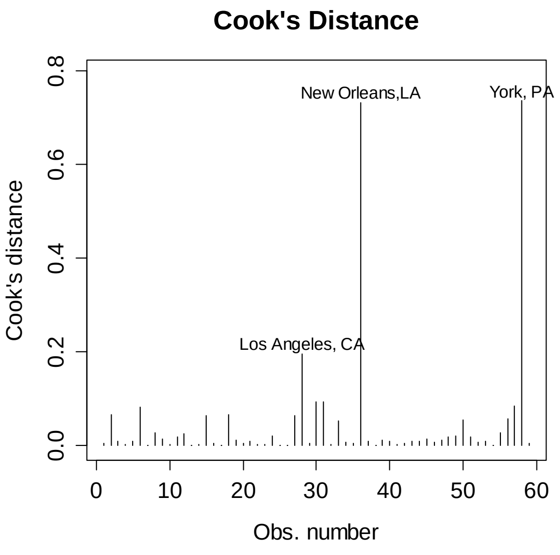
In brief summary, a leverage point tells us how strongly a data point may force the regression line to run through it. Whether it does so or not largely depends on the size of its residual. A direct measure for the change in the regression fit by a certain data point can be obtained by omitting the i^{th} data point and re-computing the fit without it. This is the basis for defining Cook's Distance:

$$D_i = \frac{\sum(\hat{y}_j - y_{j(i)})^2}{(p+1)\sigma_E^2}$$

Note that $\hat{y}_{j(i)}$ is the fitted value for the j^{th} instance, when the regression is carried out without the i^{th} data point. The sum then goes over $j = 1,...,i-1,i+1,...,n$. The computation of this measure is a bit laborious and inelegant. Fortunately, there is a direct formula for obtaining Cook's Distance which does not require running n regressions. It suffices to know the hat matrix and the standardized residuals:

$$D_i = \frac{h_{ii}}{1-h_{ii}} \cdot \frac{\tilde{r}_i^2}{(p+1)},$$





Data points with Cook's distance $D_i > 0.5$ need further investigation; because it might well be that they spoil the regression analysis. As evident from the plots on the previous page, Cook's distance contours are shown in the leverage plot. Note that in cases where they do not exist, it is because they are not visible as they do not fall within the plotting region. However, it is always possible to obtain the Cook's distance plot in R, just use `plot(fit, which=4)`. The two plots also shed light on some model deficiencies for the mortality data: there seems to be some odd systematic relation between the residuals and the leverage and there are two data points with problematic influence. These are the cities of *York (PA)* and *New Orleans (LA)*.

Dealing with Influential Data Points and Outliers

We have seen above that the "most dangerous" data points are the ones that are leverage points and outliers at the same time. Also, we explained that Cook's Distance is a well suited measure to identify such points. However, here are some more things to consider about the presence of influential data points:

1) An influential data point in one model may disappear in another where variables have been changed or transformed. One needs to reinvestigate the question of influential data points when the model is changed.

2) The error distribution may not be Gaussian and thus, larger residuals may need to be expected. For example, day-to-day relative changes in stock indices seem Gaussian over large periods of times, but large changes also happen once in a while.

3) A single or very few outliers are usually much less of a problem in larger datasets. A single point will mostly not have the leverage to affect the fit very much. It is still worth identifying outliers if these types of observations are worth knowing about in the particular application.

Suppose that you detected one or several influential data points or outliers in your data. What to do with them? The following can serve as a practical guide:

a) Check for typos first, if the original source of the data is available.

b) Examine the physical context – why did it happen? Sometimes, influential data points may be of little interest. On the other hand, it was often the case that scientific discoveries arose from noticing unexpected aberrations.

c) Exclude the influential data points from the analysis, and re-fit the model. The differences can be substantial and make the difference between getting a statistically significant result, or having some "garbage" that cannot be published. To avoid any suggestion of dishonesty always report the existence of data points that were removed from the final model.

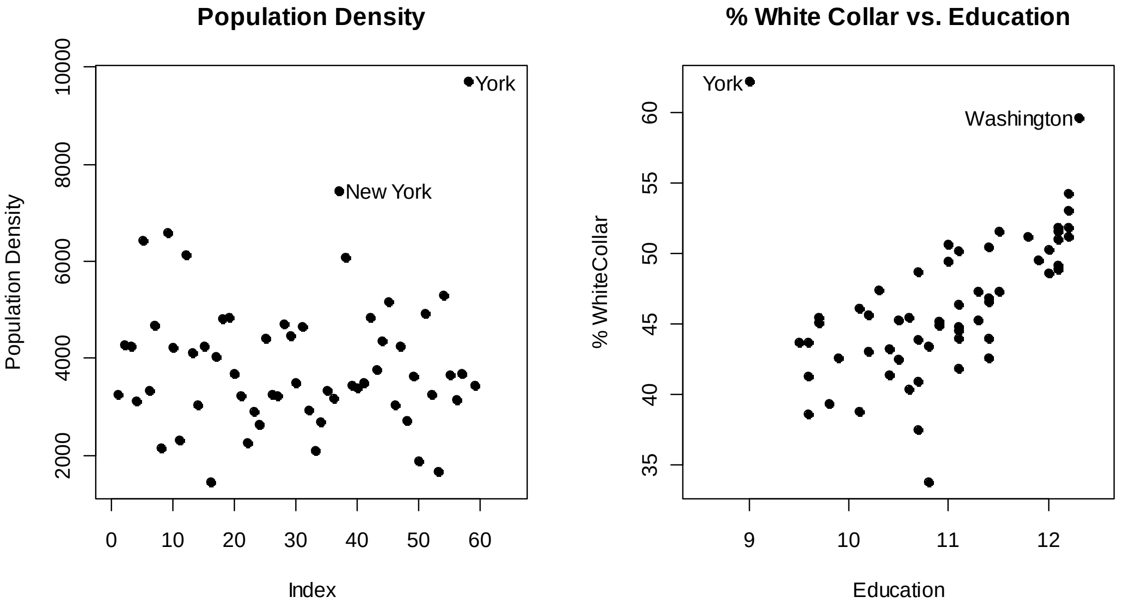
d) Suppose there are outliers that cannot be reasonably identified as mistakes or aberrations, but are viewed as naturally occurring, e.g. due to long-tailed error distribution. Rather than excluding these instances and the using least squares, it is more efficient and reliable to use robust regression.

3.7.4 Example: Mortality Dataset

From the model diagnostics, we conjecture that York and New Orleans are the most influential data points. To be on the safe side, it is reasonable to re-run the regression analysis without these two data points. The most important observations from this analysis are that the residual standard error is now smaller, and the coefficient of determination increased. Thus, the fit is better now.

We now turn our attention to the interesting question why the cities of York and New Orleans were influential data points. Plotting some of the predictors, maybe even against other predictors and identifying outlying data points may help. In the plots below, we observe that the city of York has a considerably higher population density than all the other towns. It turned out that the definition of districts with which the population density was defined was somewhat suboptimal.

Moreover, it is also striking that the average years of education in York are much lower than elsewhere, but the percentage of white collar workers is higher. This anomaly is explained by the predominance of Amish people in that region. It is thus, an inhomogeneity of the sample.



