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# **Applied Time Series Analysis**

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# Table of Contents

<b><u>1</u></b>	<b><u>INTRODUCTION</u></b>	<b><u>1</u></b>
1.1	PURPOSE	1
1.2	EXAMPLES	2
1.3	GOALS IN TIME SERIES ANALYSIS	8
<b><u>2</u></b>	<b><u>MATHEMATICAL CONCEPTS</u></b>	<b><u>11</u></b>
2.1	DEFINITION OF A TIME SERIES	11
2.2	STATIONARITY	11
2.3	TESTING STATIONARITY	13
<b><u>3</u></b>	<b><u>TIME SERIES IN R</u></b>	<b><u>15</u></b>
3.1	TIME SERIES CLASSES	15
3.2	DATES AND TIMES IN R	17
3.3	DATA IMPORT	21
<b><u>4</u></b>	<b><u>DESCRIPTIVE ANALYSIS</u></b>	<b><u>23</u></b>
4.1	VISUALIZATION	23
4.2	TRANSFORMATIONS	26
4.3	DECOMPOSITION	27
4.4	AUTOCORRELATION	46
4.5	PARTIAL AUTOCORRELATION	60
<b><u>5</u></b>	<b><u>STATIONARY TIME SERIES MODELS</u></b>	<b><u>63</u></b>
5.1	WHITE NOISE	63
5.2	ESTIMATING THE CONDITIONAL MEAN	64
5.3	AUTOREGRESSIVE MODELS	65
5.4	MOVING AVERAGE MODELS	79
5.5	ARMA(P,Q) MODELS	87
<b><u>6</u></b>	<b><u>SARIMA AND GARCH MODELS</u></b>	<b><u>91</u></b>
6.1	ARIMA MODELS	91
6.2	SARIMA MODELS	94
6.3	ARCH/GARCH MODELS	98
<b><u>7</u></b>	<b><u>TIME SERIES REGRESSION</u></b>	<b><u>103</u></b>
7.1	WHAT IS THE PROBLEM?	103
7.2	FINDING CORRELATED ERRORS	107
7.3	COCHRANE-ORCUTT METHOD	114

7.4	GENERALIZED LEAST SQUARES	115
7.5	MISSING PREDICTOR VARIABLES	121
<b>8</b>	<b>FORECASTING</b>	<b>127</b>
8.1	FORECASTING ARMA	128
8.2	EXPONENTIAL SMOOTHING	134
<b>9</b>	<b>MULTIVARIATE TIME SERIES ANALYSIS</b>	<b>143</b>
9.1	PRACTICAL EXAMPLE	143
9.2	CROSS CORRELATION	147
9.3	PREWHITENING	150
9.4	TRANSFER FUNCTION MODELS	152
<b>10</b>	<b>SPECTRAL ANALYSIS</b>	<b>157</b>
10.1	DECOMPOSING IN THE FREQUENCY DOMAIN	157
<b>11</b>	<b>STATE SPACE MODELS</b>	<b>163</b>
11.1	STATE SPACE FORMULATION	163
11.2	AR PROCESSES WITH MEASUREMENT NOISE	164
11.3	DYNAMIC LINEAR MODELS	167

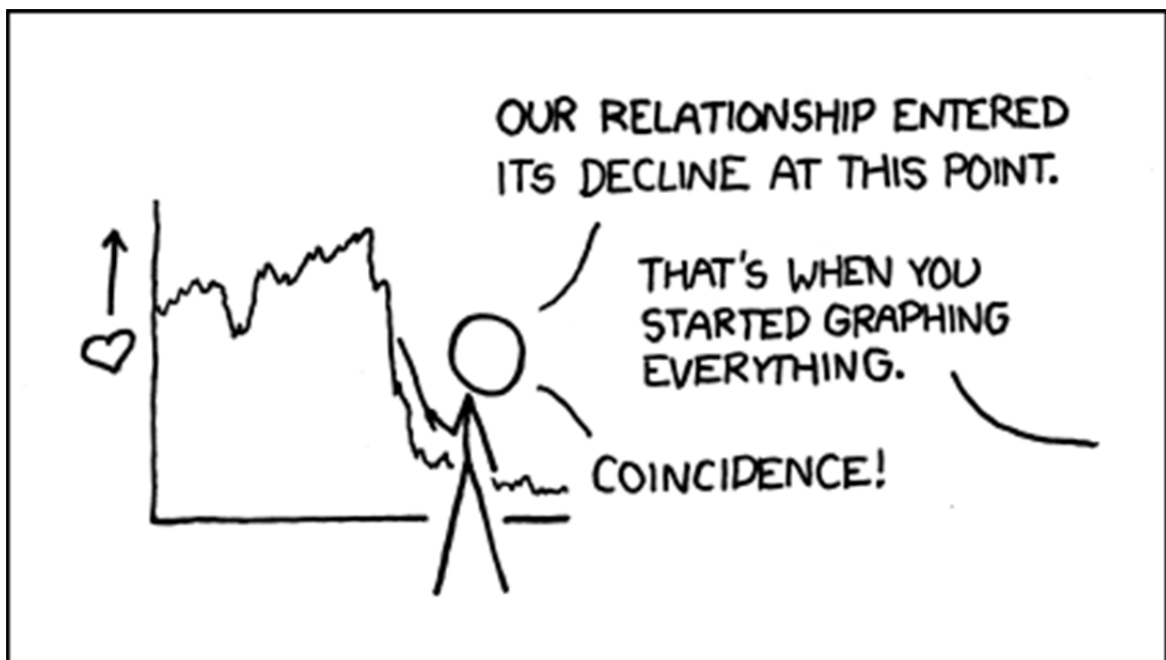
# 1 Introduction

## 1.1 Purpose

Time series data, i.e. records which are **measured sequentially over time**, are extremely common. They arise in virtually every application field, such as e.g.:

- **Business**  
*Sales figures, production numbers, customer frequencies, ...*
- **Economics**  
*Stock prices, exchange rates, interest rates, ...*
- **Official Statistics**  
*Census data, personal expenditures, road casualties, ...*
- **Natural Sciences**  
*Population sizes, sunspot activity, chemical process data, ...*
- **Environmetrics**  
*Precipitation, temperature or pollution recordings, ...*

In contrast to basic data analysis where the assumption of identically and independently distributed data is key, time series are serially correlated. The purpose of time series analysis is to **visualize and understand these dependences in past data, and to exploit them for forecasting future values**. While some simple descriptive techniques do often considerably enhance the understanding of the data, a full analysis usually involves modeling the stochastic mechanism that is assumed to be the generator of the observed time series.



Once a good model is found and fitted to data, the analyst can use that model to forecast future values and produce prediction intervals, or he can generate simulations, for example to guide planning decisions. Moreover, fitted models are used as a basis for statistical tests: they allow determining whether fluctuations in monthly sales provide evidence of some underlying change, or whether they are still within the range of usual random variation.

The dominant main features of many time series are *trend and seasonal variation*. These can either be modeled deterministically by mathematical functions of time, or are estimated using non-parametric smoothing approaches. Yet another key feature of most time series is that adjacent observations tend to be correlated, i.e. serially dependent. Much of the methodology in time series analysis is aimed at explaining this correlation using appropriate statistical models.

While the theory on mathematically oriented time series analysis is vast and may be studied without necessarily fitting any models to data, the focus of our course will be applied and directed towards data analysis. We study some basic properties of time series processes and models, but mostly focus on how to visualize and describe time series data, on how to fit models to data correctly, on how to generate forecasts, and on how to adequately draw conclusions from the output that was produced.

## 1.2 Examples

### 1.2.1 Air Passenger Bookings

The numbers of international passenger bookings (in thousands) per month on an airline (*PanAm*) in the United States were obtained from the Federal Aviation Administration for the period 1949-1960. The company used the data to predict future demand before ordering new aircraft and training aircrew. The data are available as a time series in `R`. Here, we here show how to access them, and how to first gain an impression.

```
> data(AirPassengers)
> AirPassengers
```

	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
1949	112	118	132	129	121	135	148	148	136	119	104	118
1950	115	126	141	135	125	149	170	170	158	133	114	140
1951	145	150	178	163	172	178	199	199	184	162	146	166
1952	171	180	193	181	183	218	230	242	209	191	172	194
1953	196	196	236	235	229	243	264	272	237	211	180	201
1954	204	188	235	227	234	264	302	293	259	229	203	229
1955	242	233	267	269	270	315	364	347	312	274	237	278
1956	284	277	317	313	318	374	413	405	355	306	271	306
1957	315	301	356	348	355	422	465	467	404	347	305	336
1958	340	318	362	348	363	435	491	505	404	359	310	337
1959	360	342	406	396	420	472	548	559	463	407	362	405
1960	417	391	419	461	472	535	622	606	508	461	390	432

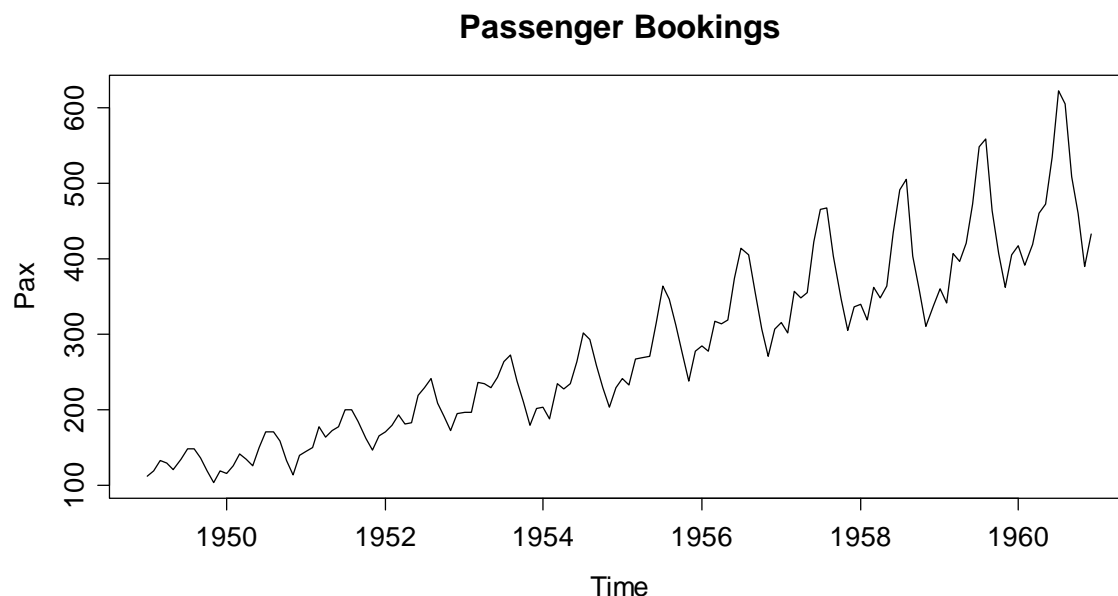
Some further information about this dataset can be obtained by typing `?AirPassengers` in **R**. The data are stored in an **R-object** of class `ts`, which is the specific class for time series data. However, for further details on how time series are handled in **R**, we refer to section 3.

One of the most important steps in time series analysis is to visualize the data, i.e. create a time series plot, where the air passenger bookings are plotted versus the time of booking. For a time series object, this can be done very simply in **R**, using the generic plot function:

```
> plot(AirPassengers, ylab="Pax", main="Passenger Bookings")
```

The result is displayed on the next page. There are a number of features in the plot which are common to many time series. For example, it is apparent that the number of passengers travelling on the airline is increasing with time. In general, a systematic change in the mean level of a time series that does not appear to be periodic is known as a *trend*. The simplest model for a trend is a linear increase or decrease, an often adequate approximation. We will discuss how to estimate trends, and how to decompose time series into trend and other components in section 4.3.

The data also show a repeating pattern within each year, i.e. in summer, there are always more passengers than in winter. This is known as a *seasonal effect*, or *seasonality*. Please note that this term is applied more generally to any repeating pattern over a fixed period, such as for example restaurant bookings on different days of week.



We can naturally attribute the increasing trend of the series to causes such as rising prosperity, greater availability of aircraft, cheaper flights and increasing population. The seasonal variation coincides strongly with vacation periods. For this reason, we here consider both trend and seasonal variation as deterministic

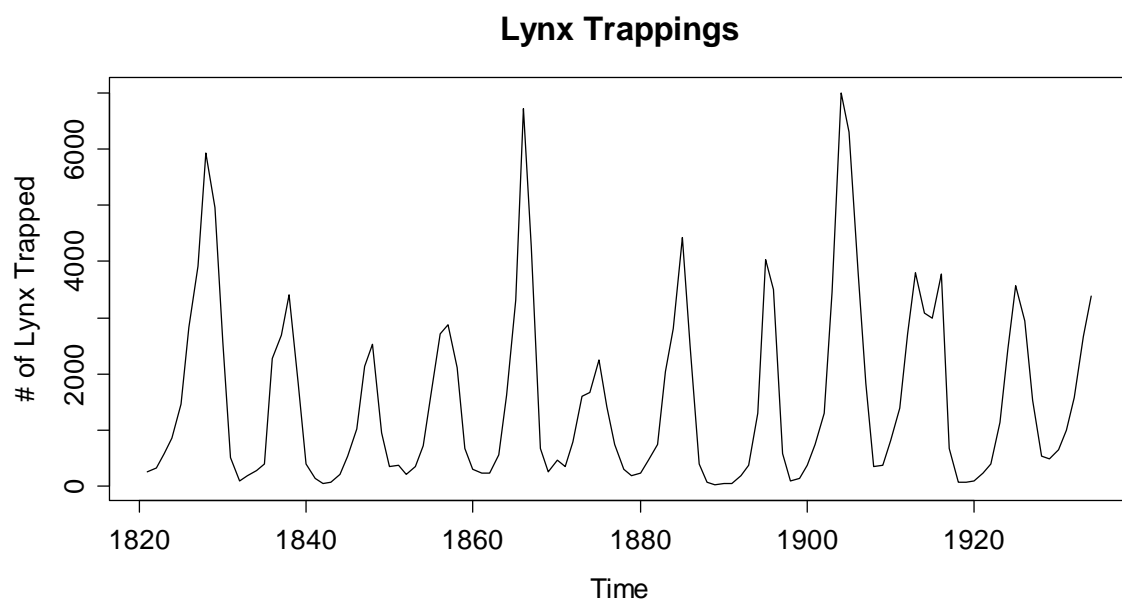
components. As mentioned before, section 4.3 discusses visualization and estimation of these components, while in section 7, time series regression models will be specified to allow for underlying causes like these, and finally section 8 discusses exploiting these for predictive purposes.

## 1.2.2 Lynx Trappings

The next series which we consider here is the annual number of lynx trappings for the years 1821-1934 in Canada. We again load the data and visualize them using a time series plot:

```
> data(lynx)
> plot(lynx, ylab="# of Lynx Trapped", main="Lynx Trappings")
```

The plot on the next page shows that the number of trapped lynx reaches high and low values every about 10 years, and some even larger figure every about 40 years. To our knowledge, there is no fixed natural period which suggests these results. Thus, we will attribute this behavior not to a deterministic periodicity, but to a random, stochastic one.



This leads us to the heart of time series analysis: while understanding and modeling trend and seasonal variation is a very important aspect, much of the time series methodology is aimed at *stationary series*, i.e. data which do not show deterministic, but only random (cyclic) variation.





### 1.2.3 Luteinizing Hormone Measurements

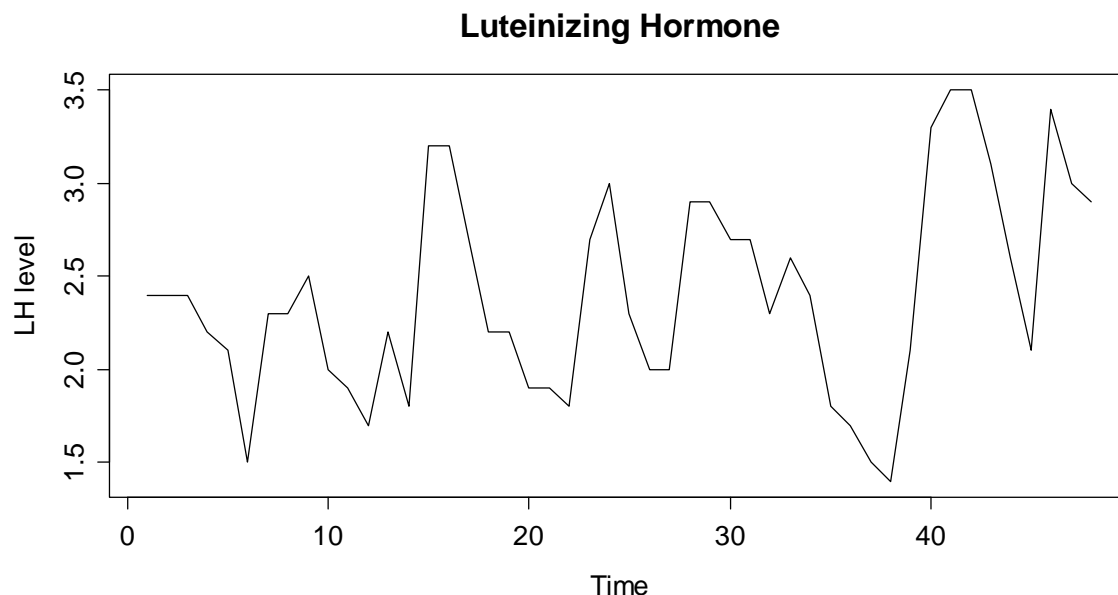
One of the key features of the above lynx trappings series is that the observations apparently do not stem from independent random variables, but there is some serial correlation. If the previous value was high (or low, respectively), the next one is likely to be similar to the previous one. To explore, model and exploit such dependence lies at the root of time series analysis.