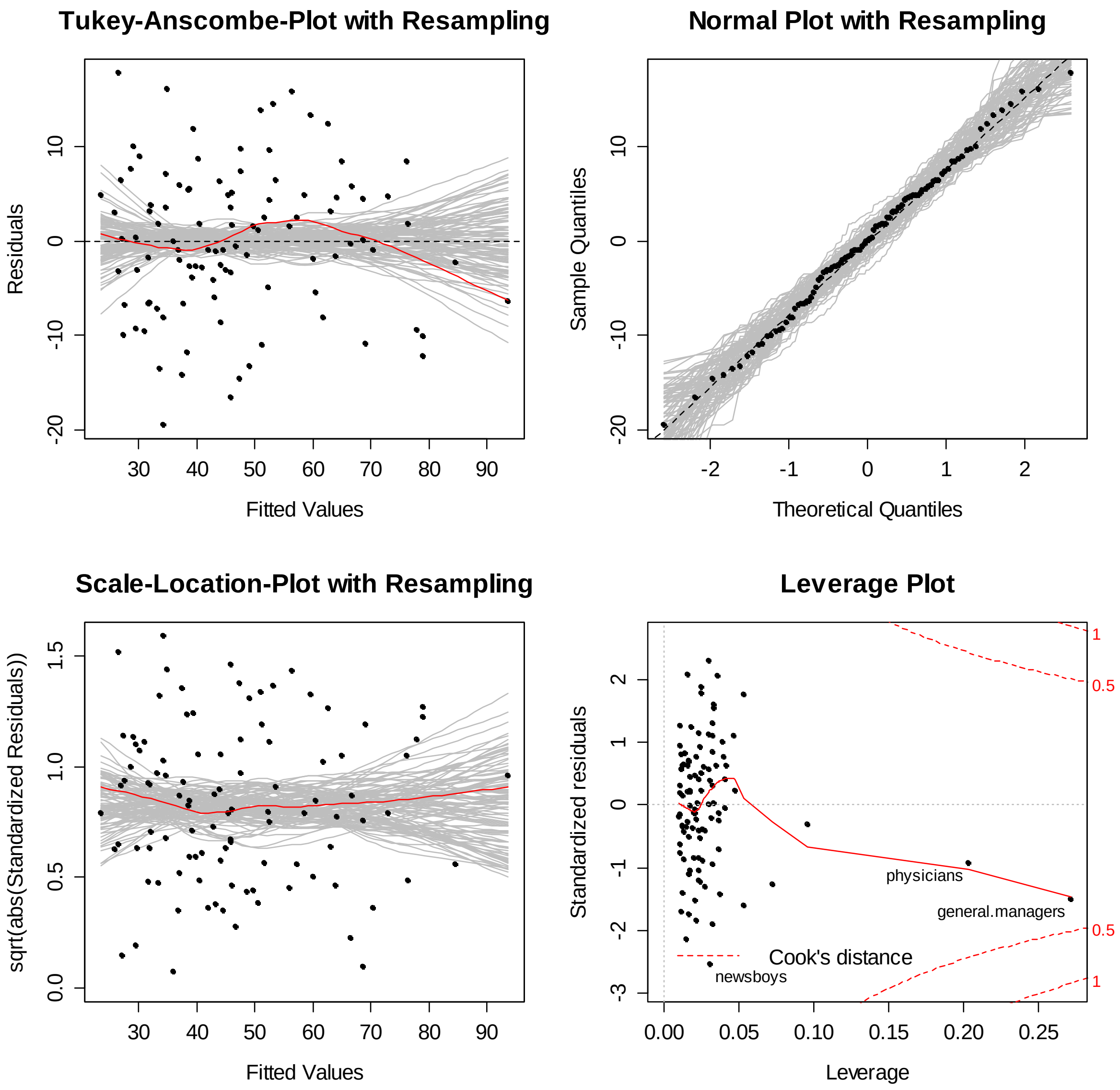
3.7.5 Further Residual Plots

It is perfectly valid to plot the residuals from a regression model against any variable we like, be it a predictor, a not yet used potential predictor or other variables such as the time or sequence of the observations. There is one important rule for all these plots: *if any non-random structure is evident, the model has deficiencies and can be improved*. We will illustrate this using a dataset where the prestige of 102 occupations was measured with a survey. The prestige score is the response variable and there are 5 potential predictors, namely the average number of years of education that people in that profession have, the average income, the percentage of women, the census (which is an occupational code) and the type, a categorical variable with the 3 levels professional/managerial, blue collar and white collar. For the purpose of exposition, we first fit a very simple model, i.e.

```
    prestige ~ income + education
```

The further three potential predictors are omitted from the model, such that we can study the deficiencies that appear. We first fit the model and study the 4 standard residual plots in R, enhanced with the resampling based confidence regions. The author has implemented that functionality in a procedure called `resplot()`:

```
> fit <- lm(prestige ~ income + education, data=Prestige)
> resplot(fit)
```



Tukey-Anscombe-Plot with Resampling

Normal Plot with Resampling

Scale-Location-Plot with Resampling

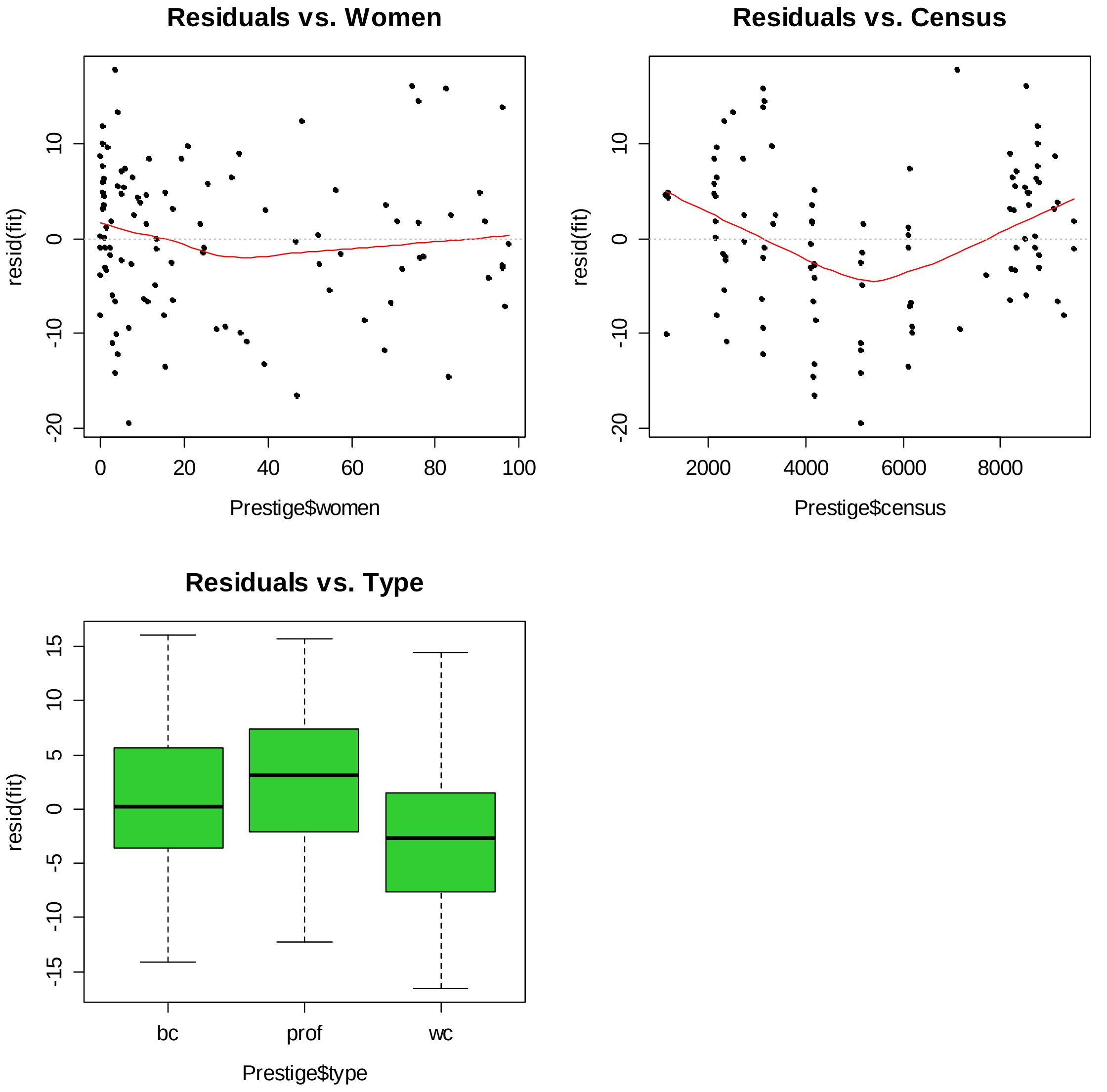
Leverage Plot

From the summary, we gather that the global F-test is highly significant and that the R-squared reaches a value close to 0.8. Also when inspecting the residual plots, the fit seems reasonable. There may be a slight systematic error visible in the Tukey-Anscombe plot and we observe two leverage points, namely physicians and general managers. These are the two professions with the highest average income. These problems are not severe and overall, the model is certainly of a reasonable quality. .However, as we will see below, it is pretty easy to come up with a better model for `prestige`.

Residuals vs. Potential Predictors

As mentioned in the introduction, we may plot the residuals against any variable we like. Here, we first study what we observe if the residuals are plotted versus the potential further predictors.