We here show another series, where 48 luteinizing hormone levels were recorded from blood samples that were taken at 10 minute intervals from a human female. This hormone, also called *lutropin*, triggers ovulation.

```
> data(lh)
> lh
Time Series:
Start = 1; End = 48; Frequency = 1
 [1] 2.4 2.4 2.4 2.2 2.1 1.5 2.3 2.3 2.5 2.0 1.9 1.7 2.2 1.8
[15] 3.2 3.2 2.7 2.2 2.2 1.9 1.9 1.8 2.7 3.0 2.3 2.0 2.0 2.9
[29] 2.9 2.7 2.7 2.3 2.6 2.4 1.8 1.7 1.5 1.4 2.1 3.3 3.5 3.5
[43] 3.1 2.6 2.1 3.4 3.0 2.9
```

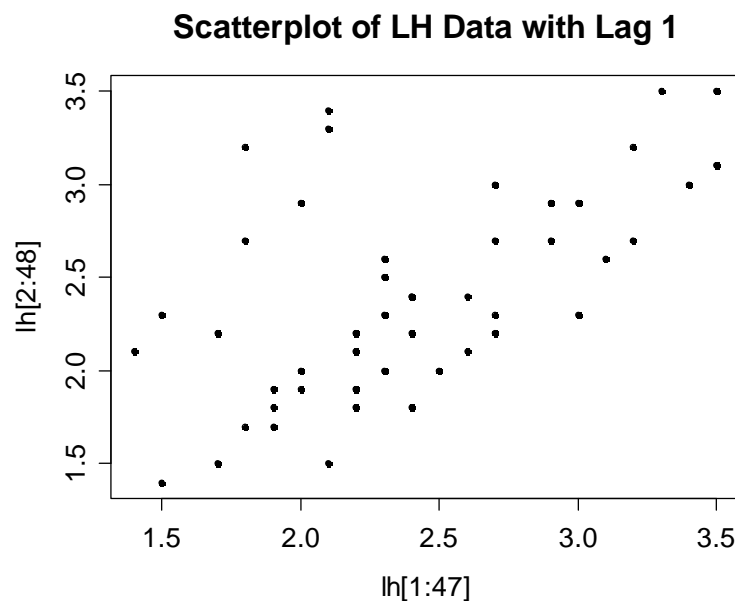
Again, the data themselves are of course needed to perform analyses, but provide little overview. We can improve this by generating a time series plot:

```
> plot(lh, ylab="LH level", main="Luteinizing Hormone")
```



For this series, given the way the measurements were made (i.e. 10 minute intervals), we can almost certainly exclude any deterministic seasonal variation. But is there any stochastic cyclic behavior? This question is more difficult to answer. Normally, one resorts to the simpler question of analyzing the correlation of subsequent records, called *autocorrelations*. The autocorrelation for lag 1 can be visualized by producing a scatterplot of adjacent observations:

```
> plot(lh[1:47], lh[2:48], pch=20)
> title("Scatterplot of LH Data with Lag 1")
```



Besides the (non-standard) observation that there seems to be an inhomogeneity, i.e. two distinct groups of data points, it is apparent that there is a positive correlation between successive measurements. This manifests itself with the clearly visible fact that if the previous observation was above or below the mean, the next one is more likely to be on the same side. We can even compute the value of the Pearson correlation coefficient:

```
> cor(lh[1:47], lh[2:48])
[1] 0.5807322
```

This figure is an estimate for the so-called *autocorrelation coefficient at lag 1*. As we will see in section 4.4, the idea of considering lagged scatterplots and computing Pearson correlation coefficients serves as a good proxy for a mathematically more sound method. We also note that despite the positive correlation of +0.58, the series seems to always have the possibility of “reverting to the other side of the mean”, a property which is common to *stationary series* – an issue that will be discussed in section 2.2.

## 1.2.4 Swiss Market Index

The *SMI* is the blue chip index of the Swiss stock market. It summarizes the value of the shares of the 20 most important companies, and currently contains nearly 90% of the total market capitalization. It was introduced on July 1, 1988 at a basis level of 1500.00 points. Daily closing data for 1860 consecutive trading days from 1991-1998 are available in `R`. We observe a more than 4-fold increase during that period. As a side note, the value in the second half of 2013 is around 8000 points, indicating a sideways movement over the latest 15 years.

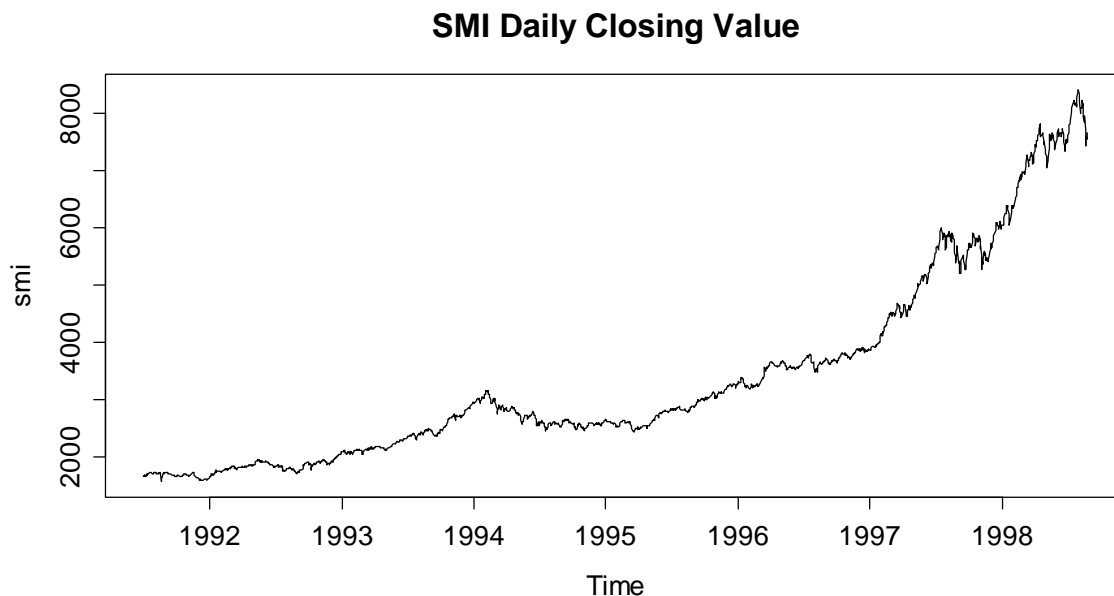
```
> data(EuStockMarkets)
> EuStockMarkets
Time Series:
Start = c(1991, 130)
End = c(1998, 169)
Frequency = 260
```

	DAX	SMI	CAC	FTSE
1991.496	1628.75	1678.1	1772.8	2443.6
1991.500	1613.63	1688.5	1750.5	2460.2
1991.504	1606.51	1678.6	1718.0	2448.2
1991.508	1621.04	1684.1	1708.1	2470.4
1991.512	1618.16	1686.6	1723.1	2484.7
1991.515	1610.61	1671.6	1714.3	2466.8

As we can see, `EuStockMarkets` is a multiple time series object, which also contains data from the German DAX, the French CAC and UK's FTSE. We will focus on the SMI and thus extract and plot the series:

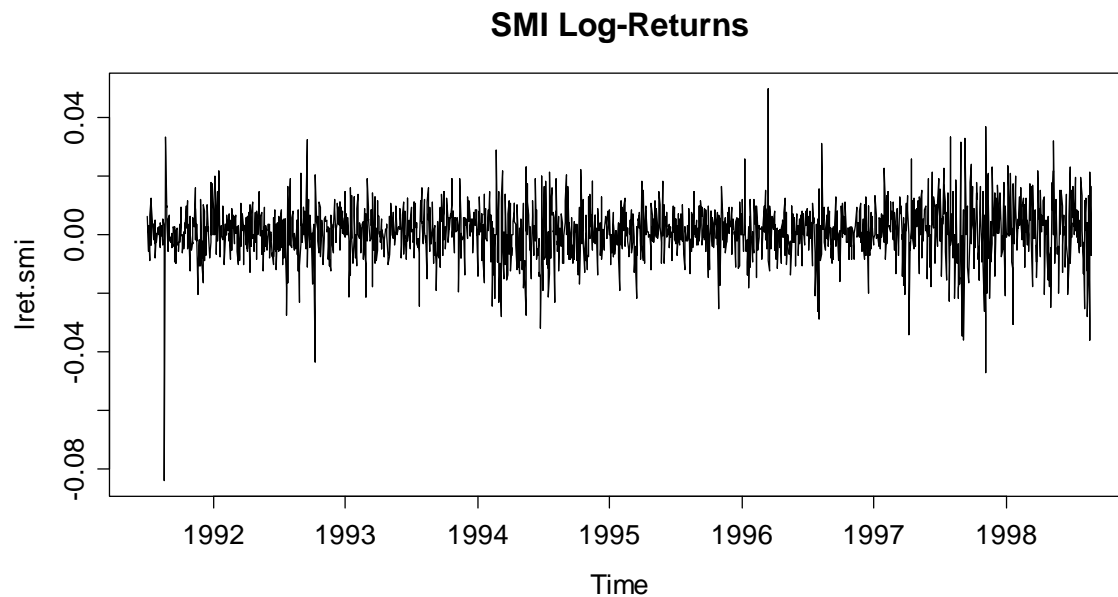
```
esm <- EuStockMarkets
tmp <- EuStockMarkets[,2]
smi <- ts(tmp, start=start(esm), freq=frequency(esm))
plot(smi, main="SMI Daily Closing Value")
```

Because subsetting from a multiple time series object results in a *vector*, but not a *time series object*, we need to regenerate a latter one, sharing the arguments of the original. In the plot we clearly observe that the series has a trend, i.e. the mean is obviously non-constant over time. This is typical for all financial time series.



Such trends in financial time series are nearly impossible to predict, and difficult to characterize mathematically. We will not embark in this, but analyze the so-called log-returns, i.e. the logged-value of today's value divided by the one of yesterday:

```
> lret.smi <- diff (log(smi))  
> plot(lret.smi, main="SMI Log-Returns")
```



The SMI log-returns are a close approximation to the relative change (percent values) with respect to the previous day. As can be seen above, they do not exhibit a trend anymore, but show some of the stylized facts that most log-returns of financial time series share. Using *lagged scatterplots* or the *correlogram* (to be discussed later in section 4.4), you can convince yourself that there is no serial correlation. Thus, there is no direct dependency which could be exploited to predict tomorrow's return based on the one of today and/or previous days.

However, it is visible that large changes, i.e. log-returns with high absolute values, imply that future log-returns tend to be larger than normal, too. This feature is also known as *volatility clustering*, and financial service providers are trying their best to exploit this property to make profit. Again, you can convince yourself of the volatility clustering effect by taking the squared log-returns and analyzing their serial correlation, which is different from zero.

## 1.3 Goals in Time Series Analysis

A first impression of the purpose and goals in time series analysis could be gained from the previous examples. We conclude this introductory section by explicitly summarizing the most important goals.

### 1.3.1 Exploratory Analysis

Exploratory analysis for time series mainly involves *visualization* with time series plots, *decomposition* of the series into deterministic and stochastic parts, and studying the *dependency structure* in the data.

### 1.3.2 Modeling

The formulation of a stochastic model, as it is for example also done in regression, can and does often lead to a deeper understanding of the series. The formulation of a suitable model usually arises from a mixture between background knowledge in the applied field, and insight from exploratory analysis. Once a suitable model is found, a central issue remains, i.e. the estimation of the parameters, and subsequent model diagnostics and evaluation.

### 1.3.3 Forecasting

An often-heard motivation for time series analysis is the prediction of future observations in the series. This is an ambitious goal, because time series forecasting relies on extrapolation, and is generally based on the assumption that past and present characteristics of the series continue. It seems obvious that good forecasting results require a very good comprehension of a series' properties, be it in a more descriptive sense, or in the sense of a fitted model.

### 1.3.4 Time Series Regression

Rather than just forecasting by extrapolation, we can try to understand the relation between a so-identified *response time series*, and one or more *explanatory series*. If all of these are observed at the same time, we can in principle employ the ordinary least squares (OLS) regression framework. However, the all-to-common assumption of (serially) uncorrelated errors in OLS is usually violated in a time series setup. We will illustrate how to properly deal with this situation, in order to generate correct confidence and prediction intervals.

### 1.3.5 Process Control

Many production or other processes are measured quantitatively for the purpose of optimal management and quality control. This usually results in time series data, to which a stochastic model is fit. This allows understanding the signal in the data, but also the noise: it becomes feasible to monitor which fluctuations in the production are normal, and which ones require intervention.



## 2 Mathematical Concepts

For performing anything else than very basic exploratory time series analysis, even from a much applied perspective, it is necessary to introduce the mathematical notion of what a time series is, and to study some basic probabilistic properties, namely the *moments* and the *concept of stationarity*.

### 2.1 Definition of a Time Series

As we have explained in section 1.2, observations that have been collected over fixed sampling intervals form a time series. Following a statistical approach, we consider such series as realizations of random variables. A sequence of random variables, defined at such fixed sampling intervals, is sometimes referred to as a *discrete-time stochastic process*, though the shorter names *time series model* or *time series process* are more popular and will mostly be used in this scriptum. It is very important to make the distinction between a time series, i.e. observed values, and a process, i.e. a probabilistic construct.

**Definition:** A *time series process* is a set of random variables  $\{X_t, t \in T\}$ , where  $T$  is the set of times at which the process was, will or can be observed. We assume that each random variable  $X_t$  is distributed according some univariate distribution function  $F_t$ . Please note that for our entire course and hence scriptum, we exclusively consider time series processes with equidistant time intervals, as well as real-valued random variables  $X_t$ . This allows us to enumerate the set of times, so that we can write  $T = \{1, 2, 3, \dots\}$ .

An observed time series, on the other hand, is seen as a realization of the random vector  $X = (X_1, X_2, \dots, X_n)$ , and is denoted with small letters  $x = (x_1, x_2, \dots, x_n)$ . It is important to note that in a multivariate sense, a time series is only *one single* realization of the  $n$ -dimensional random variable  $X$ , with its multivariate,  $n$ -dimensional distribution function  $F$ . As we all know, we cannot do statistics with just a single observation. As a way out of this situation, we need to impose some conditions on the joint distribution function  $F$ .

### 2.2 Stationarity

The aforementioned condition on the joint distribution  $F$  will be formulated as the *concept of stationarity*. In colloquial language, stationarity means that the probabilistic character of the series must not change over time, i.e. that any section of the time series is “typical” for every other section with the same length. More mathematically, we require that for any indices  $s, t$  and  $k$ , the observations  $x_t, \dots, x_{t+k}$  could have just as easily occurred at times  $s, \dots, s+k$ . If that is not the case practically, then the series is hardly stationary.

Imposing even more mathematical rigor, we introduce the concept of *strict stationarity*. A time series is said to be *strictly stationary* if and only if the  $(k+1)$ -dimensional joint distribution of  $X_t, \dots, X_{t+k}$  coincides with the joint distribution of  $X_s, \dots, X_{s+k}$  for any combination of indices  $t, s$  and  $k$ . For the special case of  $k=0$  and  $t=s$ , this means that the univariate distributions  $F_t$  of all  $X_t$  are equal. For strictly stationary time series, we can thus leave off the index  $t$  on the distribution. As the next step, we will define the unconditional moments:

$$\begin{aligned} \text{Expectation } \mu &= E[X_t], \\ \text{Variance } \sigma^2 &= \text{Var}(X_t), \\ \text{Covariance } \gamma(h) &= \text{Cov}(X_t, X_{t+h}). \end{aligned}$$

In other words, strictly stationary series have *constant (unconditional) expectation*, *constant (unconditional) variance*, and the covariance, i.e. the *dependency structure, depends only on the lag  $h$* , which is the time difference between the two observations. However, the covariance terms are generally different from 0, and thus, the  $X_t$  are usually dependent. Moreover, the conditional expectation given the past of the series,  $E[X_t | X_{t-1}, X_{t-2}, \dots]$  is typically non-constant, denoted as  $\mu_t$ . In some (rarer, e.g. for financial time series) cases, even the conditional variance  $\text{Var}(X_t | X_{t-1}, X_{t-2}, \dots)$  can be non-constant.

In practice however, except for simulation studies, we usually have no explicit knowledge of the latent time series process. Since strict stationarity is defined as a property of the process' joint distributions (all of them), it is impossible to verify from an observed time series, i.e. a single data realization. We can, however, try to verify whether a time series process shows *constant unconditional mean and variance*, and whether the *dependency only depends on the lag  $h$* . This much less rigorous property is known as *weak stationarity*.

In order to do well-founded statistical analyses with time series, weak stationarity is a necessary condition. It is obvious that if a series' observations do not have common properties such as constant mean/variance and a stable dependency structure, it will be impossible to statistically learn from it. On the other hand, it can be shown that weak stationarity, along with the additional property of ergodicity (i.e. the mean of a time series realization converges to the expected value, independent of the starting point), is sufficient for most practical purposes such as model fitting, forecasting, etc.. We will, however, not further embark in this subject.

#### Remarks:

- From now on, when we speak of *stationarity*, we strictly mean *weak stationarity*. The motivation is that weak stationarity is sufficient for applied time series analysis, and strict stationarity is a practically useless concept.
- When we analyze time series data, we need to verify whether it might have arisen from a stationary process or not. Be careful with the wording: stationarity is always a property of the process, and never of the data.



- Moreover, bear in mind that stationarity is a hypothesis, which needs to be evaluated for every series. We may be able to reject this hypothesis with quite some certainty if the data strongly speak against it. However, we can never prove stationarity with data. At best, it is plausible that a series originated from a stationary process.
- Some obvious violations of stationarity are trends, non-constant variance, deterministic seasonal variation, as well as apparent breaks in the data, which are indicators for changing dependency structure.

## 2.3 Testing Stationarity

If, as explained above, stationarity is a hypothesis which is tested on data, students and users keep asking if there are any formal tests. The answer to this question is yes, and there are even quite a number of tests. This includes the *Augmented Dickey-Fuller Test*, the *Phillips-Perron Test*, the *KPSS Test*, which are all available in  $\mathbf{R}$ 's `tseries` package. The `urca` package includes further tests such as the *Elliott-Rothenberg-Stock*, *Schmidt-Phillips* und *Zivot-Andrews*.

However, we will not discuss any of these tests here for a variety of reasons. First and foremost, they all focus on some very specific non-stationarity aspects, but do not test stationarity in a broad sense. While they may reasonably do their job in the narrow field they are aimed for, they have low power to detect general non-stationarity and in practice often fail to do so. Additionally, theory and formalism of these tests is quite complex, and thus beyond the scope of this course. In summary, these tests are to be seen as more of a pasttime for the mathematically interested, rather than a useful tool for the practitioner.

Thus, we here recommend assessing stationarity by visual inspection. The primary tool for this is the time series plot, but also the correlogram (see section 4.4) can be helpful as a second check. For long time series, it can also be useful to split up the series into several parts for checking whether mean, variance and dependency are similar over the blocks.



## 3 Time Series in R

### 3.1 Time Series Classes

In **R**, there are *objects*, which are organized in a large number of *classes*. These classes e.g. include *vectors*, *data frames*, *model output*, *functions*, and many more. Not surprisingly, there are also several classes for time series. We start by presenting `ts`, the basic class for regularly spaced time series. This class is comparably simple, as it can only represent time series with fixed interval records, and only uses numeric time stamps, i.e. (sophistically) enumerates the index set. However, it will be sufficient for most, if not all, of what we do in this course. Then, we also provide an outlook to more complicated concepts.

#### 3.1.1 The `ts` Class

For defining a time series of class `ts`, we of course need to provide the *data*, but also the *starting time* as argument `start`, and the *frequency* of measurements as argument `frequency`. If no starting time is supplied, **R** uses its default value of 1, i.e. enumerates the times by the index set  $1, \dots, n$ , where  $n$  is the length of the series. The frequency is the number of observations per unit of time, e.g. 1 for yearly, 4 for quarterly, or 12 for monthly recordings. Instead of the start, we could also provide the end of the series, and instead of the frequency, we could supply argument `deltat`, the fraction of the sampling period between successive observations. The following example will illustrate the concept.