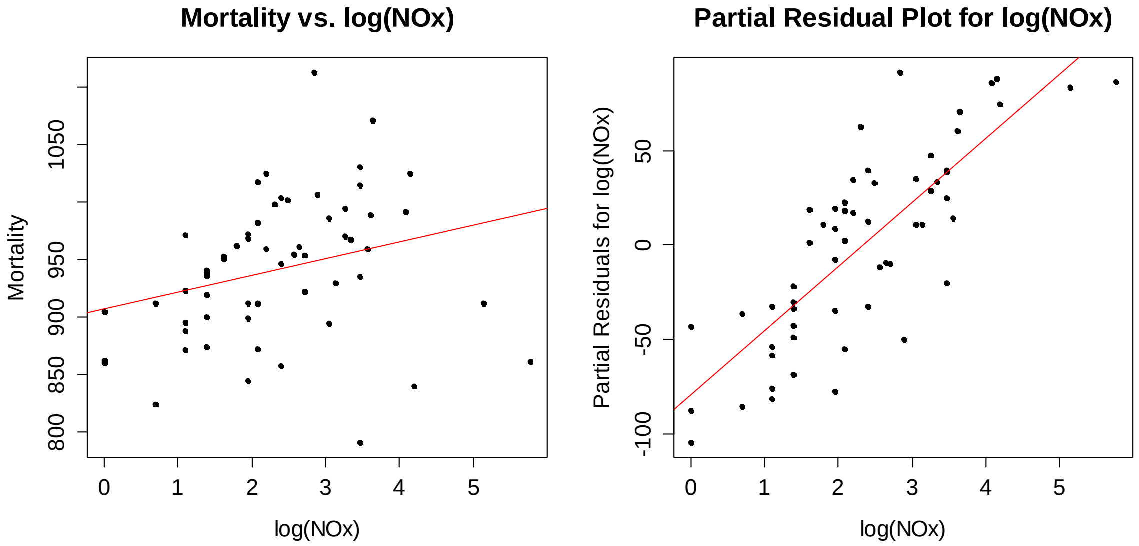
```
> plot(resid(fit) ~ Prestige$women, pch=20)
> lines(loess.smooth(Prestige$women, resid(fit)), col="red")
> abline(h=0, col="grey", lty=3)
> plot(resid(fit) ~ Prestige$census, pch=20)
> lines(loess.smooth(Prestige$census, resid(fit)), col="red")
> abline(h=0, col="grey", lty=3)
> plot(resid(fit) ~ Prestige$type, col="limegreen")
```



There does not seem to be much of a relation between the percentage of women in a profession and the residuals, but the other two variables census and type certainly have a non-random relation with the residuals. Especially for census, we quite strongly underestimate the prestige of jobs with values in the 4000-6000 range. A similar observation is made for the type: the prestige of managerial jobs is underestimated by our current model, while the one of white collar professions is overestimated. We can and should cure these problems by integrating the predictors into the model.

Partial Residual Plots

In many applied problems, it is very interesting to understand and visualize the relation between the response and some arbitrary predictor x_k. However, a plot of y vs. x_k can be deceiving, because in a multiple regression setting, all other predictors $x_1,...,x_{k-1},x_{k+1},...,x_p$ will simultaneously have an effect on the response. Hence, what we should aim for is displaying the relation of y vs. x_k under the presence of the other predictors. That is what the partial residual plot does. We try to illustrate the idea with an excerpt from the mortality dataset.



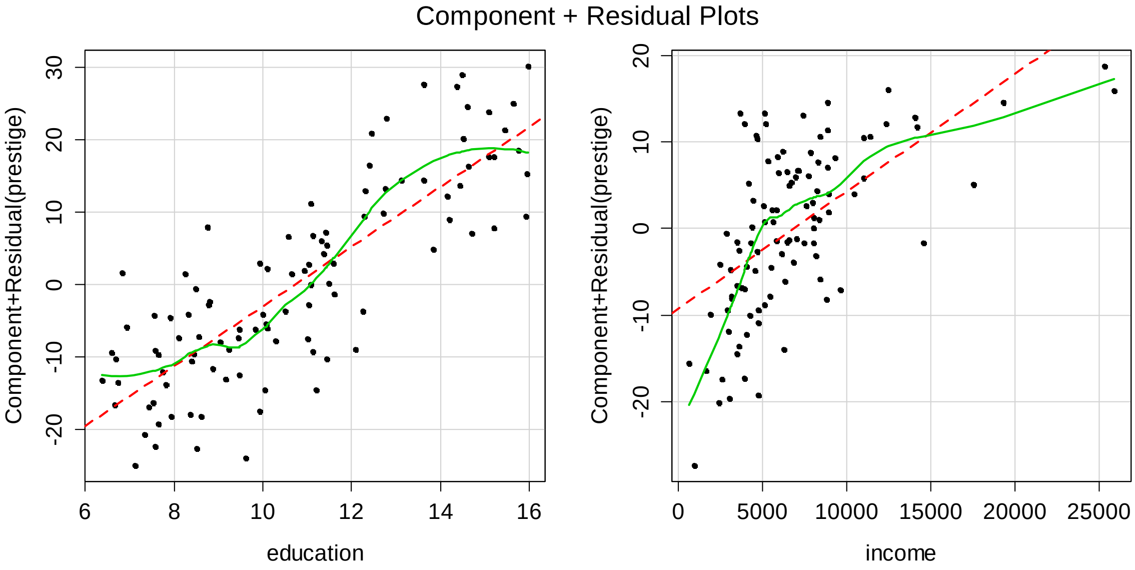
The left panel shows the plain relation between the response and the logged nitrous oxide. The problem with this plot is that mortality in the different cities is affected by other factors than $\log(NO_x)$, too. We try to improve upon this with the plot on the right. It shows the partial residual plot for $\log(NO_x)$. The basic idea is to generate an updated y variable, where the effect of all other predictors is removed from the response. This is the verbal definition of a partial residual. Mathematically, the partial residuals for predictor x_k are:

$$y-\sum_{j\neq k}\hat{\beta}_j x_j = \hat{y}+r-\sum_{j\neq k}\hat{\beta}_j x_j = \hat{\beta}_k x_k + r$$

As we can see from the formula, the initial idea is to adjust the response by the estimated effect of the other predictors. We can reformulate this as adjusting the residuals by the estimated effect of predictor x_k. While the latter is a bit more difficult to comprehend, it is much more convenient for computation. The partial residuals can easily be accessed in R by typing:

```
> residuals(fit, type="partial")
```

This yields a $n \times p$ matrix that has the partial residuals for all the predictors. Even more convenient functionality can be found in the function `crPlots()` in `library(car)`. We display the result for the prestige example:



The partial residual plots are enhanced with the red dashed line that illustrates the actual fit according to the multiple linear regression model. The green solid line is a smoother that was added for visualizing the true relation between partial residual and predictor. This allows for gaining a lot of insight into the model. As we can see, the `income` variable has a non-linear (but approximately logarithmic) relation to its partial residuals. Hence, it would be wise to use `log(income)` rather than the untransformed variable. This should not come as a surprise, as its properties with only positive values on a right-open, relative scale and a right-skewed marginal distribution speak for that, too. Even more interesting is the observation in the left hand panel. There seems to be a pronounced difference in the prestige of jobs that require >12 years of education, i.e. a university degree. Hence, adding a factor variable that codes for jobs that require a degree might improve the fit strongly. As some further experimentation shows, this is indeed the case. A similar effect is achieved if variable `type` is added to the model, as the prof/managerial jobs are the ones requiring >12 years of education.

We finish this section by summarizing that the partial residual plots allow for perceiving how the predictors act in a multiple linear regression model. If there appears a significant difference between their actual, linear fit and the true relation indicated by the smoother, one should improve the model. Sometimes, we can transform predictors to achieve this; at other times adding additional predictors and/or interaction terms may help.

3.8 Variable Selection

There is usually a wealth of predictors and potential predictors available to explain a target variable of interest. Here, we show how we can select the "best" subset of predictors. We first motivate why this is useful, then turn our attention to some strategies for finding the subset, and also discuss the meaning of the word "best" in terms of regression modeling.

3.8.1 Why Variable Selection?

Only in some rare special cases, we do already know the functional form with which a few specified predictors $x_1,...,x_p$ explain the response y. In these cases, we would still be interested in learning about the regression coefficients, do some hypothesis tests, and potentially give some prediction and confidence intervals.

Much more often however, we want to use ***regression*** in an ***explorative fashion***. This is usually when we do not know previously how the relation between response y and some potential predictors x_j is, usually we do not even know which predictors to use. In these situations it has become standard to collect data from many potential predictors. Our goal with regression analysis will then be to learn not only about the form of the relation between response and predictors, but also about required variable transformations, and probably most importantly, about the ***predictors*** that have a ***relevant impact*** on the outcome.

Thus, there is motivation for variable selection arising purely from applied aspects. However, there is some more technical reasoning for keeping a model small:

1) We generally want to explain the data in the simplest way, and thus remove redundant predictors. This follows the idea that if there are several plausible explanations (i.e. models) for a phenomenon, then the simplest is the best.

2) Unnecessary predictors in a regression model will add noise to the estimation of the coefficients for the other predictors. Or in other words: we need more observations to have the same estimation accuracy.

3) What is stated in 2) above becomes even more pronounced if there is collinearity among the predictors, i.e. if there are too many variables trying to do the same job. Removing excess predictors facilitates interpretation.

4) If the model is to be used for prediction, we will be able to save effort, time and/or money if we do not have to collect data for redundant predictors.

Please note that variable selection is not a method. It is a process that cannot even be separated from the rest of the analysis. For example, outliers and influential data points will not only change a particular model – they can even have an impact on the model we select. Also variable transformations will have an impact on the model that is selected. Some iteration and experimentation is often necessary for variable selection, i.e. to find smaller, but better models.