**Example:** We here consider a simple and short series that holds the number of days per year with traffic holdups in front of the Gotthard road tunnel north entrance in Switzerland. The data are available from the Federal Roads Office.

2004	2005	2006	2007	2008	2009	2010
88	76	112	109	91	98	139

The start of this series is in 2004. The time unit is years, and since we have just one record per year, the frequency of this series is 1. This tells us that while there may be a trend, there cannot be a seasonal effect, as the latter can only be present in periodic series, i.e. series with frequency  $> 1$ . We now define a `ts` object in **R**.

```
> rawdat <- c(88, 76, 112, 109, 91, 98, 139)
> ts.dat <- ts(rawdat, start=2004, freq=1)
> ts.dat
Time Series: Start = 2004, End = 2010
Frequency = 1
[1] 88 76 112 109 91 98 139
```

There are a number of simple but useful functions that extract basic information from objects of class `ts`, see the following examples:

```
> start(ts.dat)
[1] 2004      1

> end(ts.dat)
[1] 2010      1

> frequency(ts.dat)
[1] 1

> deltat(ts.dat)
[1] 1
```

Another possibility is to obtain the measurement times from a time series object. As class `ts` only enumerates the times, they are given as fractions. This can still be very useful for specialized plots, etc.

```
> time(ts.dat)
Time Series:
Start = 2004
End = 2010
Frequency = 1
[1] 2004 2005 2006 2007 2008 2009 2010
```

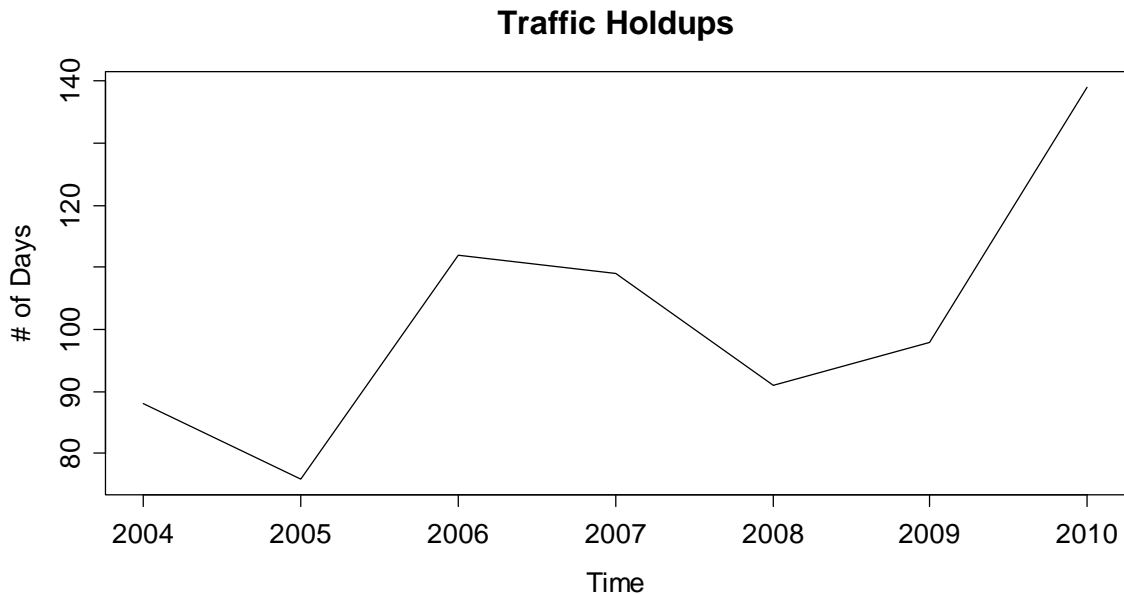
The next basic, but for practical purposes very useful function is `window()`. It is aimed at selecting a subset from a time series. Of course, also regular R-subsetting such as `ts.dat[2:5]` does work with the time series class. However, this results in a vector rather than a time series object, and is thus mostly of less use than the `window()` command.

```
> window(ts.dat, start=2006, end=2008)
Time Series:
Start = 2006
End = 2008
Frequency = 1
[1] 112 109  91
```

While we here presented the most important basic methods/functions for class `ts`, there is a wealth of further ones. This includes the `plot()` function, and many more, e.g. for estimating trends, seasonal effects and dependency structure, for fitting time series models and generating forecasts. We will present them in the forthcoming chapters of this scriptum.

To conclude the previous example, we will not do without showing the time series plot of the Gotthard road tunnel traffic holdup days, see next page. Because there are a limited number of observations, it is difficult to give statements regarding a possible trend and/or stochastic dependency.

```
> plot(ts.dat, ylab="# of Days", main="Traffic Holdups")
```



### 3.1.2 Other Classes

Besides the basic `ts` class, there are several more which offer a variety of additional options, but will rarely to never be required during our course. Most prominently, this includes the `zoo` package, which provides infrastructure for both regularly and irregularly spaced time series using arbitrary classes for the time stamps. It is designed to be as consistent as possible with the `ts` class. Coercion from and to `zoo` is also readily available.

Some further packages which contain classes and methods for time series include `xts`, `its`, `tseries`, `fts`, `timeSeries` and `tis`. Additional information on their content and philosophy can be found on CRAN.

## 3.2 Dates and Times in R

While for the `ts` class, the handling of times has been solved very simply and easily by enumerating, doing time series analysis in R may sometimes also require to explicitly working with date and time. There are several options for dealing with date and date/time data. The built-in `as.Date()` function handles dates that come without times. The contributed package `chron` handles dates and times, but does not control for different time zones, whereas the sophisticated but complex `POSIXct` and `POSIXlt` classes allow for dates and times with time zone control.

As a general rule for date/time data in R, we suggest to use the simplest technique possible. Thus, for date only data, `as.Date()` will mostly be the optimal choice. If handling dates and times, but without time-zone information, is required, the `chron` package is the choice. The `POSIX` classes are especially useful in the relatively rare cases when time-zone manipulation is important.

Apart for the `POSIXlt` class, dates/times are internally stored as the number of days or seconds from some reference date. These dates/times thus generally have a numeric mode. The `POSIXlt` class, on the other hand, stores date/time values as a list of components (hour, min, sec, mon, etc.), making it easy to extract these parts. Also the current date is accessible by typing `Sys.Date()` in the console, and returns an object of class `Date`.

### 3.2.1 The Date Class

As mentioned above, the easiest solution for specifying days in R is with the `as.Date()` function. Using the `format` argument, arbitrary date formats can be read. The default, however, is four-digit year, followed by month and then day, separated by dashes or slashes:

```
> as.Date("2012-02-14")
[1] "2012-02-14"
> as.Date("2012/02/07")
[1] "2012-02-07"
```

If the dates come in non-standard appearance, we require defining their format using some codes. While the most important ones are shown below, we reference to the **R** help file of function `strptime()` for the full list.

Code	Value
%d	Day of the month (decimal number)
%m	Month (decimal number)
%b	Month (character, abbreviated)
%B	Month (character, full name)
%y	Year (decimal, two digit)
%Y	Year (decimal, four digit)

The following examples illustrate the use of the `format` argument:

```
> as.Date("27.01.12", format="%d.%m.%Y")
[1] "2012-01-27"
> as.Date("14. Februar, 2012", format="%d. %B, %Y")
[1] "2012-02-14"
```

Internally, `Date` objects are stored as the number of days passed since the 1<sup>st</sup> of January in 1970. Earlier dates receive negative numbers. By using the `as.numeric()` function, we can easily find out how many days are past since the reference date. Also back-conversion from a number of past days to a date is straightforward:

```
> mydat <- as.Date("2012-02-14")
> ndays <- as.numeric(mydat)
> ndays
[1] 15384
```

```
> tdays <- 10000
> class(tdays) <- "Date"
> tdays
[1] "1997-05-19"
```

A very useful feature is the possibility of extracting weekdays, months and quarters from `Date` objects, see the examples below. This information can be converted to factors. In this form, they serve for purposes such as visualization, decomposition, or time series regression.

```
> weekdays(mydat)
[1] "Dienstag"
> months(mydat)
[1] "Februar"
> quarters(mydat)
[1] "Q1"
```

Furthermore, some very useful summary statistics can be generated from `Date` objects: median, mean, min, max, range, ... are all available. We can even subtract two dates, which results in a `difftime` object, i.e. the time difference in days.

```
> dat <- as.Date(c("2000-01-01", "2004-04-04", "2007-08-09"))
> dat
[1] "2000-01-01" "2004-04-04" "2007-08-09"

> min(dat)
[1] "2000-01-01"
> max(dat)
[1] "2007-08-09"
> mean(dat)
[1] "2003-12-15"
> median(dat)
[1] "2004-04-04"

> dat[3]-dat[1]
Time difference of 2777 days
```

Another option is generating time sequences. For example, to generate a vector of 12 dates, starting on August 3, 1985, with an interval of one single day between them, we simply type:

```
> seq(as.Date("1985-08-03"), by="days", length=12)
[1] "1985-08-03" "1985-08-04" "1985-08-05" "1985-08-06"
[5] "1985-08-07" "1985-08-08" "1985-08-09" "1985-08-10"
[9] "1985-08-11" "1985-08-12" "1985-08-13" "1985-08-14"
```

The `by` argument proves to be very useful. We can supply various units of time, and even place an integer in front of it. This allows creating a sequence of dates separated by two weeks:

```
> seq(as.Date("1992-04-17"), by="2 weeks", length=12)
[1] "1992-04-17" "1992-05-01" "1992-05-15" "1992-05-29"
[5] "1992-06-12" "1992-06-26" "1992-07-10" "1992-07-24"
[9] "1992-08-07" "1992-08-21" "1992-09-04" "1992-09-18"
```

### 3.2.2 The `chron` Package

The `chron()` function converts dates and times to `chron` objects. The dates and times are provided separately to the `chron()` function, which may well require some initial pre-processing. For such parsing, `R`-functions such as `substr()` and `strsplit()` can be of great use. In the `chron` package, there is no support for time zones and daylight savings time, and `chron` objects are internally stored as fractional days since the reference date of January 1<sup>st</sup>, 1970. By using the function `as.numeric()`, these internal values can be accessed. The following example illustrates the use of `chron`:

```
> library(chron)
> dat <- c("2007-06-09 16:43:20", "2007-08-29 07:22:40",
           "2007-10-21 16:48:40", "2007-12-17 11:18:50")
> dts <- substr(dat, 1, 10)
> tme <- substr(dat, 12, 19)
> fmt <- c("y-m-d", "h:m:s")
> cdt <- chron(dates=dts, time=tme, format=fmt)
> cdt
[1] (07-06-09 16:43:20) (07-08-29 07:22:40)
[3] (07-10-21 16:48:40) (07-12-17 11:18:50)
```

As before, we can again use the entire palette of summary statistic functions. Of some special interest are time differences, which can now be obtained as either fraction of days, or in weeks, hours, minutes, seconds, etc.:

```
> cdt[2]-cdt[1]
Time in days:
[1] 80.61065
> difftime(cdt[2], cdt[1], units="secs")
Time difference of 6964760 secs
```

### 3.2.3 POSIX Classes

The two classes `POSIXct` and `POSIXlt` implement date/time information, and in contrast to the `chron` package, also support time zones and daylight savings time. We recommend utilizing this functionality only when urgently needed, because the handling requires quite some care, and may on top of that be system dependent. Further details on the use of the POSIX classes can be found on CRAN.

As explained above, the `POSIXct` class also stores dates/times with respect to the internal reference, whereas the `POSIXlt` class stores them as a list of components (hour, min, sec, mon, etc.), making it easy to extract these parts.



### 3.3 Data Import

We can safely assume that most time series data are already present in electronic form; however, not necessarily in `R`. Thus, some knowledge on how to import data into `R` is required. It is beyond the scope of this scriptum to present the uncounted options which exist for this task. Hence, we will restrict ourselves to providing a short overview and some useful hints.

The most common form for sharing time series data are certainly spreadsheets, or in particular, Microsoft Excel files. While `library(RODBC)` offers functionality to directly import data from Excel files, we discourage its use. First of all, this only works on Windows systems. More importantly, it is usually simpler, quicker and more flexible to export comma- or tab-separated text files from Excel, and import them via the ubiquitous `read.table()` function, respectively the tailored version `read.csv()` (for comma separation) and `read.delim()` (for tab separation).

With packages `RODBC` and `RMySQL`, `R` can also communicate with SQL databases, which is the method of choice for large scale problems. Furthermore, after loading `library(foreign)`, it is also possible to read files from Stata, SPSS, Octave and SAS.



## 4 Descriptive Analysis

As always when working with “a pile of numbers”, also known as *data*, it is important to first gain an overview. In the field of time series analysis, this encompasses several aspects:

- understanding the context of the problem and the data source
- making suitable plots, looking for general structure and outliers
- thinking about data transformations, e.g. to reduce skewness
- judging stationarity and potentially achieve it by decomposition

We start by discussing time series plots, then discuss transformations, focus on the decomposition of time series into trend, seasonal effect and stationary random part and conclude by discussing methods for visualizing the dependency structure.

### 4.1 Visualization

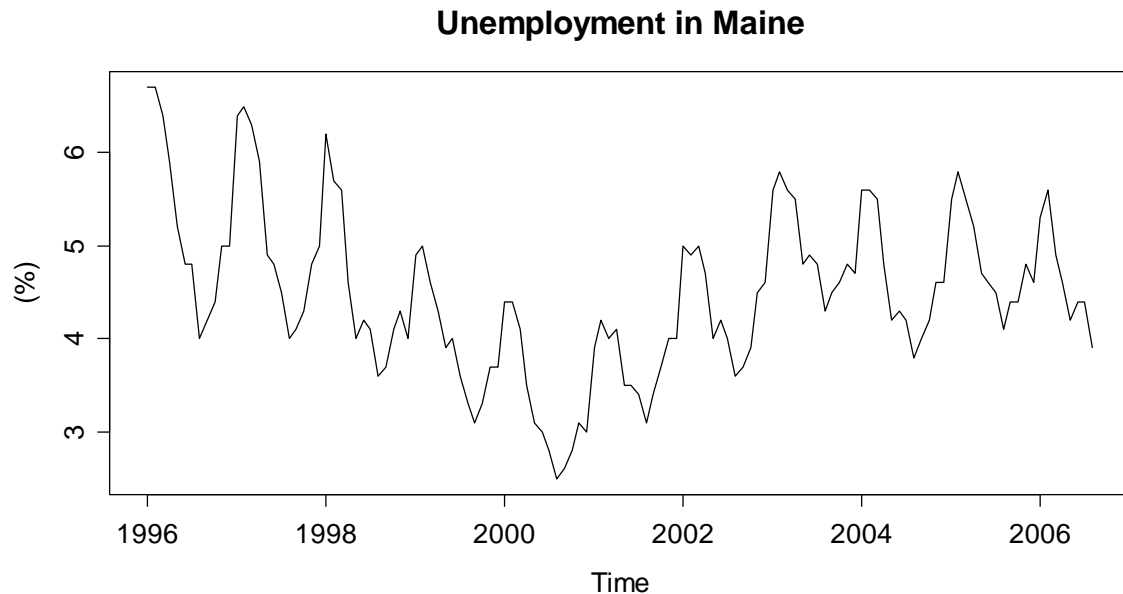
#### 4.1.1 Time Series Plot

The most important means of visualization is the time series plot, where the data are plotted versus time/index. There are several examples in section 1.2, where we also got acquainted with **R**'s generic `plot()` function. As a general rule, the data points are joined by lines in time series plots. An exception is when there are missing values. Moreover, the reader expects that the axes are well-chosen, labeled and the measurement units are given.

Another issue is the correct aspect ratio for time series plots: if the time axis gets too much compressed, it can become difficult to recognize the behavior of a series. Thus, we recommend choosing the aspect ratio appropriately. However, there are no hard and simple rules on how to do this. As a rule of the thumb, use the “banking to 45 degrees” paradigm: increase and decrease in periodic series should not be displayed at angles much higher or lower than 45 degrees. For very long series, this can become difficult on either A4 paper or a computer screen. In this case, we recommend splitting up the series and display it in different frames.

For illustration, we here show an example, the monthly unemployment rate in the US state of Maine, from January 1996 until August 2006. The data are available from a text file on the web. We can read it directly into **R**, define the data as an object of class `ts` and then do the time series plot:

```
> www <- "http://staff.elena.aut.ac.nz/Paul-Cowpertwait/ts/"
> dat <- read.table(paste(www,"Maine.dat",sep="", header=T)
> tsd <- ts(dat, start=c(1996,1), freq=12)
> plot(tsd, ylab="(%)", main="Unemployment in Maine")
```



Not surprisingly for monthly economic data, the series shows both seasonal variation and a non-linear trend. Since unemployment rates are one of the main economic indicators used by politicians/decision makers, this series poses a worthwhile forecasting problem.