Example

We will illustrate the variable selection process on data coming from the US Bureau of Census. They contain information from 50 US states recorded around 1970. The target variable is life expectancy, and there are 7 continuous predictors:

`Population`:	as of July 1, 1975
`Income`:	per capita income, estimated 1974
`Illiteracy`:	percent of populations, 1970
`Murder`:	number of murders per 100'000 people (1976)
`HS.Grad`:	percent high-school graduates (1970)
`Frost`:	number of days with minimum temperature below freezing
`Area`:	land area in square miles

Some variable transformations are required: `Population` and `Area` are very skewed, thus we apply a log-transformation on them. Moreover, `Murder` and `Frost` are counts, this is why a square root transformation is appropriate. Finally, `Illiteracy` and `HS.Grad` are proportions, for which we do an arcsine transformation. `Income` is almost symmetrically distributed, and does not need any transformation. The model diagnostics (not shown here) look fine when one is using the transformed input variables. The summary output is as follows – so now what are the driving predictors for life expectancy?

```
> summary(lm(Life.Exp ~ ., data = state.trsf)

Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept)  6.878e+01  2.806e+00  24.511  < 2e-16 ***
Population   2.799e-01  1.238e-01   2.261   0.0290 *
Income      -5.601e-05  2.345e-04  -0.239   0.8124
Illiteracy  -5.885e-01  7.663e+00  -0.077   0.9392
Murder      -1.510e+00  2.188e-01  -6.905 1.99e-08 ***
HS.Grad      5.845e+00  2.458e+00   2.378   0.0220 *
Frost       -9.968e-02  4.821e-02  -2.067   0.0449 *
Area         3.361e-02  1.036e-01   0.325   0.7472
---
Residual standard error: 0.7109 on 42 degrees of freedom
Multiple R-squared: 0.7596,   Adjusted R-squared: 0.7195
F-statistic: 18.96 on 7 and 42 DF,    p-value: 3.867e-11
```

The signs of the coefficients mostly match what we would expect. Higher murder rate decreases life expectancy which certainly confirms our a priori ideas. Additionally, we observe that there are some weakly significant variables: `Population`, `HS.Grad` and `Frost`, and a few which are non-significant: `Income`, `Illiteracy`, and `Area`.

The question is now how we could find out which ones are required in this model, and which ones can be omitted. Remember again that is not a valid approach to kick all predictors with non-significant p-values out of the model simultaneously.

3.8.2 Backward Elimination

We have seen above that reducing the model by more than one variable at a time is problematic. However, we could do some stepwise ***backward elimination***. This is the simplest of all variable selection procedures. It can easily be run without any special software. On the other hand, it can only be conducted if there is a reasonable balance between the number of predictors and the number of observations. There is a general rule of the thumb, saying that there should be at least 5 times as many observations as the number of coefficients that are estimated.

We start with a model where all potential predictors are included. We then remove the predictor with the highest p-values greater than α_{crit}. Next, we refit the model and again remove the least significant predictor, provided its p-value is greater than α_{crit}. Sooner or later, all "non-significant" predictors will be removed, and the selection process will be complete. One usually uses the arbitrary $\alpha_{crit} = 0.05$, although for prediction, often a 0.15 or 0.20 cutoff yields better results.

In our example, `Illiteracy` is the least significant predictor with a p-value of 0.939. We will omit it, and fit the model again. From the summary output (not shown here), we learn that `Income` is now the least significant predictor and has p-value of 0.804. Thus, income is omitted, and the model gets refitted. Then, `Area` has a p-value of 0.675, and is excluded. Now, the least significant predictor is `Population` with a p-value of 0.012, i.e. the backward elimination is terminated.

```
> summary(lm(Life.Exp ~ Population + Murder + HS.Grad +
                        Frost, data = state.trsf)
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) 68.78767    1.75860  39.115  < 2e-16 ***
Population   0.27663    0.10600   2.610 0.012259 *
Murder      -1.49218    0.17046  -8.754 2.83e-11 ***
HS.Grad      5.83746    1.37130   4.257 0.000104 ***
Frost       -0.09671    0.03669  -2.636 0.011477 *
---
Residual standard error: 0.6888 on 45 degrees of freedom
Multiple R-squared: 0.7582,   Adjusted R-squared: 0.7367
F-statistic: 35.28 on 4 and 45 DF,    p-value: 2.416e-13
```

When comparing this output with the full model, we observe that `Murder`, `HS.Grad`, `Frost` and `Population` have lower p-values than initially. The reason is that some of their predictive power was covered by the removed variables `Area`, `Income` and `Illiteracy`. This does not come as a surprise, because the percentage of high school graduates is correlated with illiteracy, and also income.

Moreover, it is important to understand that the removed variables are still related to the response, as a regression of `Life.Exp` on `Area`, `Income` and `Illiteracy` would show. We do not show the output here, and leave this as an exercise.

3.8.3 Forward Selection

This is an analogue to the backward elimination. However, forward selection starts with an empty model, i.e. a model where only the intercept, but no predictors are present. The, we add predictors in a stepwise manner: in every step, we add the one which is the most important one, i.e. has the lowest p-value, when added to the model. We do so, until no terms with p-values lower than α_{crit}, usually set equal to 0.05, can be added to the model.

This approach is feasible also in situations where there are more predictors than there are observations. Since it is also computationally cheap, it was popular in the early days of regression analysis.

3.8.4 Stepwise Regression

This is a combination of backward elimination and forward selection, and is what R does by default in function `step()`. It addresses the situation where variables are added or removed early in the process and we want to change our mind about them later. At each stage of the selection process, a variable may be added or removed. As before, we can base our decisions on the p-values from individual hypothesis tests.

3.8.5 Testing-Based Variable Selection

With the backward, forward and stepwise approaches, the decisions for variable selection were based on individual hypothesis tests. While this is computationally cheap, it also has some drawbacks:

1) Because of the “one-at-a-time” nature of adding/dropping predictors, it is possible to miss the “best” model.

2) The p-values should not be treated too literally. We are subject to the multiple testing problem. Moreover, the removal of less significant predictors tends to increase the significance of the remaining ones. One thus often overstates the importance of the remaining predictors.

3) The testing based variable selection procedures are not directly linked to the final objectives of prediction or explanation. With any variable selection method, it is important to keep in mind that model selection cannot be divorced from the underlying purpose of the analysis.

4) The testing based procedures tend to select models that are smaller than desirable for prediction purposes. Consider the following simple example to understand this: in a simple linear regression, we would go with the intercept only if the predictor is not significant. However, for prediction it could still be better to use it.

3.8.6 Criterion Based Variable Selection: AIC/BIC

On the other hand, if we have some idea about the purpose for which a model is intended, we might propose some measure of how well a given model meets that purpose. It would be appealing to scan a big variety of different models. In the case where there are a fixed number of m predictors, we can build 2^m different regression models: for each variable we can decide, whether it will be included in the model or not.

Obviously, this ***all subsets regression*** approach only works when the number of potential predictors is limited, else it will be too time consuming and we need to economize on computing time. Also note that we here cannot any longer use the p-values from individual hypothesis tests as a criterion, but we need something, that judges the quality of the model more generally. The following quantities are potential candidates:

a) Coefficient of determination R^2

b) Test statistic or p-value of the global F-test

c) Estimated error variance $\hat{\sigma}_E^2$

For a fixed number of predictors m', they will all lead to the same order among all possible models. Another property they share is that they judge the goodness-of-fit, and thus generally tend to improve if more terms are added to the model. However, as we can easily imagine, bigger models are not necessarily better than smaller ones. It would thus be preferable to employ a criterion which is not only based on goodness-of-fit, but also penalizes for the model size. A potential candidate is the adjusted R^2. In practice, one nowadays almost exclusively uses the ***Akaike*** or ***Bayes Information Criteria*** (AIC/BIC), which are defined as follows:

$$\begin{aligned} AIC &= -2\max(\log likelihood) + 2p \\ &= const + n\log(RSS/n) + 2p \end{aligned}$$

and

$$\begin{aligned} BIC &= -2\max(\log likelihood) + p\log n \\ &= const + n\log(RSS/n) + p\log n \end{aligned}$$

Because the constant ($const$) is the same for a given dataset and any assumed error distribution, it can be ignored for model comparisons on the same data.

The goal in practice is to find the model which minimizes AIC or BIC. Larger models will fit better, and thus have smaller residual sum of squares RSS. However, they use more parameter and are thus penalized by the terms $2p$ (AIC) and $p\log n$ (BIC). Note that BIC punishes larger models more heavily and so will tend to prefer smaller models in comparison to AIC.