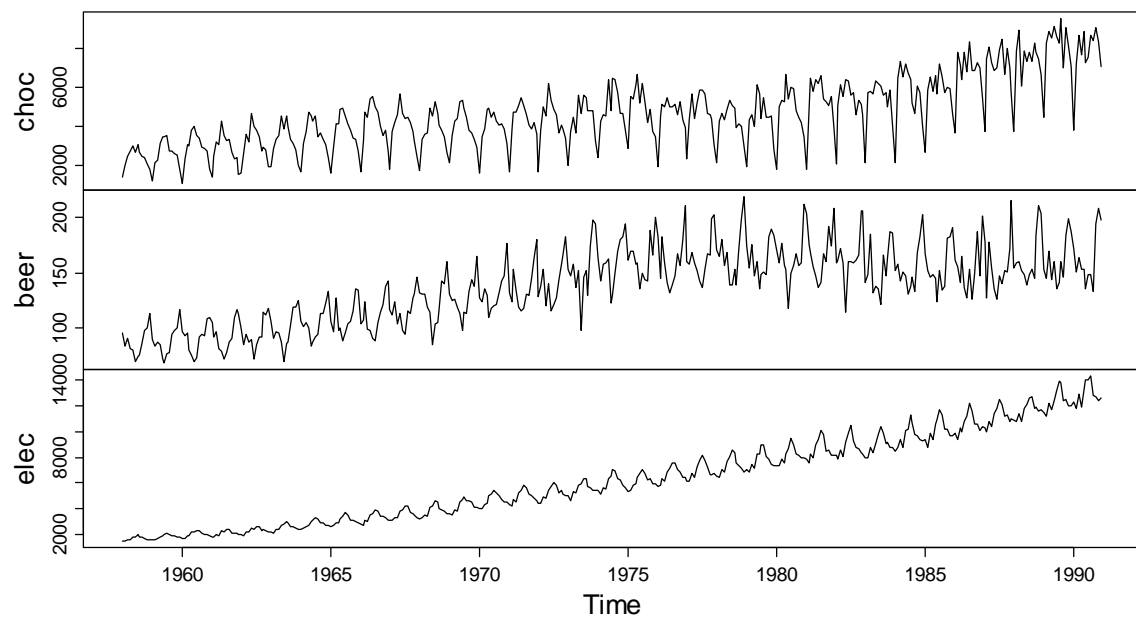
### 4.1.2 Multiple Time Series Plots

In applied problems, one is often provided with multiple time series. Here, we illustrate some basics on import, definition and plotting. Our example exhibits the monthly supply of electricity (millions of kWh), beer (millions of liters) and chocolate-based production (tonnes) in Australia over the period from January 1958 to December 1990. These data are available from the Bureau of Australian Statistics and are, in pre-processed form, accessible as a text-file online.

```
www <- "http://staff.elena.aut.ac.nz/Paul-Cowpewartwait/ts/"
dat <- read.table(paste(www,"cbe.dat",sep="", header=T)
tsd <- ts(dat, start=1958, freq=12)
plot(tsd, main="Chocolate, Beer & Electricity")
```

All three series show a distinct seasonal pattern, along with a trend. It is also instructive to know that the Australian population increased by a factor of 1.8 during the period where these three series were observed. As visible in the bit of code above, plotting multiple series into different panels is straightforward. As a general rule, using different frames for multiple series is the most recommended means of visualization. However, sometimes it can be more instructive to have them in the same frame. Of course, this requires that the series are either on the same scale, or have been indexed, resp. standardized to be so. While R offers function `ts.plot()` to include multiple series in the same frame, that function does not allow color coding. For this reason, we prefer doing some manual work.

### Chocolate, Beer & Electricity

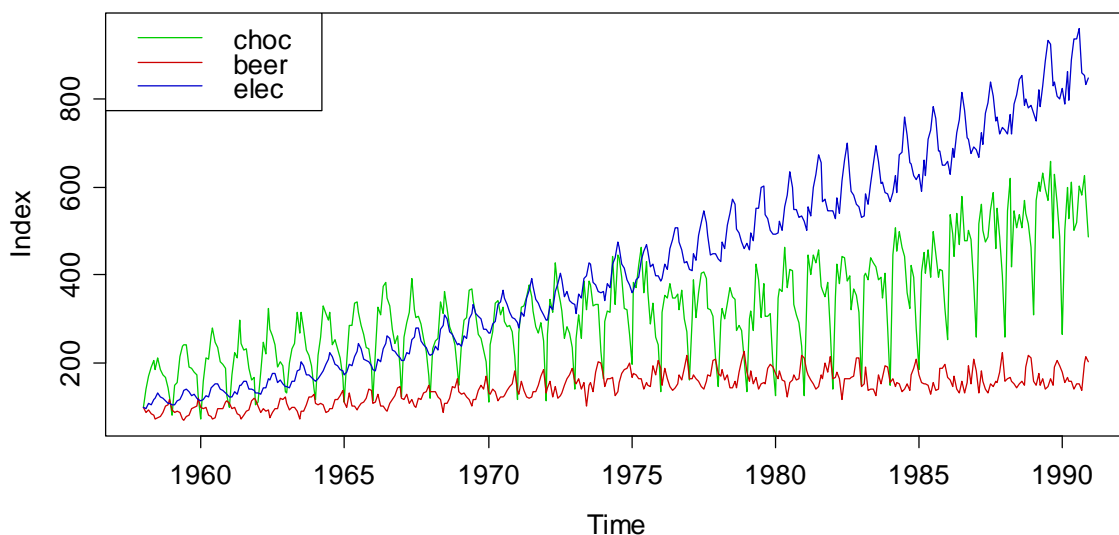


```
## Indexing the series
tsd[,1] <- tsd[,1]/tsd[1,1]*100
tsd[,2] <- tsd[,2]/tsd[1,2]*100
tsd[,3] <- tsd[,3]/tsd[1,3]*100

## Plotting in one single frame
clr <- c("green3", "red3", "blue3")
plot.ts(tsd[,1], ylim=range(tsd), ylab="Index", col=clr[1])
title("Indexed Chocolate, Beer & Electricity")
lines(tsd[,2], col=clr[2]); lines(tsd[,3], col=clr[3])

## Legend
ltx <- names(dat)
legend("topleft", lty=1, col=clr, legend=ltx)
```

### Indexed Chocolate, Beer & Electricity

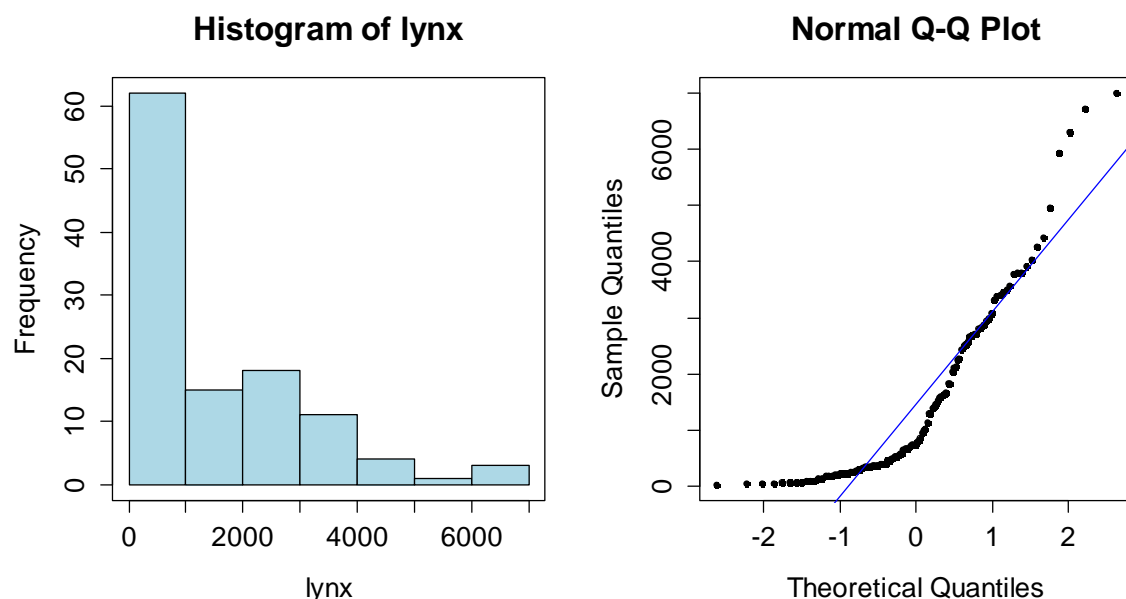


In the indexed single frame plot above, we can very well judge the relative development of the series over time. Due to different scaling, this was nearly impossible with the multiple frames on the previous page. We observe that electricity production increased around 8x during 1958 and 1990, whereas for chocolate the multiplier is around 4x, and for beer less than 2x. Also, the seasonal variation is most pronounced for chocolate, followed by electricity and then beer.

## 4.2 Transformations

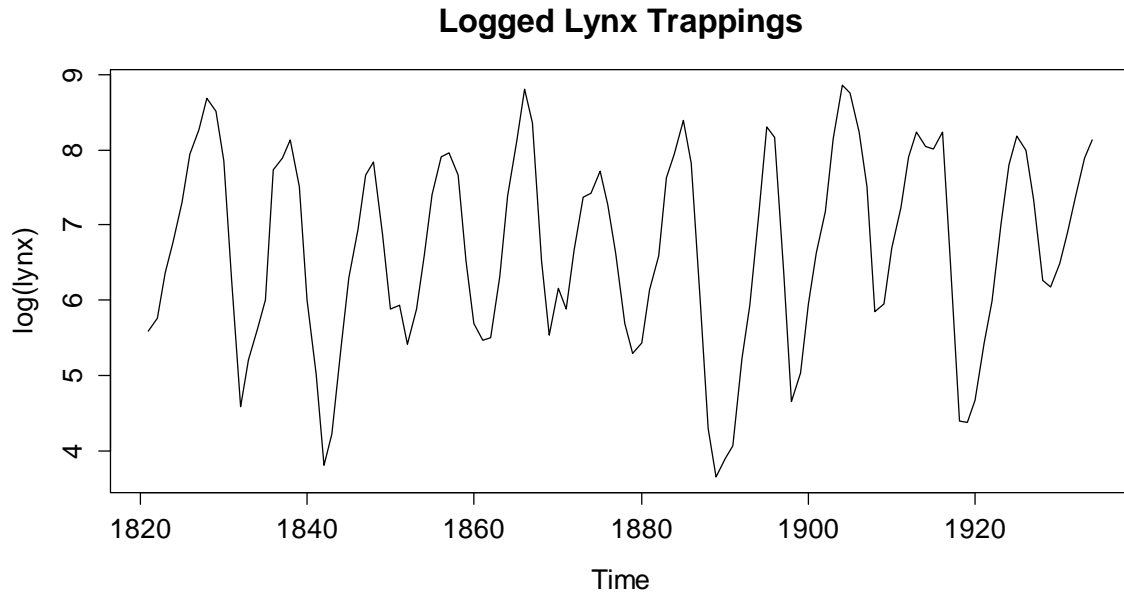
Many popular time series models are based on the Gaussian distribution and linear relations between the variables. However, data may exhibit different behavior. In such cases, we can often improve the fit by not using the original data  $x_1, \dots, x_n$ , but a transformed version  $g(x_1), \dots, g(x_n)$ . The most popular and practically relevant transformation is  $g(\cdot) = \log(\cdot)$ . It is indicated if either the variation in the series grows with increasing mean, or if the marginal distribution appears to be right-skewed. Both properties often appear in data that can take positive values only, such as the lynx trappings from section 1.2.2. It is easy to spot right-skewness by histograms and QQ-plots:

```
> hist(lynx, col="lightblue")
> qqnorm(lynx, pch=20); qqline(lynx, col="blue")
```



The lynx data show some very strong right-skewness and hence, a log-transformation is indicated. Of course, it was not wrong to use the original scale for a time series plot, but when it comes to estimating autocorrelations or estimating time series models, it is clearly better to log-transform the data first. This is very easy in R:

```
> plot(log(lynx))
> title("Logged Lynx Trappings")
```



The data now follow a more symmetrical pattern; the extreme upward spikes are all gone. We will use these transformed data to determine the autocorrelation and to generate forecasts. However, please be aware of the fact that back-transforming fitted or predicted (model) values to the original scale by just taking  $\exp(\cdot)$  usually leads to biased results, unless a correction factor is used. An in-depth discussion of that issue is contained in chapter 8.

## 4.3 Decomposition

### 4.3.1 The Basics

We have learned in section 2.2 that stationarity is an important prerequisite for being able to statistically learn from time series data. However, many of the example series exhibit either trend and/or seasonal effect, and thus are non-stationary. In this section, we will learn how to deal with that. It is achieved by using *decomposition models*, the easiest of which is the *simple additive* one:

$$X_t = m_t + s_t + R_t,$$

where  $X_t$  is the time series process at time  $t$ ,  $m_t$  is the trend,  $s_t$  is the seasonal effect, and  $R_t$  is the remainder, i.e. a sequence of usually correlated random variables with mean zero. The goal is to find a decomposition such that  $R_t$  is a stationary time series process. Such a model might be suitable for all the monthly-data series we got acquainted with so far: air passenger bookings, unemployment in Maine and Australian production. However, closer inspection of all these series exhibits that the seasonal effect and the random variation increase as the trend increases. In such cases, a multiplicative decomposition model is better:

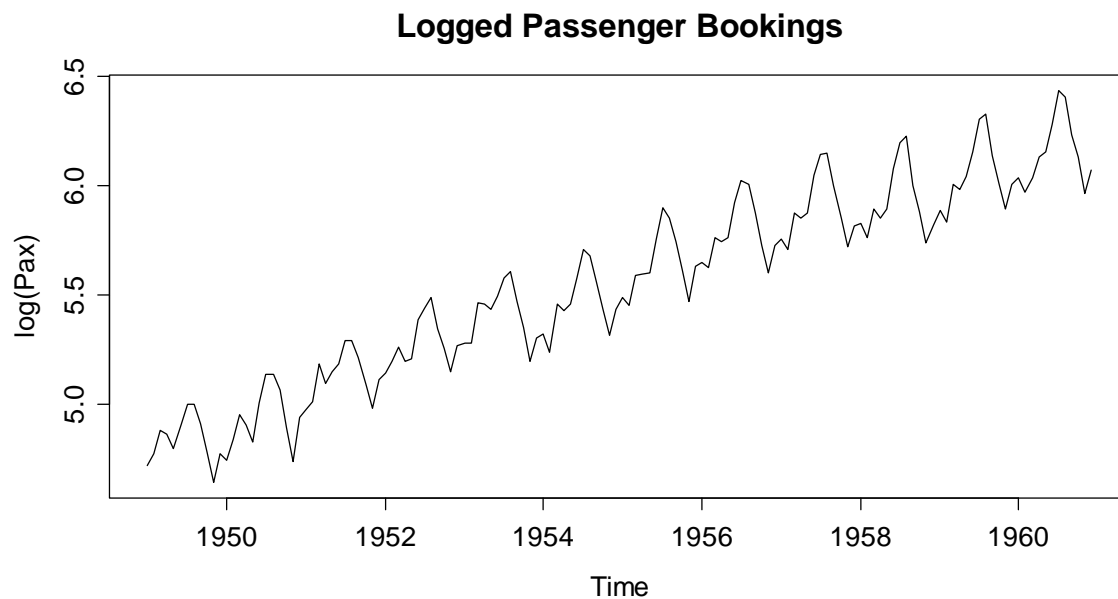
$$X_t = m_t \cdot s_t \cdot R_t$$

Empirical experience says that taking logarithms is beneficial for such data. Also, some basic math shows that this brings us back to the additive case:

$$\log(X_t) = \log(m_t \cdot s_t \cdot R_t) = \log(m_t) + \log(s_t) + \log(R_t) = m'_t + s'_t + R'_t$$

For illustration, we carry out the log-transformation on the air passenger bookings:

```
> plot(log(AirPassengers), ylab="log(Pax)", main=...)
```



Indeed, seasonal effect and random variation now seem to be independent of the level of the series. Thus, the multiplicative model is much more appropriate than the additive one. However, a further snag is that the seasonal effect seems to alter over time rather than being constant. That issue will be addressed later.

### 4.3.2 Differencing

A simple approach for removing deterministic trends and/or seasonal effects from a time series is by taking differences. A practical interpretation of taking differences is that by doing so, the changes in the data will be monitored, but no longer the series itself. While this is conceptually simple and quick to implement, the main disadvantage is that it does not result in explicit estimates of the trend component  $m_t$  and the seasonal component  $s_t$ .

We will first turn our attention to series with an additive trend, but without seasonal variation. By taking first-order differences with lag 1, and assuming a trend with little short-term changes, i.e.  $m_t \approx m_{t-1}$ , we have:

$$\begin{aligned} X_t &= m_t + R_t \\ Y_t &= X_t - X_{t-1} \approx R_t - R_{t-1} \end{aligned}$$



In practice, this kind of differencing approach “mostly works”, i.e. manages to reduce presence of a trend in the series in a satisfactory manner. However, the trend is only fully removed if it is exactly linear, i.e.  $m_t = \alpha + \beta t$ . Then, we obtain:

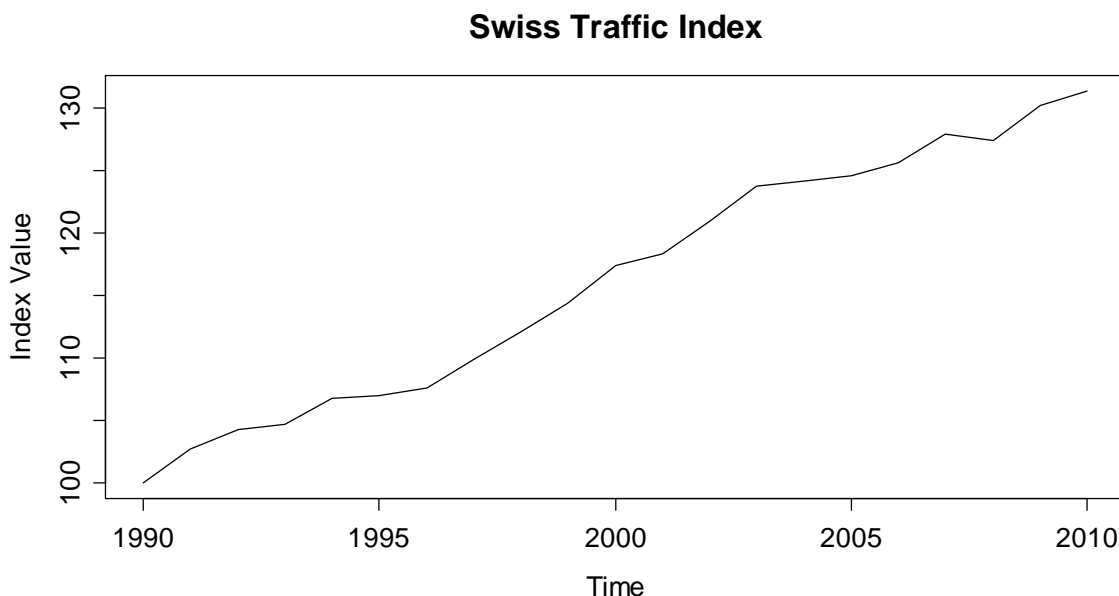
$$Y_t = X_t - X_{t-1} = \beta + R_t - R_{t-1}$$

Another somewhat disturbing property of the differencing approach is that strong, artificial new dependencies are created, meaning that the autocorrelation in  $Y_t$  is different from the one in  $R_t$ . For illustration, consider a stochastically independent remainder  $R_t$ : the differenced process  $Y_t$  has autocorrelation!

$$\begin{aligned} \text{Cov}(Y_t, Y_{t-1}) &\approx \text{Cov}(R_t - R_{t-1}, R_{t-1} - R_{t-2}) \\ &= -\text{Cov}(R_{t-1}, R_{t-1}) \\ &\neq 0 \end{aligned}$$

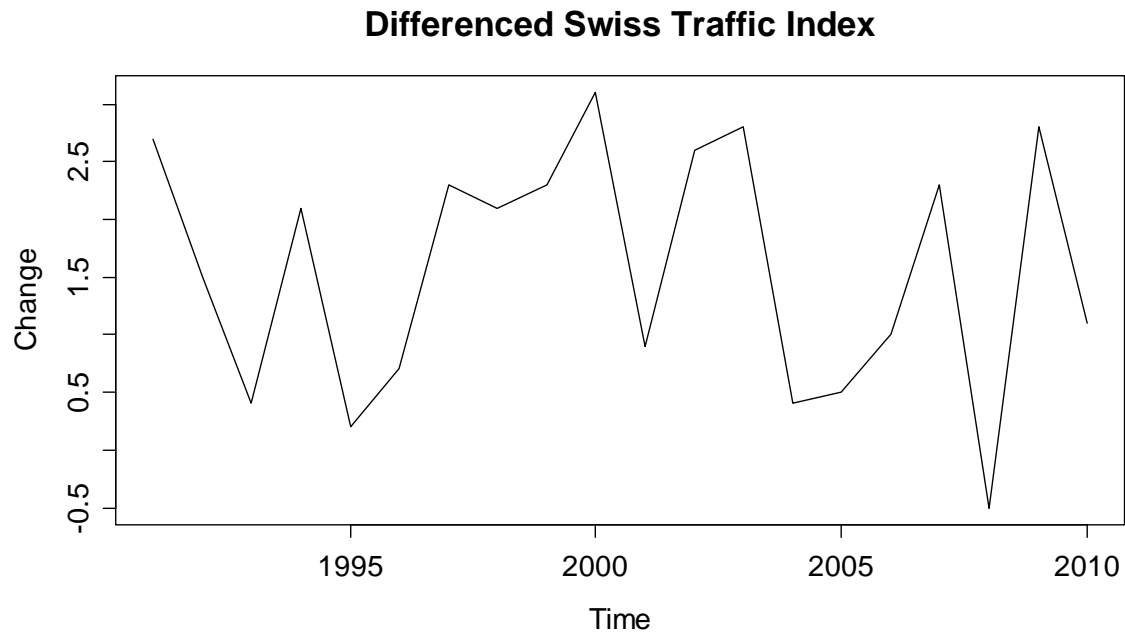
We illustrate how differencing works by using a dataset that shows the traffic development on Swiss roads. The data are available from the federal road office (ASTRA) and show the indexed traffic amount from 1990-2010. We type in the values and plot the original series:

```
> SwissTraffic <- ts(c(100.0, 102.7, 104.2, 104.6, 106.7,
                      106.9, 107.6, 109.9, 112.0, 114.3,
                      117.4, 118.3, 120.9, 123.7, 124.1,
                      124.6, 125.6, 127.9, 127.4, 130.2,
                      131.3), start=1990, freq=1)
> plot(SwissTraffic)
```



There is a clear trend, which is close to linear, thus the simple approach should work well here. Taking first-order differences with lag 1 shows the yearly changes in the Swiss Traffic Index, which must now be a stationary series. In **R**, the job is done with function `diff()`.

```
> diff(SwissTraffic)
Time Series:
Start = 1991
End = 2010
Frequency = 1
[1] 2.7 1.5 0.4 2.1 0.2 0.7 2.3 2.1 2.3 3.1
[11] 0.9 2.6 2.8 0.4 0.5 1.0 2.3 -0.5 2.8 1.1
```



Please note that the time series of differences is now 1 instance shorter than the original series. The reason is that for the first year, 1990, there is no difference to the previous year available. The differenced series now clearly has a constant mean, i.e. the trend was successfully removed.

### Log-Transformation and Differencing

On a sidenote, we consider a series that was log-transformed first, before first-order differences with lag 1 were taken. An example is the SMI data that were shown in section 1.2.4. The result is the so-called *log return*, which is an approximation to the relative change, i.e. the percent in- or decrease with respect to the previous instance. In particular:

$$Y_t = \log(X_t) - \log(X_{t-1}) = \log\left(\frac{X_t}{X_{t-1}}\right) = \log\left(\frac{X_t - X_{t-1}}{X_{t-1}} + 1\right) \approx \frac{X_t - X_{t-1}}{X_{t-1}}$$

The approximation of the log return to the relative change is very good for small changes, and becomes a little less precise with larger values. For example, if we have a 0.00% relative change, then  $Y_t = 0.00\%$ , for 1.00% relative change we obtain  $Y_t = 0.995\%$  and for 5.00%,  $Y_t = 4.88\%$ . We conclude with summarizing that for any non-stationary series which is also due to a log-transformation, the transformation is always carried out first, and then followed by the differencing!

### The Backshift Operator

We here introduce the backshift operator  $B$  because it allows for convenient notation. When the operator  $B$  is applied to  $X_t$  it returns the instance at lag 1, i.e.

$$B(X_t) = X_{t-1}.$$

Less mathematically, we can also say that applying  $B$  means “go back one step”, or “increment the time series index  $t$  by -1”. The operation of taking first-order differences at lag 1 as above can be written using the backshift operator:

$$Y_t = (1 - B)X_t = X_t - X_{t-1}$$

However, the main aim of the backshift operator is to deal with more complicated forms of differencing, as will be explained below.

### Higher-Order Differencing

We have seen that taking first-order differences is able to remove linear trends from time series. What has differencing to offer for polynomial trends, i.e. quadratic or cubic ones? We here demonstrate that it is possible to take higher order differences to remove also these, for example, in the case of a quadratic trend.

$$\begin{aligned} X_t &= \alpha + \beta_1 t + \beta_2 t^2 + R_t, \quad R_t \text{ stationary} \\ Y_t &= (1 - B)^2 X_t \\ &= (X_t - X_{t-1}) - (X_{t-1} - X_{t-2}) \\ &= R_t - 2R_{t-1} + R_{t-2} + 2\beta_2 \end{aligned}$$

We see that the operator  $(1 - B)^2$  means that after taking “normal” differences, the resulting series is again differenced “normally”. This is a discretized variant of taking the second derivative, and thus it is not surprising that it manages to remove a quadratic trend from the data. As we can see,  $Y_t$  is an additive combination of the stationary  $R_t$ ’s terms, and thus itself stationary. Again, if  $R_t$  was an independent process, that would clearly not hold for  $Y_t$ , thus taking higher-order differences (strongly!) alters the dependency structure.

Moreover, the extension to cubic trends and even higher orders  $d$  is straightforward. We just use the  $(1 - B)^d$  operator applied to series  $X_t$ . In  $\mathbf{R}$ , we can employ function `diff()`, but have to provide argument `differences=d` for indicating the order of the difference  $d$ .

### Removing Seasonal Effects by Differencing

For time series with monthly measurements, seasonal effects are very common. Using an appropriate form of differencing, it is possible to remove these, as well as potential trends. We take first-order differences with lag  $p$ :

$$Y_t = (1 - B^p)X_t = X_t - X_{t-p},$$

Here,  $p$  is the period of the seasonal effect, or in other words, the frequency of series, which is the number of measurements per time unit. The series  $Y_t$  then is made up of the changes compared to the previous period's value, e.g. the previous year's value. Also, from the definition, with the same argument as above, it is evident that not only the seasonal variation, but also a strictly linear trend will be removed.

Usually, trends are not exactly linear. We have seen that taking differences at lag 1 removes slowly evolving (non-linear) trends well due to  $m_t \approx m_{t-1}$ . However, here the relevant quantities are  $m_t$  and  $m_{t-p}$ , and especially if the period  $p$  is long, some trend will usually be remaining in the data. Then, further action is required.

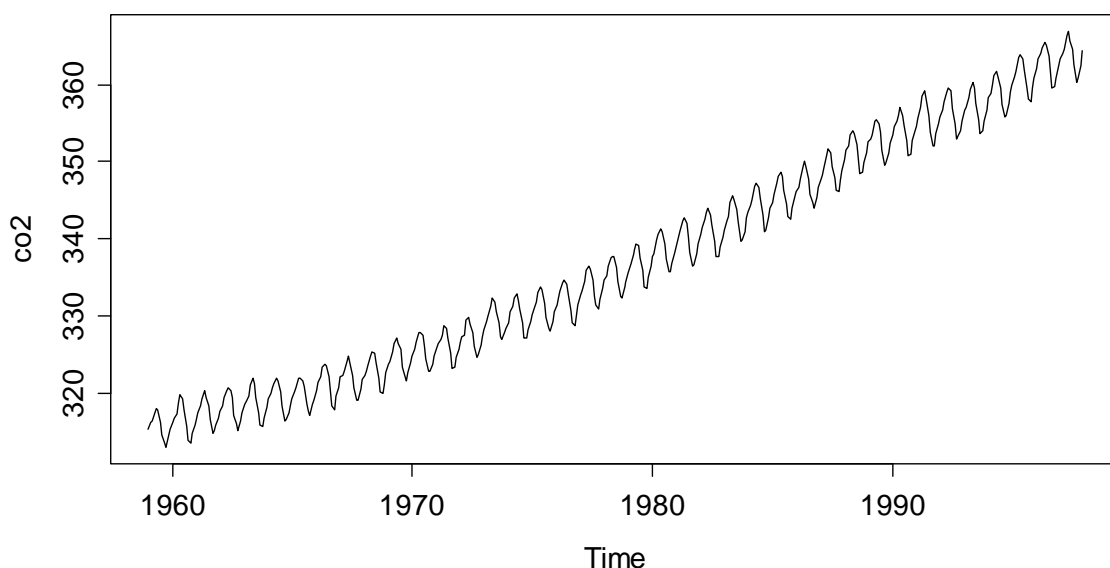
### Example

We are illustrating seasonal differencing using the Mauna Loa atmospheric  $CO_2$  concentration data. This is a time series with monthly records from January 1959 to December 1997. It exhibits both a trend and a distinct seasonal pattern. We first load the data and do a time series plot:

```
> data(co2)
> plot(co2, main="Mauna Loa CO2 Concentrations")
```

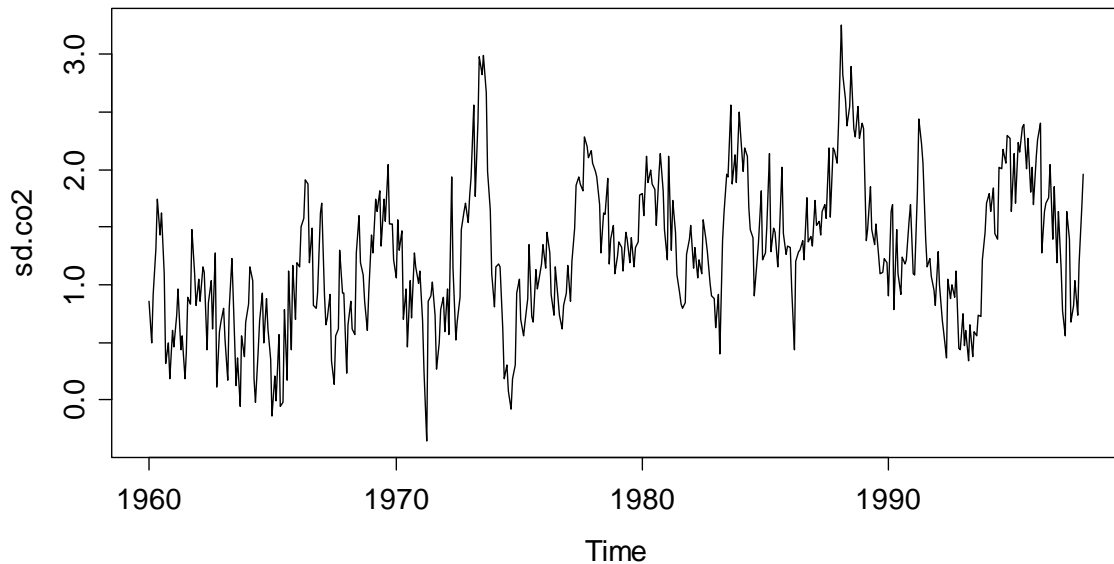
Seasonal differencing is very conveniently available in **R**. We use function `diff()`, but have to set argument `lag=...`. For the Mauna Loa data with monthly measurements, the correct lag is 12. This results in the series shown on the next page. Because we are comparing every record with the one from the previous year, the resulting series is 12 observations shorter than the original one. It is pretty obvious that some trend is remaining and thus, the result from seasonal differencing cannot be considered as stationary. As the seasonal effect is gone, we could try to add some first-order differencing at lag 1.

### Mauna Loa CO2 Concentrations



```
> sd.co2 <- diff(co2, lag=12)
> plot(sd.co2, main="Differenced Mauna Loa Data (p=12)")
```

### Differenced Mauna Loa Data (p=12)

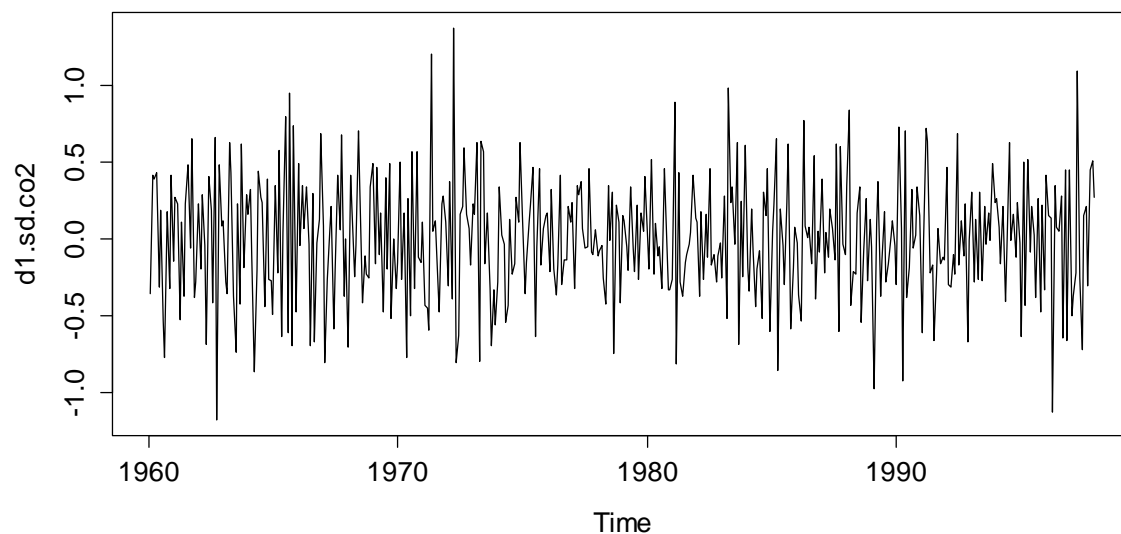


The second differencing step indeed manages to produce a stationary series, as can be seen below. The equation for the final series is:

$$Z_t = (1 - B)Y_t = (1 - B)(1 - B^{12})X_t.$$

The next step would be to analyze the autocorrelation of the series below and fit an  $ARMA(p, q)$  model. Due to the two differencing steps, such constructs are also named *SARIMA* models. They will be discussed in chapter 6.

### Twice Differenced Mauna Loa Data (p=12, p=1)



We conclude this section by emphasizing that while differencing is quick and simple, and (correctly done) manages to remove any trend and/or seasonality, we do not obtain explicit estimates for trend  $m_t$ , seasonal effect  $s_t$  and remainder  $R_t$  which proves problematic in many applications.

### 4.3.3 Smoothing, Filtering

Our next goal is to define a decomposition procedure that yields explicit trend, seasonality and remainder estimates  $\hat{m}_t$ ,  $\hat{s}_t$  and  $\hat{R}_t$ . In the absence of a seasonal effect, the trend of a time series can simply be obtained by applying an *additive linear filter*:

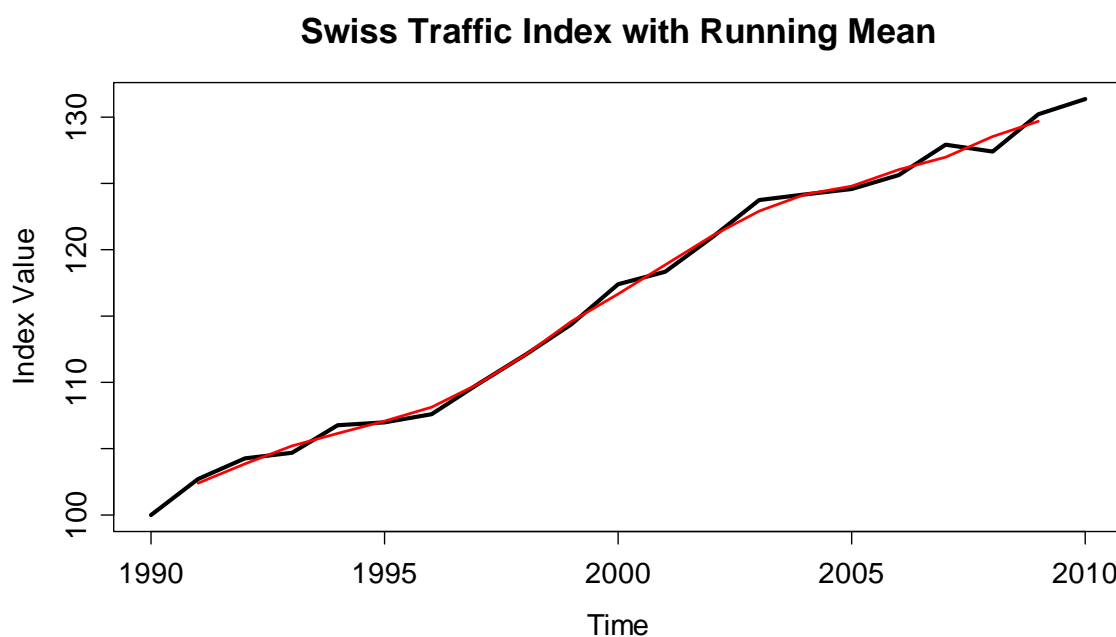
$$\hat{m}_t = \sum_{i=-p}^q a_i X_{t+i}$$

This definition is general, as it allows for arbitrary weights and asymmetric windows. The most popular implementation, however, relies on  $p=q$  and  $a_i = 1/(2p+1)$ , i.e. a *running mean estimator* with symmetric window and uniformly distributed weights. The window width is the smoothing parameter.

#### Example: Trend Estimation with Running Mean

We here again consider the Swiss Traffic data that were already exhibited before. They show the indexed traffic development in Switzerland between 1990 and 2010. Linear filtering is available with function `filter()` in **R**. With the correct settings, this function becomes a running mean estimator.