Finally, we note here that the use of AIC/BIC is not limited to all subset regression. These criteria can also be applied in the backward, forward or stepwise approaches. In R, variable selection is generally performed by function `step()`, which by default employs the stepwise approach with AIC as a criterion. We illustrate this with the state data:

Example

```
> step(lm(Life.Exp ~ ., data=state.trsf))
Start:  AIC=-26.84
Life.Exp ~ Population + Income + Illiteracy + Murder +
           HS.Grad + Frost + Area

             Df Sum of Sq    RSS      AIC
- Illiteracy  1    0.0030 21.231 -28.8291
- Income      1    0.0288 21.256 -28.7682
- Area        1    0.0532 21.281 -28.7109
<none>                    21.228 -26.8361
- Frost       1    2.1603 23.388 -23.9903
- Population  1    2.5844 23.812 -23.0918
- HS.Grad     1    2.8591 24.087 -22.5183
- Murder      1   24.0982 45.326   9.0927

[Output partly omitted...]

Step:  AIC=-32.55
Life.Exp ~ Population + Murder + HS.Grad + Frost

             Df Sum of Sq    RSS     AIC
<none>                    21.347 -32.555
- Population  1     3.231 24.578 -27.508
- Frost       1     3.296 24.643 -27.376
- HS.Grad     1     8.596 29.944 -17.635
- Murder      1    36.352 57.699  15.161
```

When we did a backward elimination based on the AIC criterion, the sequence of predictor removal was exactly the same as when our decision was based on hypothesis testing. The process also stops at the same spot, and the resulting model is exactly equal to the one we found before. Please note that this is a coincidence – one generally does observe differences when using different variable selection schemes.

A final remark on variable selection: every procedure may yield a different "best" model. However, if we could obtain another sample from the same population, even a fixed procedure might result in another "best" model. Thus, there is an element of chance in this declaration. How can we mitigate this in practice? It is usually advisable to not only consider the "best" model according to a particular procedure, but to check a few more models that did nearly as good, if they exist.

3.8.7 Correct Treatment of Hierarchical Models

For models with interactions, it does not result in a valid model if a main effect is removed, but the interaction is kept within the model. The reasons are similar as with the polynomial models above. We leave it as an exercise to study the effects of removing a main effect, but keeping the interaction.

When there are categorical predictors, we need dummy variables to incorporate them into the model. Now if a single dummy coefficient is non-significant, we cannot just kick this term out of the model! Thus, we have to test the entire block of indicator variables. When we work manually and testing based, this will be done with a partial F-test, whose p-value can be compared against the ones from the other variables (even if they may arise from individual hypothesis tests).

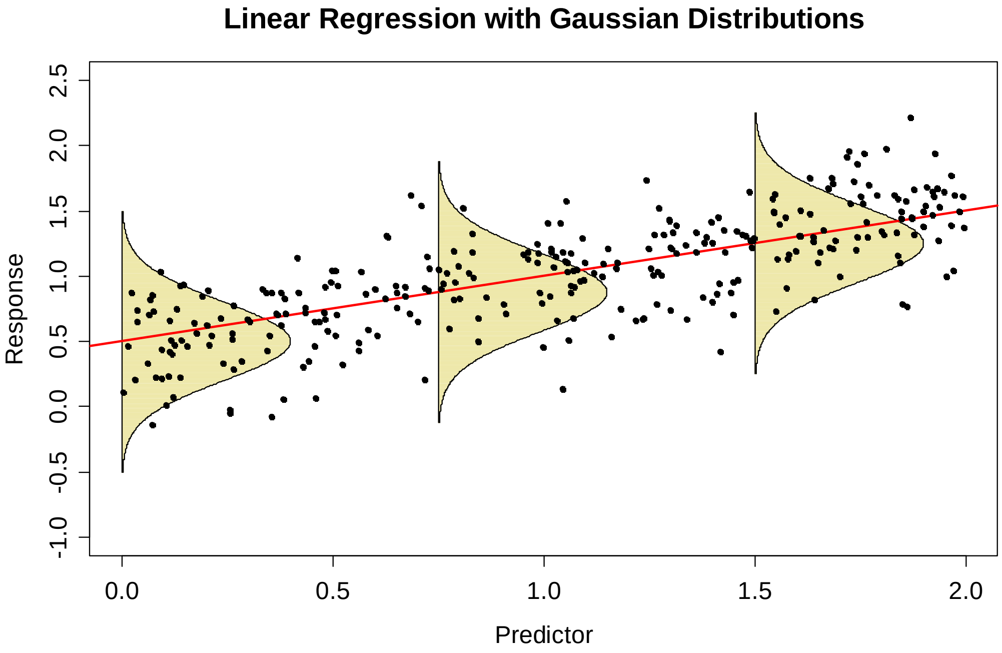
When we use a criterion based approach with function `step()`, then `R` deals correctly with categorical predictors, and also with interactions and hierarchical models. Be careful with other software though – not all statistics packages can correctly handle variable selection with such input.

4 Extending the Linear Model

Linear models are central to the practice of statistics and can be seen as part of the core knowledge of any applied statistician. While they are very versatile, there are situations that cannot be handled within the standard framework. Here, we will take care of some of these.

4.1 What is the Problem?

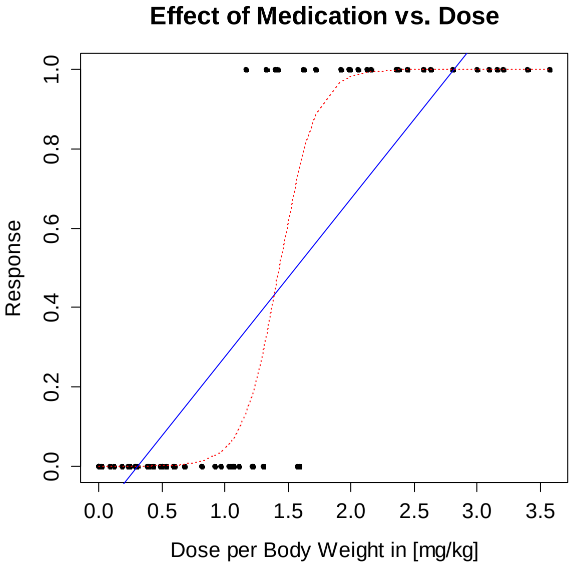
In all our previous theory, the response y_i was assumed to be a continuous random variable whose range was (at least theoretically) reaching from minus to plus infinity. The principal goal was to estimate and predict the conditional expectation, i.e. $\hat{y}_i = E[y_i \mid X_i]$ from the data. All theory, algorithms, tests and confidence intervals operated under the assumption that the conditional distribution was Gaussian, i.e. $y_i \mid X_i \sim N(\hat{y}_i, \sigma_E^2)$. The figure below shows the density of these in a simple linear regression at $x = 0$, $x = 0.75$ and $x = 1.50$.



On the other hand, there are response variables that are not continuous, but binary, i.e. with values in $\{0,1\}$, or which are a proportion in $[0,1]$. Still, it can be very worthwhile to study the dependence of this response on a number of predictors with a regression approach. However, applying the standard multiple regression framework will ultimately result in responses that are beyond the set of values which are foreseen in that problem. Thus, we need some additional techniques which can deal with these types of situations. Depending on how exactly the response variable is, there are several different approaches, which all fit within the framework of a more widely formulated concept entitled *generalized linear modeling* (GLM). Here follows a brief overview of the covered topics:

4.1.1 Binary Response

In toxicological studies, one tries to infer whether a lab mouse survives when it is given a particular dose of some poisonous medication. In human medicine, we are often interested in the contrary case: how much “dose” has an effect, i.e. reduces pain or other symptoms. Here, the response variable is a binary variable in $\{0,1\}$, standing for either *survival vs. death*, or *status quo vs. reduction*. The conditional distribution of the response is $y_i \mid X_i \sim Bernoulli(p_i)$ and hence much different from a Gaussian. Our interest lies in modeling the expectation of this conditional distribution which is $E[y_i \mid X_i] = p_i$, the probability of death resp. pain reduction. We illustrate this with an example where we acquired the response for a cohort of 72 patients and also the dose given per bodyweight (in $[mg/kg]$) was known. The data present themselves as follows:



The naïve approach is to use simple linear regression with the 0/1 outcome as response and the dose as predictor. This yields the blue regression line. Obviously, this results in fitted values outside of the interval $[0,1]$, whose interpretation is unclear. A good statistical model for the above example must yield a $[0,1]$-restricted probability for positive response. This is a coherent approach and takes into account that for a given (intermediate) concentration, we will only have an effect on some of the subjects, but not on all of them. A potential solution is offered by the red dotted line in the above plot. The question is how the curved red line is obtained/estimated. While the full details are covered in section 4.2, we briefly mention that fitting such a logistic regression model is based on estimating the positive response probability $p_i = P(y_i = 1 \mid x_i)$ for each observation i such that:

$$\log\left(\frac{p_i}{1-p_i}\right) = \beta_0 + \beta_1 \cdot x_i \text{, or equivalently } p_i = \frac{\exp(\beta_0 + \beta_1 x_i)}{1+\exp(\beta_0 + \beta_1 x_i)}$$

The regression parameters β_0, β_1 are determined by optimizing the goodness-of-fit of the p_i with a maximum likelihood approach, for details see section 4.2.