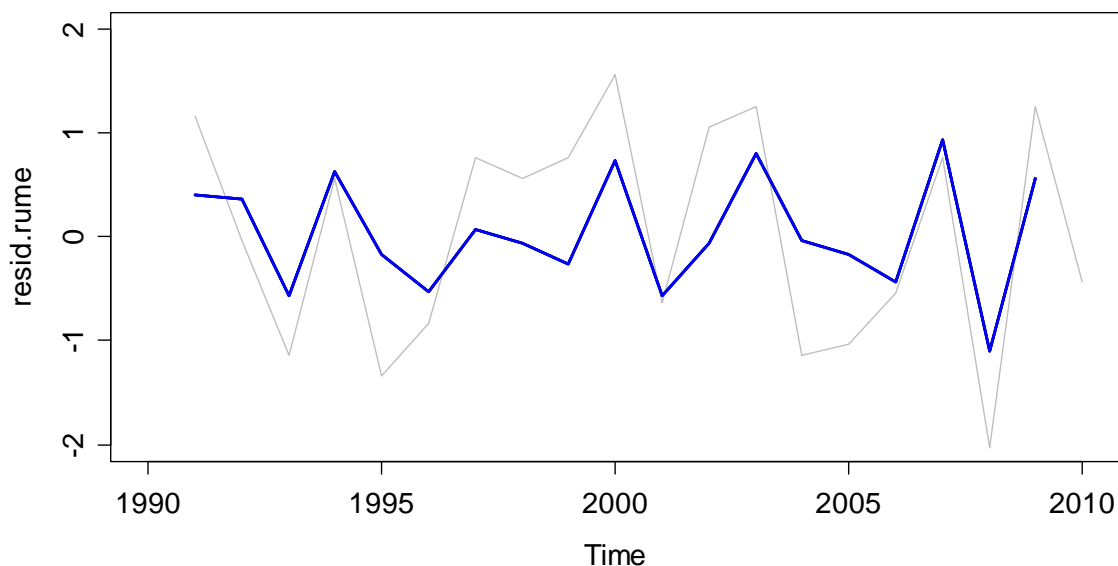
```
> trend.est <- filter(SwissTraffic, filter=c(1,1,1)/3)
```



```
> trend.est
Time Series: Start = 1990, End = 2010, Frequency = 1
[1]      NA 102.3000 103.8333 105.1667 106.0667 107.0667
[7] 108.1333 109.8333 112.0667 114.5667 116.6667 118.8667
[13] 120.9667 122.9000 124.1333 124.7667 126.0333 126.9667
[19] 128.5000 129.6333      NA
```

In our example, we chose the trend estimate to be the mean over three consecutive observations. This has the consequence that for both the first and the last instance of the time series, no trend estimate is available. Also, it is apparent that the Swiss Traffic series has a very strong trend signal, whereas the remaining stochastic term is comparably small in magnitude. We can now compare the estimated remainder term from the running mean trend estimation to the result from differencing:

### Estimated Stochastic Remainder Term



The blue line is the remainder estimate from running mean approach, while the grey one resulted from differencing with lag 1. We observe that the latter has bigger variance; and, while there are some similarities between the two series, there are also some prominent differences – please note that while both seem stationary, they are different.

### Trend Estimation for Seasonal Data

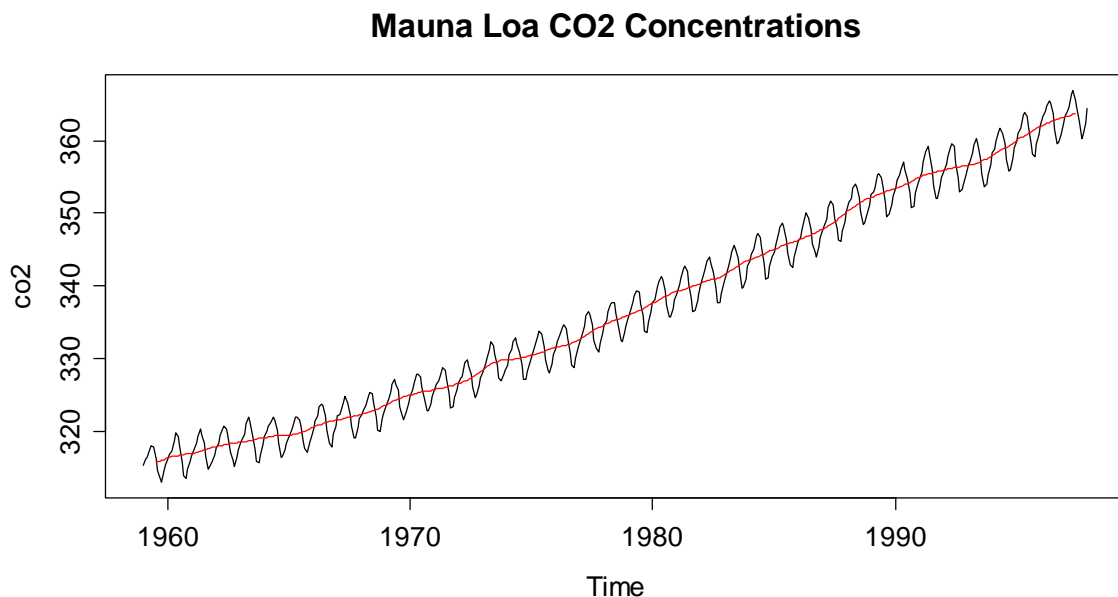
We now turn our attention to time series that show both trend *and* seasonal effect. The goal is to specify a filtering approach that allows trend estimation for periodic data. We still base this on the running mean idea, but have to make sure that we average over a full period. For monthly data, the formula is:

$$\hat{m}_t = \frac{1}{12} \left( \frac{1}{2} X_{t-6} + X_{t-5} + \dots + X_{t+5} + \frac{1}{2} X_{t+6} \right), \text{ for } t = 7, \dots, n-6$$

Be careful, as there is a slight snag if the frequency is even: if we estimate the trend for December, we use data from July to May, and then also add half of the value of the previous June, as well as half of the next June. This is required for having a window that is centered at the time we wish to estimate the trend. Using **R**'s function `filter()`, with appropriate choice of weights, we can compute the seasonal running mean. We illustrate this with the Mauna Loa  $CO_2$  data.

```
> wghts      <- c(.5,rep(1,11),.5)/12
> trend.est <- filter(co2, filter=wghts, sides=2)
> plot(co2, main="Mauna Loa CO2 Concentrations")
> lines(trend.est, col="red")
```

We obtain a trend which fits well to the data. It is not a linear trend, rather it seems to be slightly progressively increasing, and it has a few kinks, too.



We finish this section about trend estimation using linear filters by stating that other smoothing approaches, e.g. *running median estimation*, the *loess smoother* and many more are valid choices for trend estimation, too.

### Estimation of the Seasonal Effect

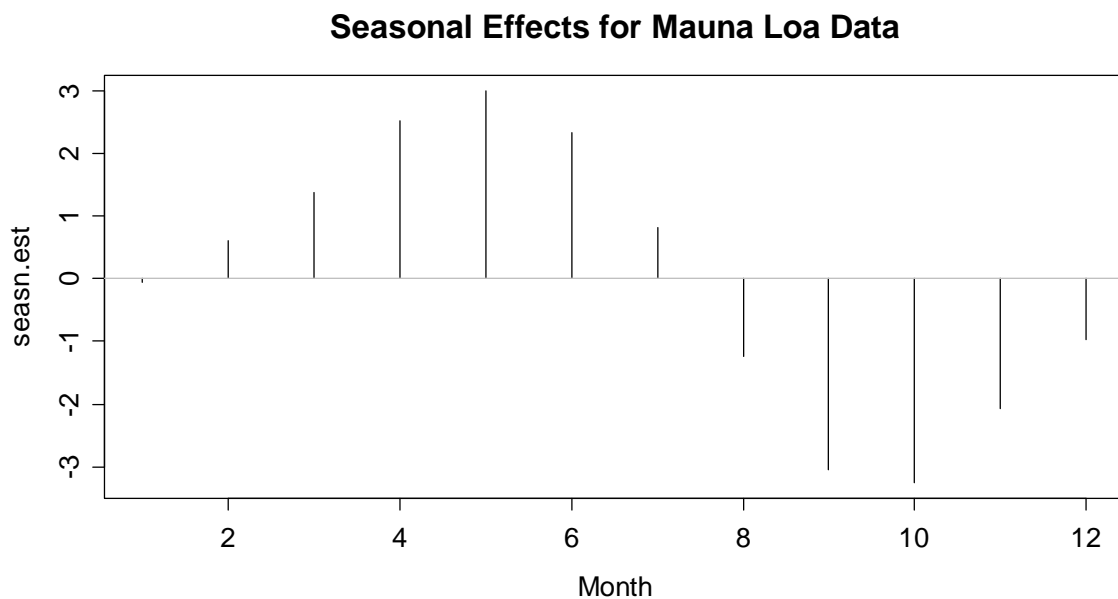
For fully decomposing periodic series such as the Mauna Loa data, we also need to estimate the seasonal effect. This is done on the basis of the trend adjusted data: simple averages over all observations from the same seasonal entity are taken. The following formula shows the January effect estimation for the Mauna Loa data, a monthly series which starts in January and has 39 years of data.

$$\hat{s}_{Jan} = \hat{s}_1 = \hat{s}_{13} = \dots = \frac{1}{39} \cdot \sum_{j=0}^{38} (x_{12j+1} - \hat{m}_{12j+1})$$



In **R**, a convenient way of estimating such seasonal effects is by generating a factor for the months, and then using the `tapply()` function. Please note that the seasonal running mean naturally generates NA values at the start and end of the series, which we need to remove in the seasonal averaging process.

```
> trend.adj <- co2-trend.est
> month      <- factor(rep(1:12,39))
> seasn.est <- tapply(trend.adj, month, mean, na.rm=TRUE)
> plot(seasn.est, type="h", xlab="Month")
> title("Seasonal Effects for Mauna Loa Data")
> abline(h=0, col="grey")
```



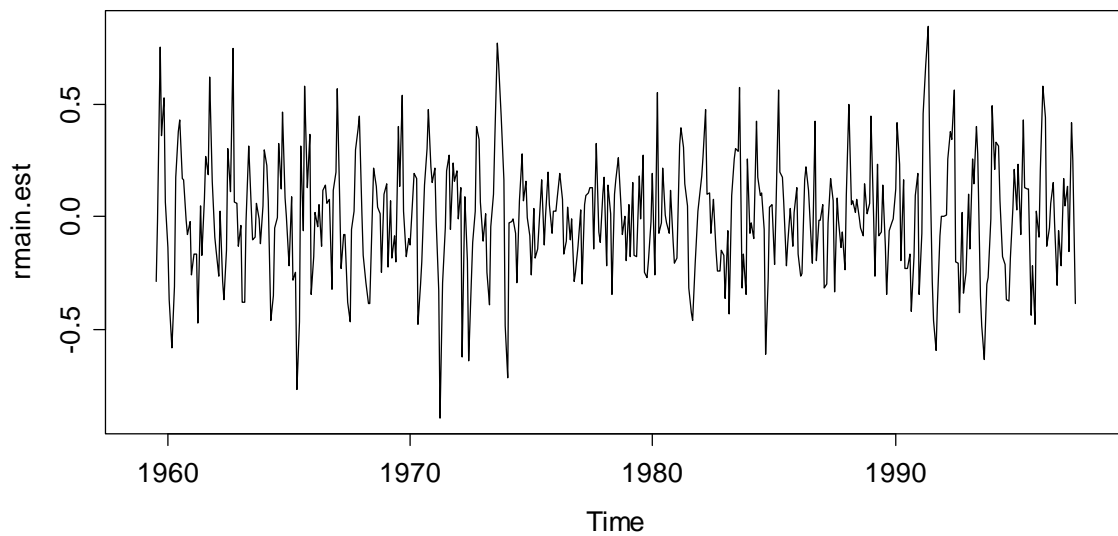
In the plot above, we observe that during a period, the highest values are usually observed in May, whereas the seasonal low is in October. The estimate for the remainder at time  $t$  is simply obtained by subtracting estimated trend and seasonality from the observed value.

$$\hat{R}_t = x_t - \hat{m}_t - \hat{s}_t$$

From the plot on the next page, it seems as if the estimated remainder still has some periodicity and thus it is questionable whether it is stationary. The periodicity is due to the fact that the seasonal effect is not constant but slowly evolving over time. In the beginning, we tend to overestimate it for most months, whereas in the end, we underestimate. We will address the issue on how to visualize evolving seasonality below in section 4.3.4 about STL-decomposition. A further option for dealing with non-constant seasonality is given by the exponential smoothing approach which is covered in chapter 8.3.

```
> rmain.est <- co2-trend.est-rep(seasn.est,39)
> plot(rmain.est, main="Estimated Stochastic Remainder Term")
```

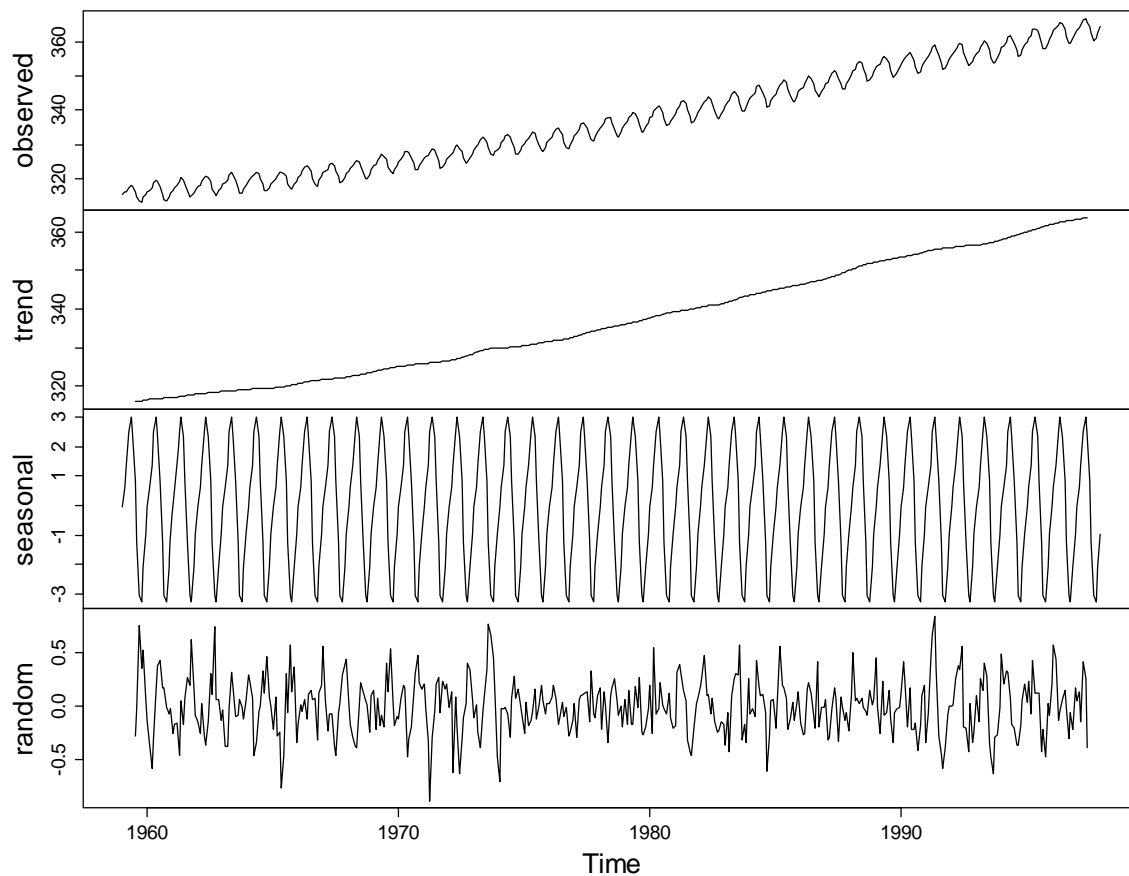
### Estimated Stochastic Remainder Term



Moreover, we would like to emphasize that R offers the convenient `decompose()` function for running mean estimation and seasonal averaging.

```
> co2.dec <- decompose(co2)
> plot(co2.dec)
```

### Decomposition of additive time series



Please note that `decompose()` only works with periodic series where at least two full periods were observed; else it is not mathematically feasible to estimate trend and seasonality from a series. The `decompose()` function also offers the neat plotting method shown above that generates the four frames above with the series, and the estimated trend, seasonality and remainder. Except for the different visualization, the results are exactly the same as what we had produced with our do-it-yourself approach.

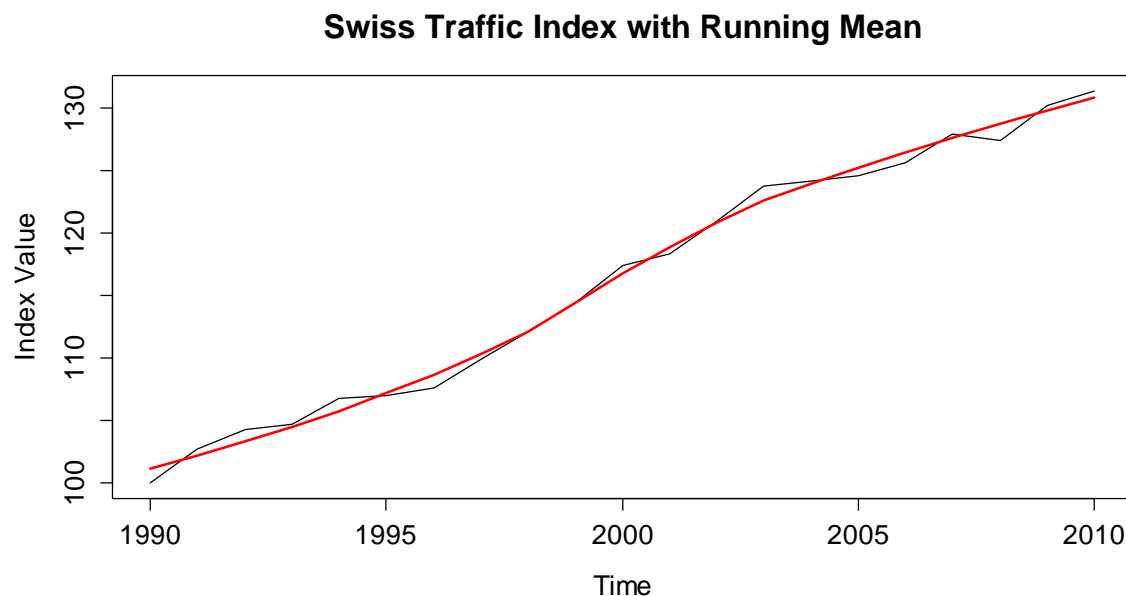
### 4.3.4 Seasonal-Trend Decomposition with LOESS

It is well known that the running mean is not the best smoother around. Thus, potential for improvement exists. While there is a dedicated R procedure for decomposing periodic series into trend, seasonal effect and remainder, we have to do some handwork in non-periodic cases.