4.1.2 Count Response

What are predictors for the abundance of starfish (*in German: Seestern*) at several locations in the sea? For answering this question, we could analyze a dataset consisting of counts in different areas, plus the values of several predictors. Obviously, the response y_i is a count – the simplest and natural model for the conditional distribution $y_i \mid X_i$ is a Poisson distribution. We then assume that the parameter λ_i at location i depends on the predictors. Since $\lambda_i > 0$, we must use a log-transformation to link it to the linear combination:

$$y_i \mid X \sim Pois(\lambda_i) \text{ where } \log(\lambda_i) = \beta_0 + \beta_1 x_{i1} + ... + \beta_p x_{ip}.$$

4.1.3 Categorical Response

Another extension of the linear model is necessary for the case where we try to predict a nominal response variable. For example, we may be interested in giving probabilities for the favorite political party of a person, depending on predictors such as education, age, etc. Such data can be summarized and displayed in contingency tables. The goal is modeling conditional probabilities $P(y_i = k \mid X_i)$ for the categories $k = 1,...,K$.

4.1.4 Generalized Linear Models

The above mentioned models for binary, count and categorical response all fit within the framework of generalized linear models, which also encompasses the multiple linear regression approach from chapter 3. GLMs are based on the notion that the suitably transformed conditional expectation of the response y_i has a linear relation to the predictors, i.e.:

$$g(E[y_i \mid X_i]) = \beta_0 + \beta_1 x_{i1} + ... + \beta_p x_{ip}.$$

As we had argued above, in case of multiple linear regression the link $g(\cdot)$ will be the identity function, and the conditional distribution $y_i \mid X_i$ is a Gaussian. The specifics of the model extensions for counts and categorical response will be discussed on the following pages. Please note that formally, GLMs also require that the responses' variance y_i is of the form $\phi \cdot v(E[y])$, where ϕ is an additional parameter, and $v(\cdot)$ a specific function. Moreover, the choice of conditional distributions $y_i \mid X_i$ that are tractable within the limits of GLMs is restricted.

While the GLM formulation and the restrictions may sound complicated, they allow for formulating a unified mathematical theory that encompasses common basic principles for estimation, inference and model diagnostics. We will not deeply embark into the formal aspects, but limit ourselves to the practically relevant do's and dont's of applied generalized linear modeling. For readers who are interested in pursuing the theory on GLMs, we refer to the seminal work "Generalized Linear Models" by McCullagh and Nelder (Chapman and Hall, 1989).

4.2 Logistic Regression

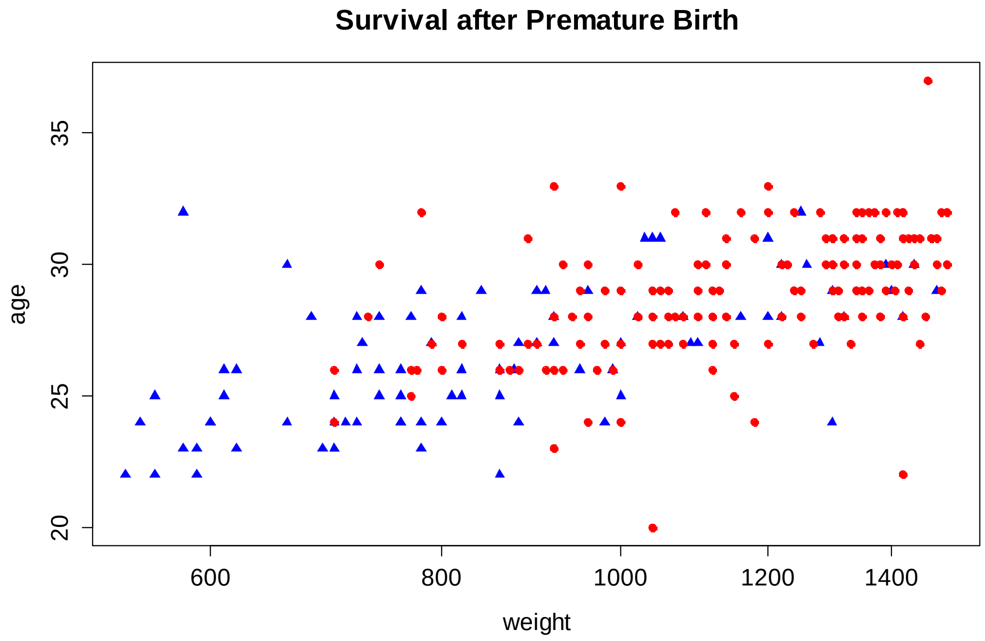
As explained above, datasets with a binary response variable are not multiple linear regression problems. Here, we will discuss the necessary extension. While in many aspects, techniques and ideas are similar to what is already known, some novel issues appear as well. We will take care of model formulation, estimation, inference, diagnostics, prediction and model choice.

4.2.1 Example: Survival after Premature Birth

We discuss an example dealing with survival after premature birth. A study of Hubbard (1986) contains data of 247 early born babies. Predictors for survival are *birth weight* (in grams), *birth age* (in weeks of pregnancy), the *apgar scores* (judging the vital functions one and five minutes after birth) and the *pH-value* of the babies' blood (providing information on oxygen saturation). For reasons of simplicity, we limit ourselves to the two most informative predictors, *age* and *weight*. Due to positive skewness, we perform a log-transformation for the latter.

If we color-code the response, i.e. *survival with red dots* and *death with blue triangles*, the data can be displayed in a 2d-scatterplot, see below. It is apparent that the proportion of surviving babies depends on age and weight: the older and heavier a baby is born prematurely, the better the odds for surviving are. The goal with our logistic regression analysis will be the quantitatively model the probability for survival conditional on the two predictors weight and age.

```
> plot(age ~ weight, data=baby, log="x", type="n")
> points(age ~ weight, subset=(survival==0), data=baby, ...)
> points(age ~ weight, subset=(survival==1), data=baby, ...)
> title("Survival after Premature Birth")
```



4.2.2 Model and Estimation

In the premature birth example, the response is binary: $y_i \in \{0,1\}$. Hence y_i follows a *Bernoulli distribution*, whose parameter (called the “success probability”) is denoted by p_i. Typically, the parameter and the distribution are conditional on the predictor(s), for which we use the general notation X_i:

$$p_i = P(y_i = 1 \mid X_i) = E[y_i \mid X_i] = \mu_i ,$$

It is important to note that p_i is not only the parameter of the responses’ Bernoulli distribution, but also the conditional expectation μ_i of the response variable y_i. In that situation, the logistic regression model is defined as

$$\log\left(\frac{p_i}{1-p_i}\right) = \beta_0 + \beta_1 x_{i1} + ... + \beta x_{ip}$$

As we can see, the linear predictor $\eta_i = \beta_0 + \beta_1 x_{i1} + ... + \beta_p x_{ip}$ is linked to the conditional expectation $p_i = \mu_i$ via the logit function $p \mapsto \log(p/(1-p))$, which maps from $[0,1]$ to $(-\infty,+\infty)$. Thus, we are “safe” to use a linear combination of the predictors, i.e. it is certain that the output will always be a $[0,1]$-restricted probability. The logit function has a descriptive interpretation: $p/(1-p)$ is called the *odds* (*“Wettverhältnis”* in German) for an event. A probability of $1/2$ yields to a $1:1$ odds, i.e. both outcomes are equally likely. If we have $p_i = 1/4$, then the odds turns out to be $1:3$, i.e. the second outcome is three times as likely. Odds are always positive, so that we require a log-transformation to obtain a full real-valued scale. Thus, logistic regression equals describing the *log-odds* with a linear model.

A peculiarity of logistic regression is that there is no explicit, additive error term as in multiple linear regression. It is not needed because we model p_i: the variation in the babies’ survival for a given combination of birth age and weight is already dealt with by the Bernoulli distribution of the response variable with parameter p_i.

Estimation

For practical application, it is important to estimate the regression coefficients $\beta_0,...,\beta_p$ on a given dataset. While it would conceptually be possible to minimize the sum of squared raw residuals $r_i = p_i - y_i$, this approach is not theoretically sound and does not prove to be fruitful in practice. Instead, we perform *maximum likelihood estimation* (MLE) where the regression coefficients β_j are determined such that the likelihood of the observed data is maximized. By assuming independence of the cases, this boils down to determine the parameters such that the Bernoulli log-likelihood

$$l(\beta) = \sum_{i=1}^{n} \left(y_i \log(p_i) + (1-y_i)\log(1-p_i) \right)$$

is maximized. Note that this is a sensible goodness-of-fit measure. For all observations with $y_i = 1$ we aspire for high p_i to keep the contribution to $l(\beta)$ low, and vice versa for the observations with $y_i = 0$. The dependence of $l(\beta)$ on the data and the regression coefficients becomes more obvious if p_i is replaced with:

$$p_i = \frac{\exp(\beta_0 + \beta_1 x_{i1} + ... + \beta_p x_{ip})}{1 + \exp(\beta_0 + \beta_1 x_{i1} + ... + \beta_p x_{ip})}$$

The log-likelihood maximization can be approached by taking partial derivatives of $l(\beta)$ with respect to $\beta_0, ..., \beta_p$. This still yields an equation system, but in contrast to multiple linear regression, it is no longer a linear one that is easy to solve. However, under some mild conditions, the maximum exists, though it cannot be written in closed form. We thus require numerical optimization. It turns out that a good method is to employ linear approximations that are solved using a sequence of *iteratively reweighted least squares regressions* (the *IRLS algorithm*). We do without giving further details, but instead focus on the practical application.