#### Trend Estimation with LOESS

We here consider again the Swiss Traffic dataset, for which the trend had already been estimated above. Our goal is to re-estimate the trend with *LOESS*, a smoothing procedure that is based on local, weighted regression. The aim of the weighting scheme is to reduce potentially disturbing influence of outliers. Applying the LOESS smoother with (the often optimal) default settings is straightforward:

```
> fit <- loess(SwissTraffic~time(SwissTraffic))  
> trend <- predict(fit)
```

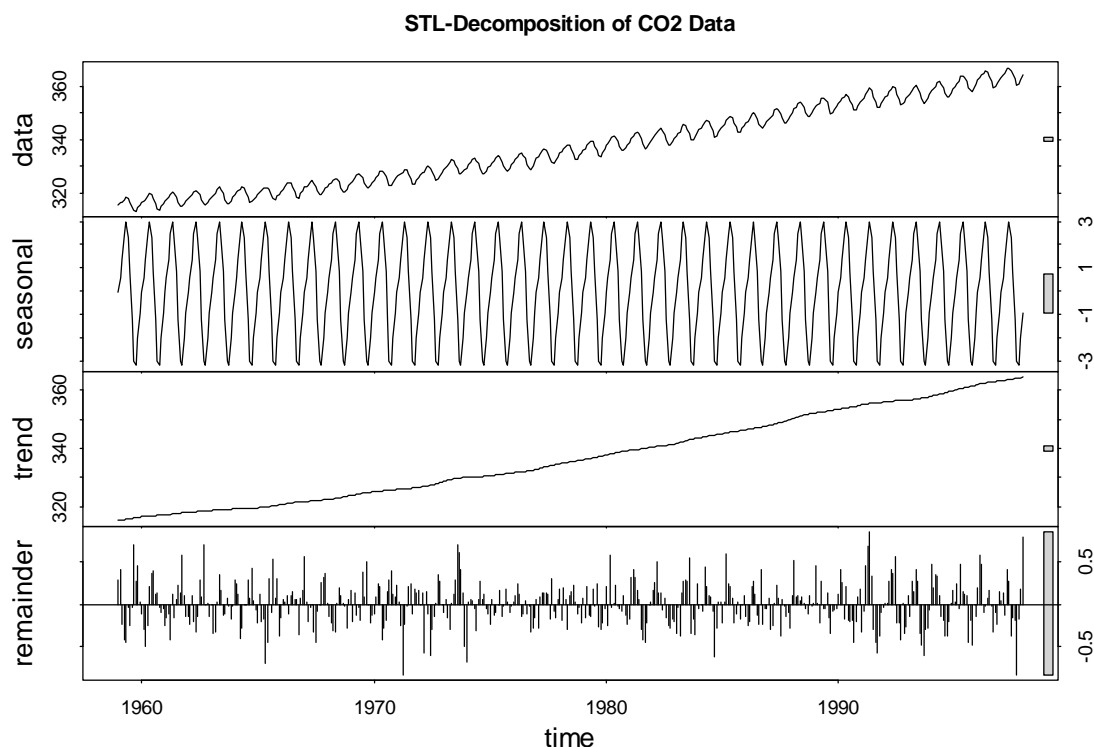


We observe that the estimated trend, in contrast to the running mean result, is now smooth and allows for interpolation within the observed time. Also, the `loess()` algorithm returns trend estimates which extend to the boundaries of the dataset. In summary, we recommend to always perform trend estimation with LOESS.

## Using the `stl()` Procedure for Periodic Series

R's `stl()` procedure offers a decomposition of a periodic time series into trend, seasonality and remainder. All estimates are based on the LOESS smoother. While the output is (nearly) equivalent to what we had obtained above with `decompose()`, we recommend to use this procedure only, because the results are more trustworthy. We do here without giving the full details on the procedure, but only state that it works iteratively. The commands are as follows:

```
> co2.stl <- stl(co2, s.window="periodic")
> plot(co2.stl, main="STL-Decomposition of CO2 Data")
```

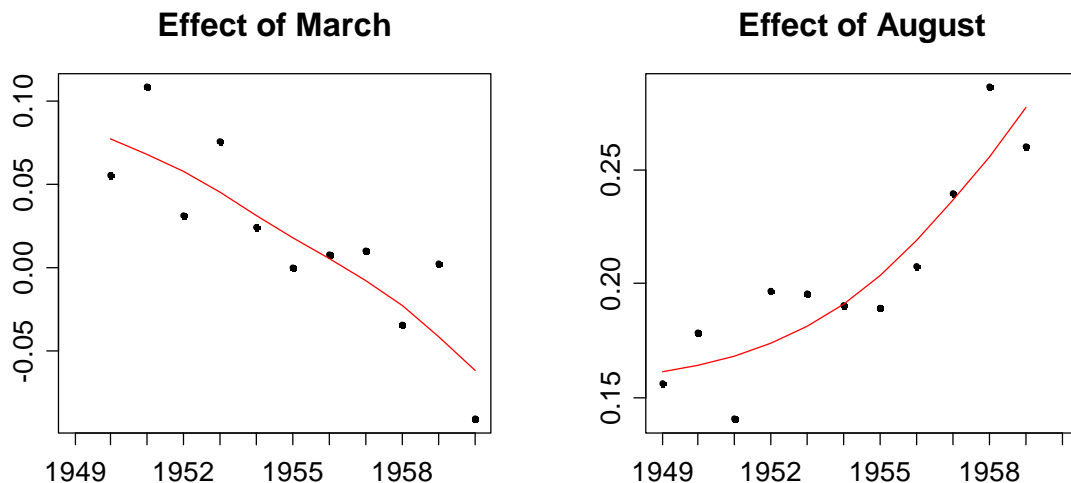


The graphical output is similar to the one from `decompose()`. The grey bars on the right hand side facilitate interpretation of the decomposition: they show the relative magnitude of the effects, i.e. cover the same span on the y-scale in all of the frames. The two principal arguments in function `stl()` are `t.window` and `s.window`: `t.window` controls the amount of smoothing for the trend, and has a default value which often yields good results. The value used can be inferred with:

```
> co2.stl$win[2]
t
19
```

The result is the number of lags used as a window for trend extraction in LOESS. Increasing it means the trend becomes smoother; lowering it makes the trend rougher, but more adapted to the data. The second argument, `s.window`, controls the smoothing for the seasonal effect. When set to "periodic" as above, the seasonality is obtained as a constant value from simple (monthly) averaging.

However, `stl()` offers better functionality. If `s.window` is set to a numeric value, the procedure can accommodate for evolving seasonality. The assumption behind is that the change in the seasonal effect happens slowly and smoothly. We visualize what is meant with the logged air passenger data. For quick illustration, we estimate the trend with a running mean filter; subtract it from the observed series and display all March and all August values of the trend adjusted series:



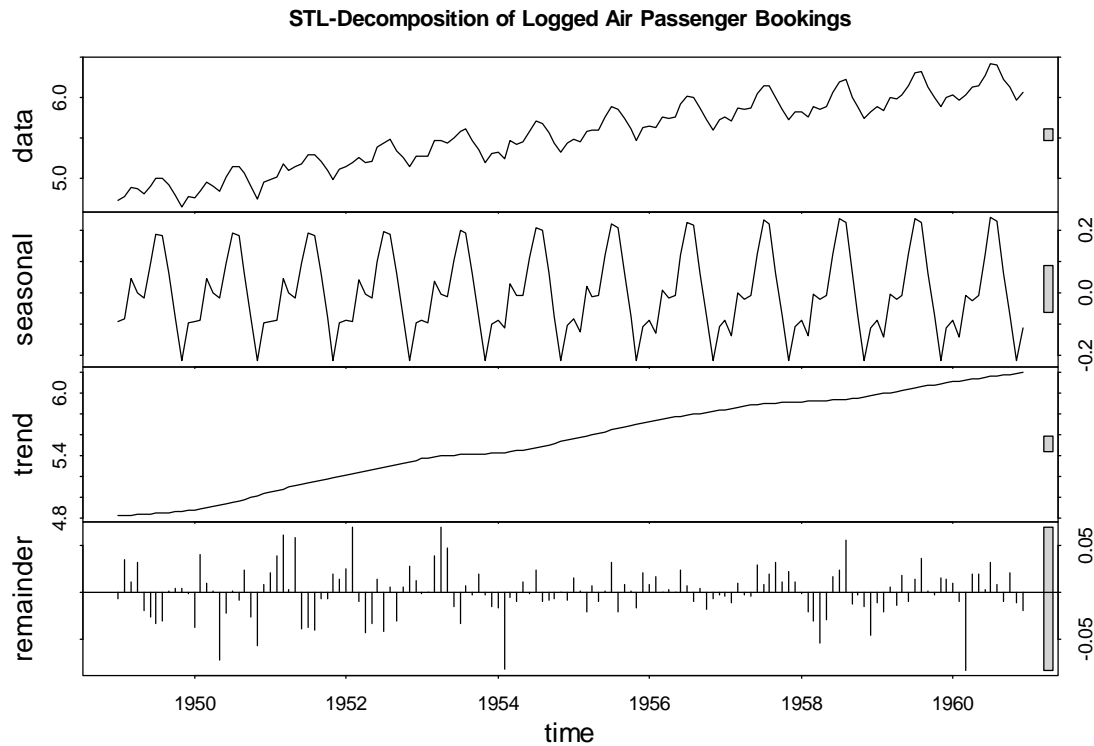
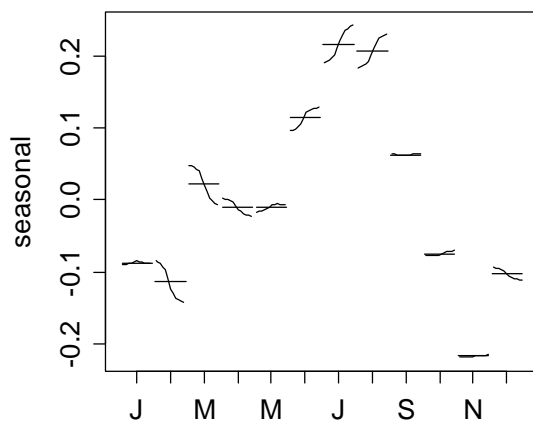
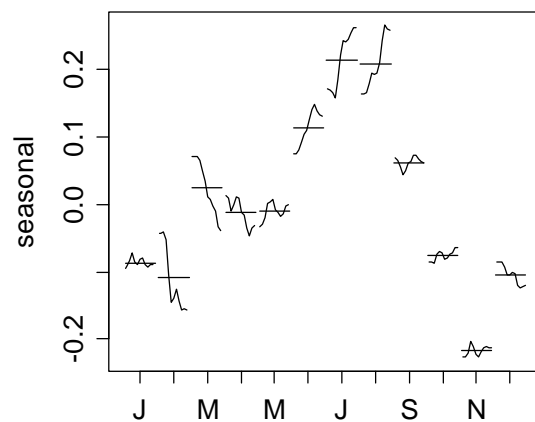
When assuming a non-changing seasonal effect, the standard procedure would be to take the mean of the data points in the above scatterplots and declare that as the seasonal effect for March and August, respectively. This is a rather crude way of data analysis, and can of course be improved. We achieve a better decomposition of the logged air passenger bookings by employing the `stl()` function and setting `s.window=13`. The resulting output is displayed below.

```
> fit.05 <- stl(lap, s.window= 5)
> fit.13 <- stl(lap, s.window=13)
> plot(fit.13, main="STL-Decomposition ...")
```

Please note that there is no default value for the seasonal span, and the optimal choice is left to the user upon visual inspection. An excellent means for doing so is the `monthplot()` function which shows the seasonal effects that were estimated by `stl()`.

```
> monthplot(fit.13, main="Monthplot, s.window=13")
> monthplot(fit.05, main="Monthplot, s.window=5")
```

The output, which can be found on the next page shows an appropriate amount of smoothing in the left panel, with `s.window=13`. However on the right, with smaller span, i.e. `s.window=5`, we observe overfitting – the seasonal effects do not evolve in a smooth way, and it means that this is not a good decomposition estimate.

**Monthplot, s.window=13****Monthplot, s.window=5**

### 4.3.5 Parametric Modeling

A powerful approach for decomposing time series is parametric modeling. It is based on the assumption of a functional form for the trend, usually a polynomial. For the seasonal effect, we can either use the dummy variable approach that amounts to averaging. Or, in some special cases, a sine/cosine seasonality may be appropriate. We illustrate the parametric modeling approach by two examples and use them for discussing some specifics.

We consider the Maine unemployment data from section 4.1.1. Our goal is to fit a polynomial trend, along with a seasonal effect that is obtained from averaging. We write down this model for a polynomial of grade 4.

$$X_t = \beta_0 + \beta_1 \cdot t + \beta_2 \cdot t^2 + \beta_3 \cdot t^3 + \beta_4 \cdot t^4 + \alpha_{i(t)} + E_t,$$

where  $t = 1, \dots, 128$  and  $i(t) \in \{1, \dots, 12\}$ , i.e.  $\alpha_{i(t)}$  is a factor variable encoding for the month the observation was made in, see the `R` code below. Two questions immediately pop up, namely what polynomial order is appropriate, and how this model can be fit.

As for the fitting, this will usually be done with the ordinary least squares (OLS) algorithm. This requires some prudence, because when working with time series, the remainder term  $E_t$  may not necessarily be stochastically independent. Thus, we might have some violated assumption for the OLS estimation. Since the estimated coefficients are still unbiased, OLS is a valid approach. However, be careful with the standard errors, as well as tests and confidence intervals derived from them, because they can be grossly misleading.

For the grade of the polynomial, we determine by eyeballing from the time series plot that the hypothesized trend in the unemployment series has at least 3 extrema. This means that a polynomial with grade below 4 will not result in a sensible trend estimate. Thus, we try orders 4, 5 and 6, and discuss how an appropriate choice can be made from residual analysis. However, we first focus on the `R` code for fitting such models. In the first step below, we lay the basics. From time series `maine`, we extract the times of observation, i.e. the predictor. As always when fitting polynomial regression models, it is crucial to center the  $x$ -values to mitigate potential collinearity among the terms. Furthermore, we define a factor variable for modeling the seasonality.

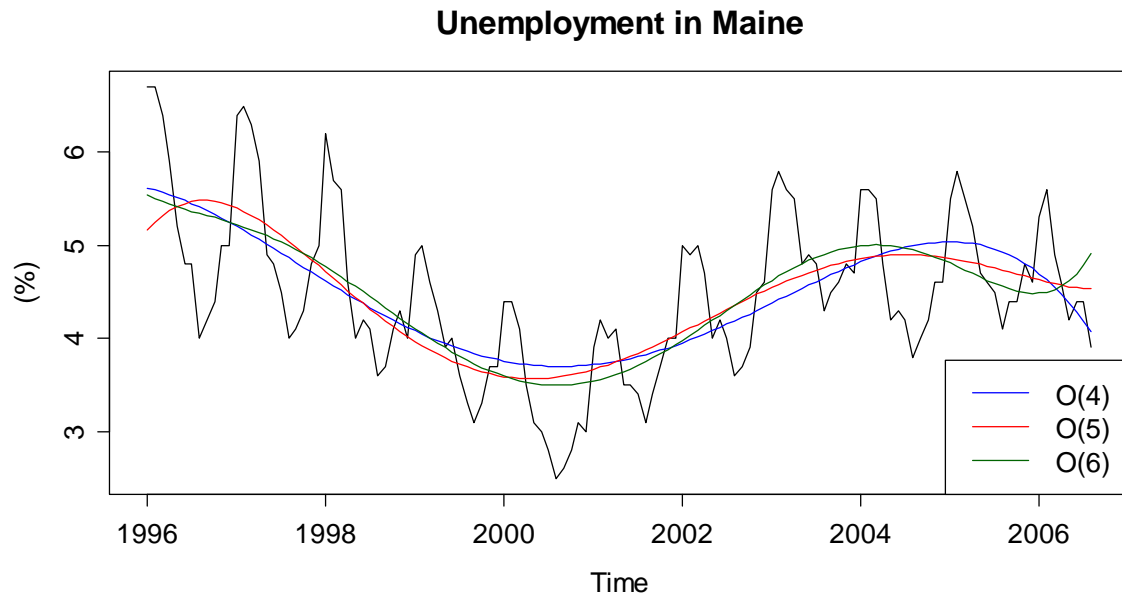
```
> maine <- ts(dat, start=c(1996,1), freq=12)
> tr      <- as.numeric(time(maine))
> tc      <- tr-mean(tr)
> mm      <- rep(c("Jan", "Feb", "Mar", "Apr", "May", "Jun",
                  "Jul", "Aug", "Sep", "Oct", "Nov", "Dec"))
> mm      <- factor(rep(mm,11),levels=mm)[1:128]
```

We can then obtain an OLS-fit of the decomposition model with `R`'s `lm()` procedure, as shown below. The `I()` notation in the formula assures that the `"^"` are interpreted as arithmetical operators, i.e. powers of the predictor, rather than as formula operators. Thereafter, we can use the estimated coefficients for determining the trend estimate `t.est.04`. Because the seasonal factor uses the month of January as a reference, and thus generally has a mean different from zero, we need to shift the trend to make run through "the middle of the data".

```
> fit04    <- lm(maine~tc+I(tc^2)+I(tc^3)+I(tc^4)+mm)
> cf       <- coef(fit04)
> t.est.04 <- cf[1]+cf[2]*tc+cf[3]*tc^2+cf[4]*tc^3+cf[5]*tc^4
> t04.adj  <- t.est.04-mean(t.est.04)+mean(maine)
```

```
> plot(maine, ylab="(%)", main="Unemployment in Maine")
> lines(tr, t.04.adj)
```

The time series plot below is enhanced with polynomial trend lines of order 4 (blue), 5 (red) and 6 (green). From this visualization, it is hard to decide which of the polynomials is most appropriate as a trend estimate. Because there are some boundary effects for orders 5 and 6, we might guess that their additional flexibility is not required. As we will see below, this is treacherous.