R-Code for Estimating Logistic Regression Models

In R, routines for estimating logistic regression models are readily available. We illustrate their syntax on the premature birth example:

```
> glm(survival~log10(weight)+age, family=binomial, data=baby)

Coefficients:
  (Intercept)  log10(weight)            age
     -33.9711        10.1685         0.1474
```

This is only a part of the output, but for the moment the most interesting one, namely the estimated coefficients $\hat{\beta}_0, \hat{\beta}_1$ and $\hat{\beta}_2$. Please note that this is a numerically optimized solution, so it may happen that the following warning message appears:

```
Warning message:
glm.fit: algorithm did not converge
```

It obviously means that the IRLS algorithm did not converge, and hence the coefficients are not trustworthy. Unfortunately, it is not possible to make general statements on how to achieve convergence. On the other hand, convergence problems are rare in well-posed regression problems. Another issue (and warning) that can arise is the one of fitted 0 or 1 probabilites:

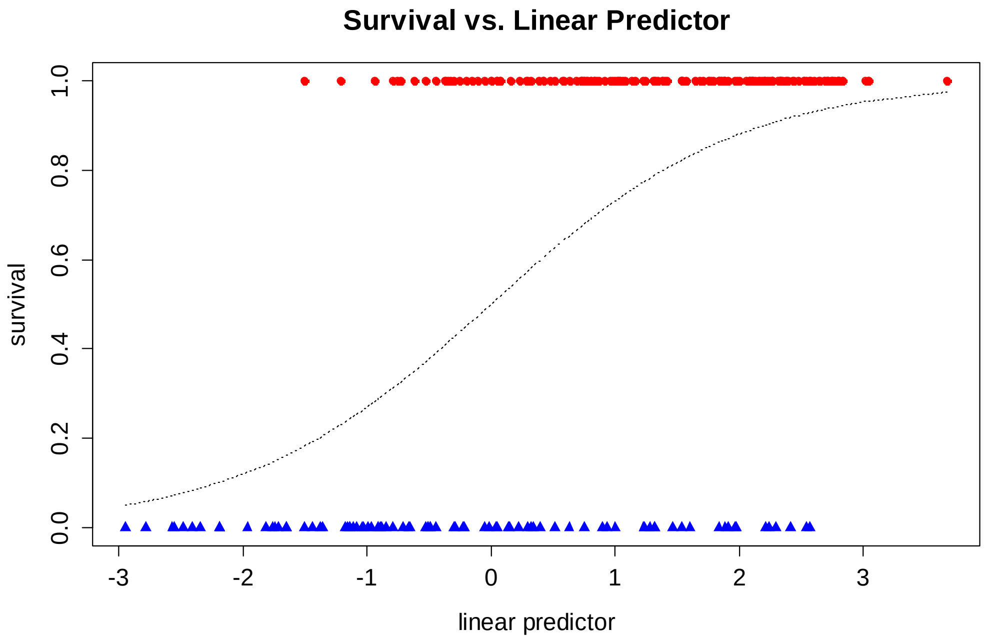
```
Warning message:
glm.fit: fitted probabilities numerically 0 or 1 occurred
```

This is also known as the *Hauck-Donner phenomenon* and indicates that there is a subspace in predictor space with perfect separation of observations with $y = 0$ and $y = 1$. If that is the case, the optimal regression coefficient estimates could be arbitrarily large what makes it difficult to explicitly determine them. As a way out, R artificially limits the estimated coefficients to a maximum of +/- 10 and issues the above warning. Working with such models is usually fine despite the warning.

Displaying the Fit

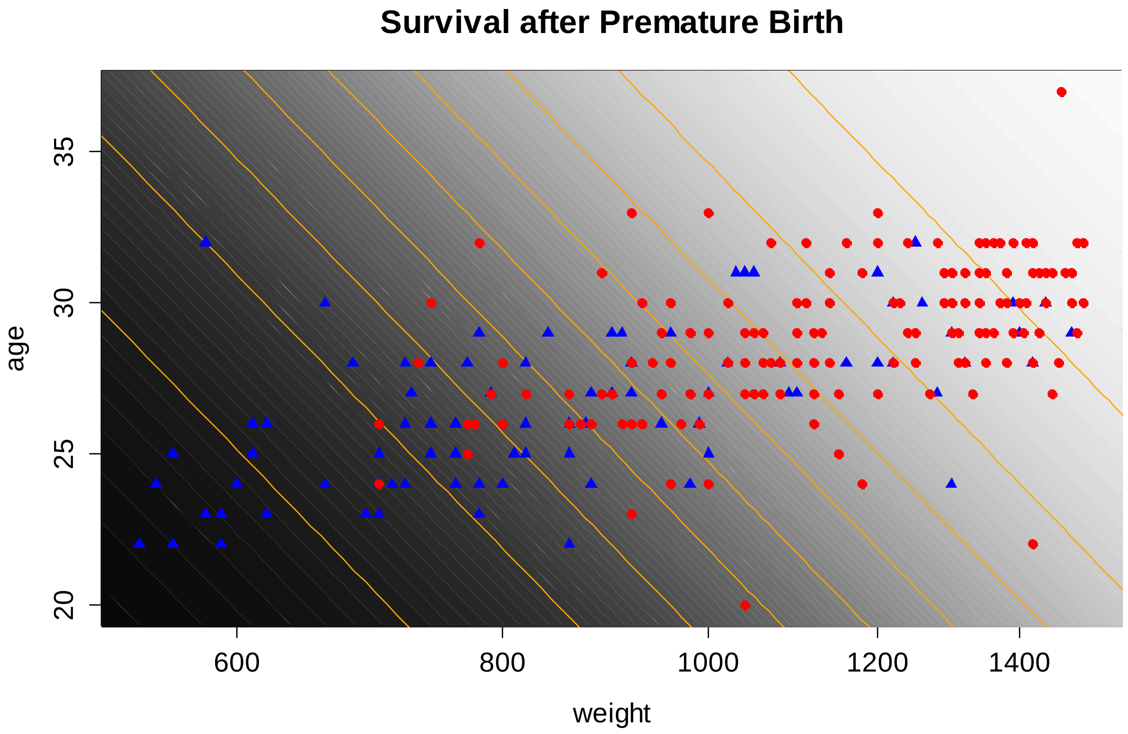
A simple option for displaying the GLM fit is to plot the response vs. the linear predictor. This always works, no matter how many predictor variables ones uses. The following code is required:

```
> fit <- glm(survival ~ log10(weight) + age, family=binomial)
> fvl <- predict(fit, type="link")
> fpr <- predict(fit, type="response")
> plot(fvl, survival, type="n", xlab="linear predictor")
> points(fvl[survival==0], survival[survival==0])
> points(fvl[survival==1], survival[survival==1], col="red")
> lines(sort(fvl), sort(fpr), lty=3)
> title("Survival vs. Linear Predictor")
```



Small values in the linear predictor correspond to low survival probability, and vice versa. The fitted values show their typical S-shaped curve that is created by the inverse of the logit function. The value 0 always marks the midpoint: it corresponds to an odds of 1 and hence equal chances for survival vs. death.

Another option for displaying the results (that is restricted to examples with two predictors as in premature birth) is to color code the probability of survival. By keeping the probability of survival fixed, we can express the *age* value as function of *log10(weight)*. Some quick calculations show that the resulting function is linear, hence the contours of equal probability are given by parallel straight lines. The frame on the next page illustrates this for the age vs. weight plot: black background color would correspond to a survival probability of 0, and white to 1. The orange contours stand for probability 0.1, 0.2, …, 0.9. As we can observe, there are babies who survive with estimated probabilities below 0.9, whereas other die despite of estimated survival probabilities above 0.9.



Interpretation of the Regression Coefficients

We now turn our attention to the interpretation of the regression coefficients β_j. As we had stated above, the log-odds for $y_i = 1$ are a linear function of the predictors. Thus, if predictor x_j is increased by 1 unit, then the log-odds in favor of $y = 1$ increase by β_j if all other predictors remain unchanged. We illustrate this with the premature birth example, where we consider an individual with $\log_{10}(weight) = 3$ and birth age of 30 weeks. We have:

$$\eta = -33.9711 + 10.1685 \cdot 3.0 + 0.1474 \cdot 30 = 0.957 \text{ ,}$$

which are the log-odds for survival. If we take $\exp(0.957) = 2.604$, we obtain the odds for survival. It is thus 2.604 times more likely to survive than die when born at this particular combination of age and weight. On the other hand, the probability for survival is:

$$g^{-1}(\eta) = \frac{\exp(\eta)}{1+\exp(\eta)} = \frac{\exp(0.957)}{1+\exp(0.957)} = 0.723$$

Now, if we compare to an individual with birth age 31 weeks (and the rest remaining as above), we obtain the odds as $\exp(1.104) = 3.017$. If we divide the two odds, we obtain the odds-ratio:

$$\frac{3.017}{2.604} = 1.159 = \exp(\hat{\beta}_2)$$

The odds for surviving increase by $\exp(\hat{\beta}_2)$ (i.e. about 15%) when a baby of the same weight is born one week later – this is a more illustrative way to see the parameter $\hat{\beta}_2$. In other words, we can say that the coefficients from logistic regression models are *log-odds ratios*.

Alternative Link Functions

The role of the link function is to map between the conditional expectation $E[y \mid X]$ and the linear predictor η. In logistic regression, we must ensure that this mapping is between the intervals $[0,1]$ and $(-\infty,+\infty)$. Above, we had argued that the logit function can play this part and is attractive due to its clear interpretation. However, we could use any function that maps between these intervals and in fact, the inverse of any *cumulative distribution function (cdf)* will do so.

Hence, an intuitive alternative choice for the link function is $\eta = \Phi^{-1}(p)$, the inverse of the Gaussian cdf. The resulting procedure is known as *Probit Regression*. In most applied problems, the difference between probit and logistic regression are negligible. Unless you know exactly that you are in a setting where one needs to use with the probit link function, it is probably better to stick to logit link. Even more exotic is the complementary log-log link $\eta = \log(-\log(1-p))$. There are some special cases where it is useful, but giving the details is far beyond the scope of this course.

4.2.3 Inference for Logistic Regression

We base our discussion about inferring a logistic regression model on the summary output in R. Most concepts are already known from our previous discussion about multiple linear regression, but reappear in slightly different form.

```
> summary(fit)

Call: glm(survival ~ log10(weight) + age, family = binomial)

Deviance Residuals:
    Min       1Q   Median       3Q      Max
-2.2983  -0.7451   0.4303   0.7557   1.8459

Coefficients:
               Estimate Std. Error z value Pr(>|z|)
(Intercept)   -33.97108    4.98983  -6.808 9.89e-12 ***
log10(weight)  10.16846    1.88160   5.404 6.51e-08 ***
age             0.14742    0.07427   1.985   0.0472 *
---
Dispersion parameter for binomial family taken to be 1

    Null deviance: 319.28  on 246  degrees of freedom
Residual deviance: 235.94  on 244  degrees of freedom
AIC: 241.94
Number of Fisher Scoring iterations: 4
```

Perhaps the most important difference is that the multiple R-squared and the global F-test are missing here, and only some information about the deviance is given. For deeper insight, we need to consider the goodness-of-fit measure that is used here, which is the so-called deviance:

$$D(y,\hat{p}) = -2 \cdot \sum_{i=1}^{n} \left(y_i \log(\hat{p}_i) + (1-y_i)\log(1-\hat{p}_i) \right)$$

We can see that $D = -2l(\hat{\beta})$, i.e. minus twice the log-likelihood of our model. The summary output lists the value under `Residual deviance`, together with the degrees of freedom of that model, which are $df = n-(p+1)$. The `Null deviance` conceptually is the same, but for the simplest possible model that only has no predictors but only the intercept, and which fits the a-priori probability (i.e. the relative frequency of observations with $y_i = 1$) to all observations.

Coefficient of Determination

In multiple linear regression, the multiple R-squared was an intuitive concept for the explanatory content in the predictors. We might consider applying the same idea for logistic regression models by measuring the proportion of deviance explained. In particular, this would yield $1-235.94/319.28 = 0.26$, or in R:

```
> 1-fit$dev/fit$null
[1] 0.2610193
```

This simple measure is often reasonable for practical application, though the proportion of deviance explained is an often debated topic. A better statistic to measure the explanatory content is:

$$R^2 = \frac{1-\exp((D_{res} - D_{null})/n)}{1-\exp(-D_{null}/n)},$$

where D_{res} and D_{null} are the residual resp. null deviance and n is the number of observations. When this alternative measure is implemented in R, we obtain:

```
> (1-exp((fit$dev-fit$null)/247))/(1-exp(-fit$null/247))
[1] 0.3947567
```

Individual Hypothesis Tests and Confidence Intervals

In multiple linear regression, when assuming Gaussian errors, it is quite easy to show that the estimated regression coefficients $\hat{\beta}_j$ are normally distributed. That property can be used for constructing the individual hypothesis test and the confidence interval. Both require the use of the standard error $\hat{\sigma}_{\hat{\beta}_j}$ for standardization, hence the t-distribution comes into play. All this is no longer true for logistic regression. Maximum likelihood theory tells us that under some mild conditions, the $\hat{\beta}_j$ are asymptotically Gaussian. In practice, we are of course lacking infinitely many observations, but the asymptotic result is used for concluding that the regression coefficients are approximately Gaussian.

This property can be used to assess the individual hypothesis tests and to determine the confidence intervals for the coefficients. We simply assume that under the null hypothesis $H_0 : \beta_j = b$

$$Z = \frac{\hat{\beta}_j - b}{\hat{\sigma}_{\hat{\beta}_j}} \sim N(0,1)$$

The p-values of the individual hypothesis tests for $H_0 : \beta_j = 0$ are given in the summary output. Due to the normal assumption, the respective columns are entitled “z-value” rather than the “t-value” we had in multiple linear regression. A 95%-confidence interval for β_1 can be hand-constructed via:

```
> 10.16846+qnorm(c(0.025,0.975))*1.88160
[1] 6.480592 13.856328
```

A convenient way for obtaining the confidence interval is with the R command `confint()`. However, it uses a more sophisticated method for deriving the result, hence it is not numerically identical to the hand-constructed one.

```
> confint(fit, "log10(weight)")
Waiting for profiling to be done...
    2.5 %    97.5 %
 6.618496 14.032741
```

Comparing Hierachical Models

This section discusses the analogue to the partial F-test of multiple linear regression. The idea behind is still the same, namely comparing two hierarchical models by their goodness-of-fit measure and their difference in degrees of freedom. However, some adjustments are necessary here, because we are now using the deviance rather than the residual sum of squares which leads to a different distribution in the test statistic. Let us assume that we have Big and $Small$ models where $(p+1)$ resp $(q+1)$ parameters are estimated. Our interest lies in the null hypothesis $H_0 : \beta_{q+1} = \beta_{q+2} = ... = \beta_p = 0$. This means that the additional predictors in the big model have zero coefficients and thus are useless. The MLE theory suggest to use the likelihood ratio (or log-likelihood difference) as the test statistic:

$$2 \cdot (ll^{Big} - ll^{Small}) = D(y, \hat{p}_{Small}) - D(y, \hat{p}_{Big}) \sim \chi^2_{p-q}$$

The log-likelihood difference can be computed from the difference in deviance between the two models. Under the null hypothesis, it asymptotically follows a Chisquare distribution with $p-q$ degrees of freedom. We illustrate the procedure by performing the **global test** against the null model. This is the easiest model that is possible and contains the intercept term only. In our example about baby survival, the null model fits the overall survival proportion $\hat{p}_{Null} = \sum y_i / n$ to all observations, no matter what the birth weight or age were. Our goal is now to compare against the full model with age- and weight-specific survival probabilities.

The two deviances are reported in the summary output. We observe a value of 319.28 for the null model (the `Null deviance`) and 235.94 for the model with two predictors (the `Residual deviance`). The full model has two parameters more, and hence the difference of the deviances follows a χ_2^2 distribution. We can thus compute the p-value for the null hypothesis $H_0 : \beta_1 = \beta_2 = 0$:

```
> 1-pchisq(fit$null-fit$dev, df=(fit$df.null-fit$df.res))
[1] 0
```

We obtain a p-value that is (numerically) zero; hence there is a strongly significant contribution of the two predictors on the odds for survival. While typing the above command into R is not a big effort, there is a quick check that can be done by looking at the summary output. The Chisquare distribution with $p-q$ degrees of freedom has an expectation of $p-q$ and standard deviation $\sqrt{2(p-q)}$. The consequence is that if the difference between null and residual deviance is large with respect to the difference in degrees of freedom, then the predictors do yield a significant contribution.

For factor variables with multiple levels, where a hierarchical model comparison is required to test their contribution to the model, the R command `drop1()` is very useful. The difference of deviance test is implemented there. We type:

```
> drop1(fit, test="Chisq")
Single term deletions

Model:
survival ~ log10(weight) + age
              Df Deviance    AIC    LRT  Pr(>Chi)
<none>             235.94 241.94
log10(weight)  1   270.19 274.19 34.247 4.855e-09 ***
age            1   239.89 243.89  3.948   0.04694 *
```

The function tests the exclusion of all model terms, using the difference of deviance as a test statistic. Please note that for all variables with one degree of freedom only, this is a special case of hierarchical model comparison, namely an individual hypothesis test. However, in case of GLMs the results will be slightly different to the ones that are reported in the summary. The latter are based on the approximation of the estimated coefficients' distribution to the Gaussian, whereas here the comparison is against the Chisquare. Hence, the p-values are not equal, though the difference is relatively small. Asymptotically, it will even vanish – the two tests will be one and the same when infinitely many datapoints are available.