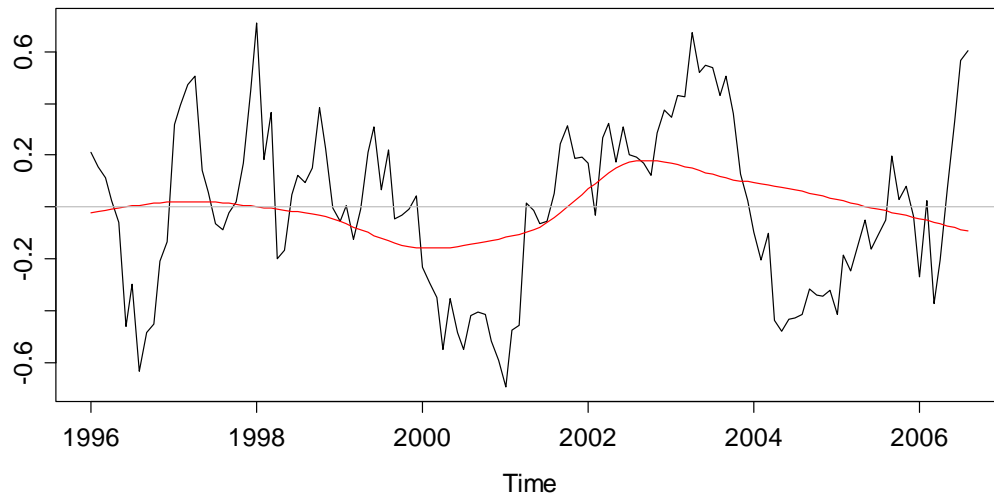
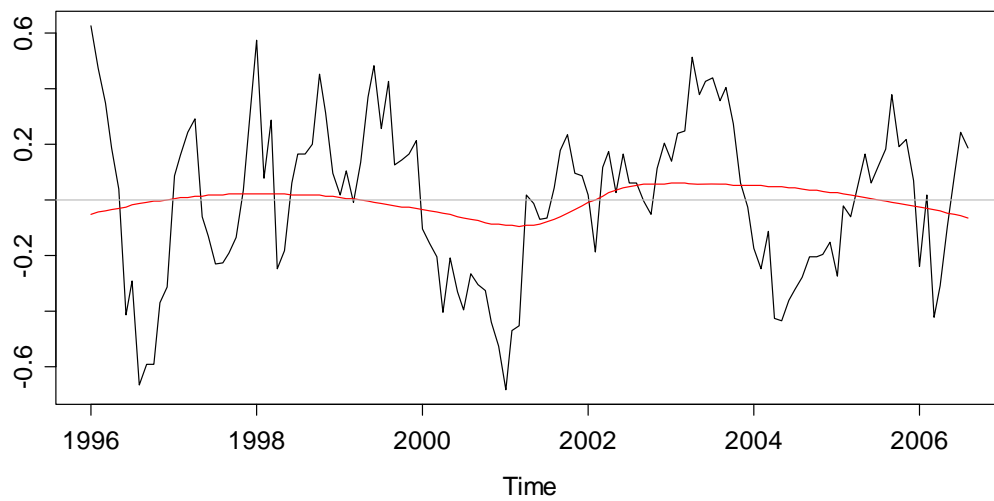
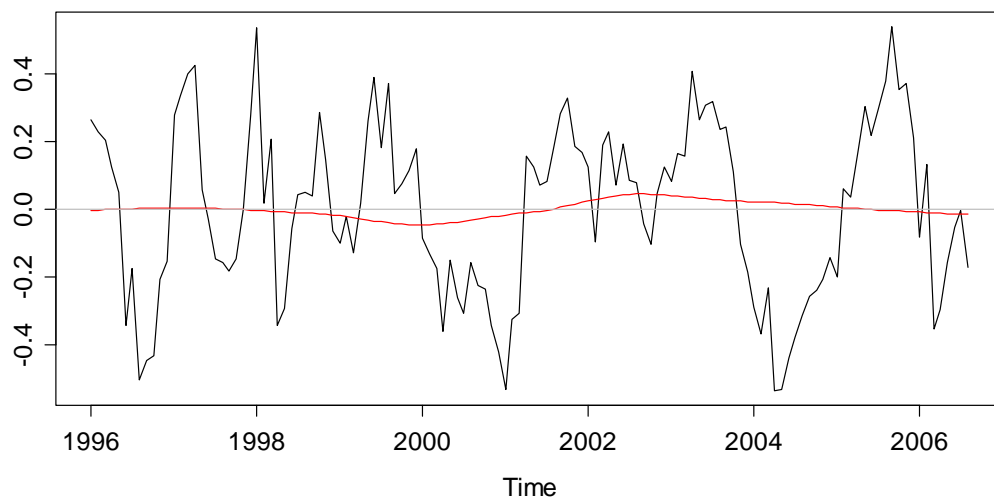


A better way for judging the fit of a parametric model is by residual analysis. We plot the remainder term  $\hat{E}_t$  versus time and add a LOESS smoother. The following bit of code shows this for the grade 4 polynomial.

```
> re.est <- maine-fitted(fit04)
> plot(re.est, ylab="", main="Residuals vs. Time, O(4)")
> fit <- loess(re.est~tr)
> lines(tr, fitted(fit), col="red")
> abline(h=0, col="grey")
```

We repeat the procedure for polynomial orders 5 and 6 and display all results on the next page. In the top plot, the remainder term still features a slight trend, owing to a too low polynomial grade. The middle panel looks better, but there is another clear improvement with order 6, which is the best choice for this series. It is also striking that the remainder is not an i.i.d. series, the serial correlation is clearly standing out. Its estimation and visualization will be discussed in the next section. We conclude this chapter on parametric modeling by issuing a warning: while the explicit form of the trend can be useful, it shall never be interpreted as causal for the evolvement of the series. Also, much care needs to be taken if forecasting is the goal. Extrapolating high-order polynomials beyond the range of observed times can yield very poor results. We will discuss some simple methods for trend extrapolation later in section 8 about forecasting.



**Residuals vs. Time, O(4)****Residuals vs. Time, O(5)****Residuals vs. Time, O(6)**

## 4.4 Autocorrelation

An important feature of time series is their (potential) serial correlation. This section aims at analyzing and visualizing these correlations. We first display the autocorrelation between two random variables  $X_{t+k}$  and  $X_t$ , which is defined as:

$$\text{Cor}(X_{t+k}, X_t) = \frac{\text{Cov}(X_{t+k}, X_t)}{\sqrt{\text{Var}(X_{t+k})\text{Var}(X_t)}}$$

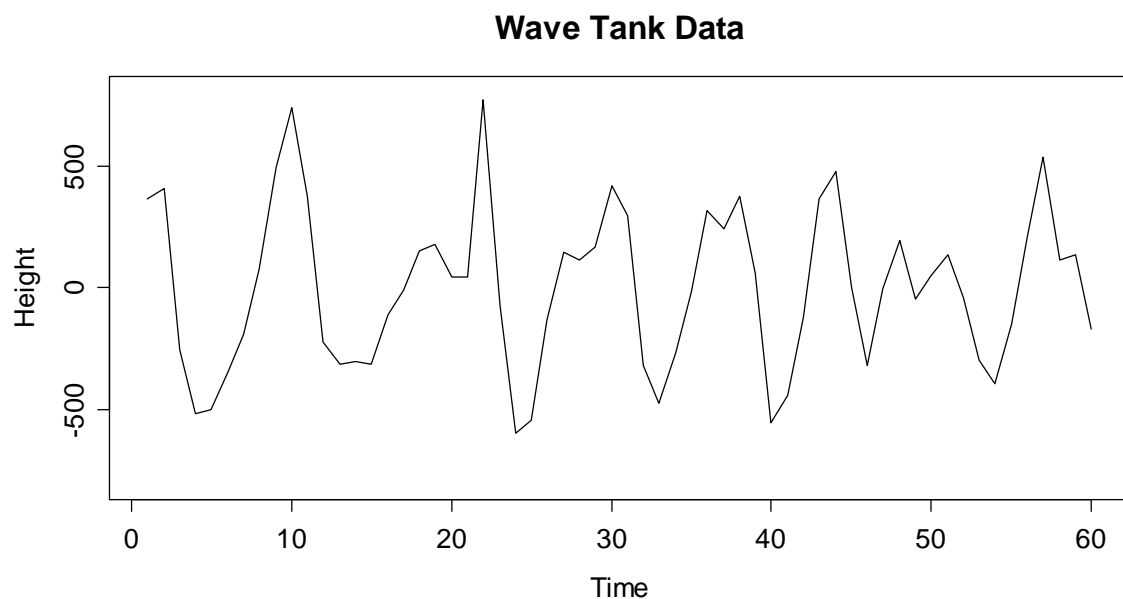
This is a dimensionless measure for the linear association between the two random variables. Since for stationary series, we require the moments to be non-changing over time, we can drop the index  $t$  for these, and write the autocorrelation as a function of the lag  $k$ :

$$\rho(k) = \text{Cor}(X_{t+k}, X_t)$$

The goals in the forthcoming sections are estimating these autocorrelations from observed time series data, and to study the estimates' properties. The latter will prove useful whenever we try to interpret sample autocorrelations in practice.

The example we consider in this chapter is the wave tank data. The values are wave heights in millimeters relative to still water level measured at the center of the tank. The sampling interval is 0.1 seconds and there are 396 observations. For better visualization, we here display the first 60 observations only:

```
> www <- "http://staff.elena.aut.ac.nz/Paul-Cowpewartwait/ts/"
> dat <- read.table(paste(www, "wave.dat", sep=" ", header=T))
> wave <- ts(dat$waveht)
> plot(window(wave, 1, 60), ylim=c(-800,800), ylab="Height")
> title("Wave Tank Data")
```

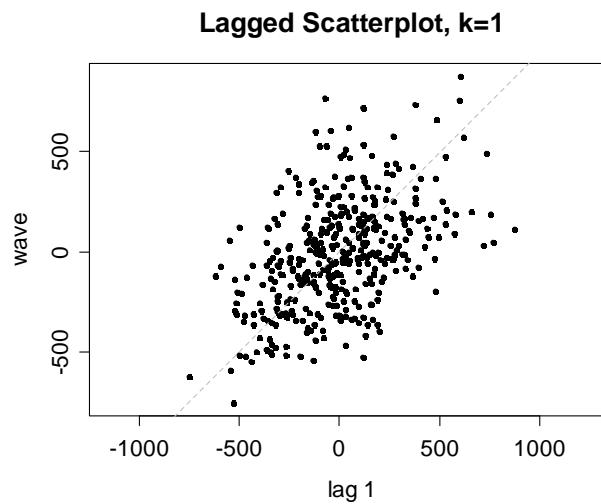


These data show some pronounced cyclic behavior. This does not come as a surprise, as we all know from personal experience that waves do appear in cycles. The series shows some very clear serial dependence, because the current value is quite closely linked to the previous and following ones. But very clearly, it is also a stationary series.

### 4.4.1 Lagged Scatterplot

An appealing idea for analyzing the correlation among consecutive observations in the above series is to produce a scatterplot of  $(x_t, x_{t+1})$  for all  $t = 1, \dots, n-1$ . There is a designated function `lag.plot()` in **R**. The result is as follows:

```
> lag.plot(wave, do.lines=FALSE, pch=20)
> title("Lagged Scatterplot, k=1")
```



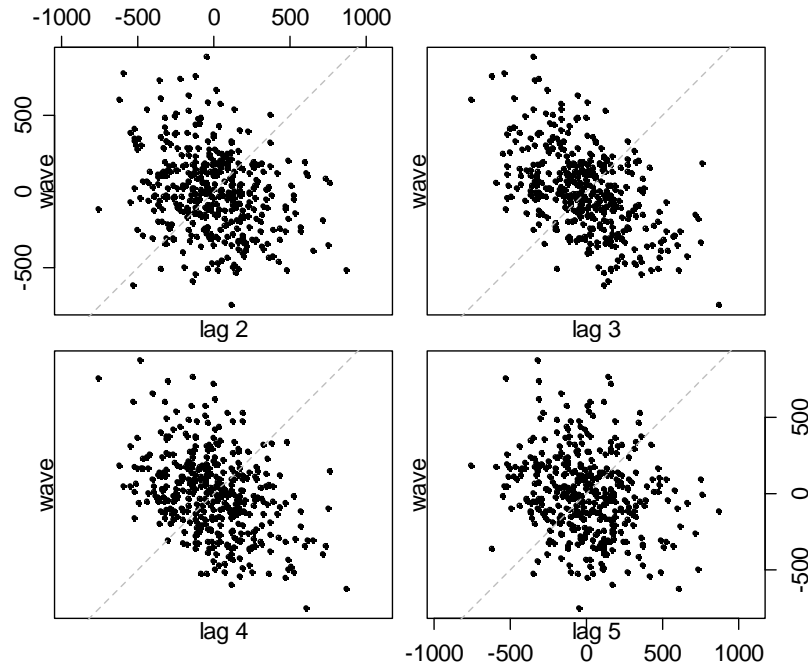
The association seems linear and is positive. The Pearson correlation coefficient turns out to be 0.47, thus moderately strong. How to interpret this value from a practical viewpoint? Well, the square of the correlation coefficient,  $0.47^2 = 0.22$ , is the percentage of variability explained by the linear association between  $x_t$  and its respective predecessor. Here in this case,  $x_{t-1}$  explains roughly 22% of the variability observed in  $x_t$ .

We can of course extend the very same idea to higher lags. We here analyze the lagged scatterplot correlations for lags  $k = 2, \dots, 5$ , see below. When computed, the estimated Pearson correlations turn out to be -0.27, -0.50, -0.39 and -0.22, respectively. The formula for computing them is:

$$\tilde{\rho}(k) = \frac{\sum_{s=1}^{n-k} (x_{s+k} - \bar{x}_{(k)})(x_s - \bar{x}_{(1)})}{\sqrt{\sum_{s=k+1}^n (x_s - \bar{x}_{(k)})^2 \cdot \sum_{t=1}^{n-k} (x_t - \bar{x}_{(1)})^2}} \quad \text{for } k = 1, \dots, n-2,$$

$$\text{where } \bar{x}_{(1)} = \frac{1}{n-k} \sum_{i=1}^{n-k} x_i \text{ and } \bar{x}_{(k)} = \frac{1}{n-k} \sum_{i=k+1}^n x_i$$

It is important to notice that while there are  $n-1$  data pairs for computing  $\tilde{\rho}(1)$ , there are only  $n-2$  for  $\tilde{\rho}(2)$ , and then less and less, i.e.  $n-k$  pairs for  $\tilde{\rho}(k)$ . Thus for the last autocorrelation coefficient which can be estimated,  $\tilde{\rho}(n-2)$ , there is only one single data pair which is left. Of course, they can always be interconnected by a straight line, and the correlation in this case is always  $\pm 1$ . Of course, this is an estimation snag, rather than perfect linear association for the two random variables.



Intuitively, it is clear that because there are less and less data pairs at higher lags, the respective estimated correlations are less and less precise. Indeed, by digging deeper in mathematical statistics, one can prove that the variance of  $\tilde{\rho}(k)$  increases with  $k$ . This is undesired, as it will lead to instable results and spurious effects. The remedy is discussed in the next section.

#### 4.4.2 Plug-In Estimation

For mitigating the above mentioned problem with the lagged scatterplot method, autocorrelation estimation is commonly done using the so-called plug-in approach, using estimated autocovariances as the basis. The formula is as follows:

$$\hat{\rho}(k) = \frac{\hat{\gamma}(k)}{\hat{\gamma}(0)}, \text{ for } k = 1, \dots, n-1,$$

$$\text{where } \hat{\gamma}(k) = \frac{1}{n} \sum_{s=1}^{n-k} (x_{s+k} - \bar{x})(x_s - \bar{x}), \text{ with } \bar{x} = \frac{1}{n} \sum_{t=1}^n x_t.$$

Note that here,  $n$  is used as a denominator irrespective of the lag and thus the number of summands. This has the consequence that  $\hat{\gamma}(0)$  is not an unbiased estimator for  $\gamma(0) = \sigma_x^2$ , but as explained above, there are good reasons to do so. When plugging in the above terms, the estimate for the  $k$ th autocorrelation coefficient turns out to be:

$$\hat{\rho}(k) = \frac{\sum_{s=1}^{n-k} (x_{s+k} - \bar{x})(x_s - \bar{x})}{\sum_{t=1}^n (x_t - \bar{x})^2}, \text{ for } k = 1, \dots, n-1.$$

It is straightforward to compute these in **R**, function `acf()` does the job, and we below do so for the wave tank data. As for the moment, we are interested in the numerical results, we set argument `plot=FALSE`. However, as we will see below, it is usually better to visualize the estimated autocorrelation coefficients graphically, as it will be explained below in section 4.4.3. Also note that **R** by default does not return all autocorrelations which are estimable in this series with 396 observations, but only the first 25.

```
> acf(wave, plot=FALSE)
```

Autocorrelations of series 'wave', by lag

0	1	2	3	4	5	6	7
1.000	0.470	-0.263	-0.499	-0.379	-0.215	-0.038	0.178
8	9	10	11	12	13	14	15
0.269	0.130	-0.074	-0.079	0.029	0.070	0.063	-0.010
16	17	18	19	20	21	22	23
-0.102	-0.125	-0.109	-0.048	0.077	0.165	0.124	0.049
24	25						
-0.005	-0.066						

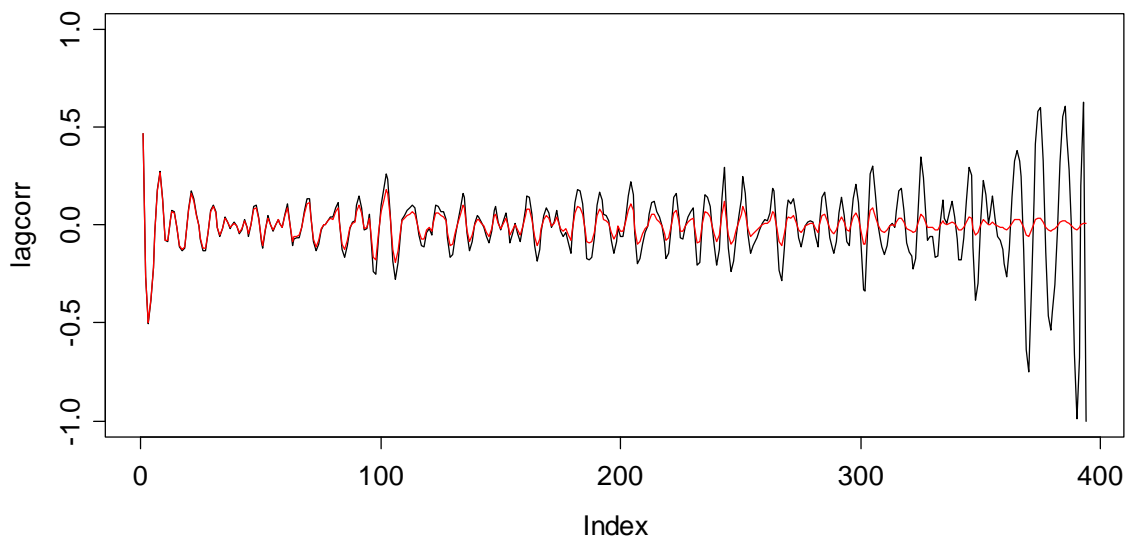
Next, we compare the autocorrelations from lagged scatterplot estimation vs. the ones from the plug-in approach. These are displayed on the next page. While for the first 50 lags, there is not much of a difference, the plug-in estimates are much more damped for higher lags. As claimed above, the lagged scatterplot estimate shows a value of  $-1$  for lag 394, and some generally very erratic behavior in the few lags before.

We can “prove”, or rather, provide evidence that this is an estimation artifact only if we restrict the series to the first 60 observations and then repeat the estimation of autocorrelations. Again, for the highest few lags which are estimable, the lagged scatterplot approach shows erratic behavior – and this was not present at the same lags, when the series was still longer. We do not observe this kind of effect with the plug-in based autocorrelations, thus this is clearly the method of choice.

We finish this chapter by repeating that the bigger the lag, the fewer data pairs remain for estimating the autocorrelation coefficient. We discourage of the use of the lagged scatterplot approach. While the preferred plug-in approach is biased

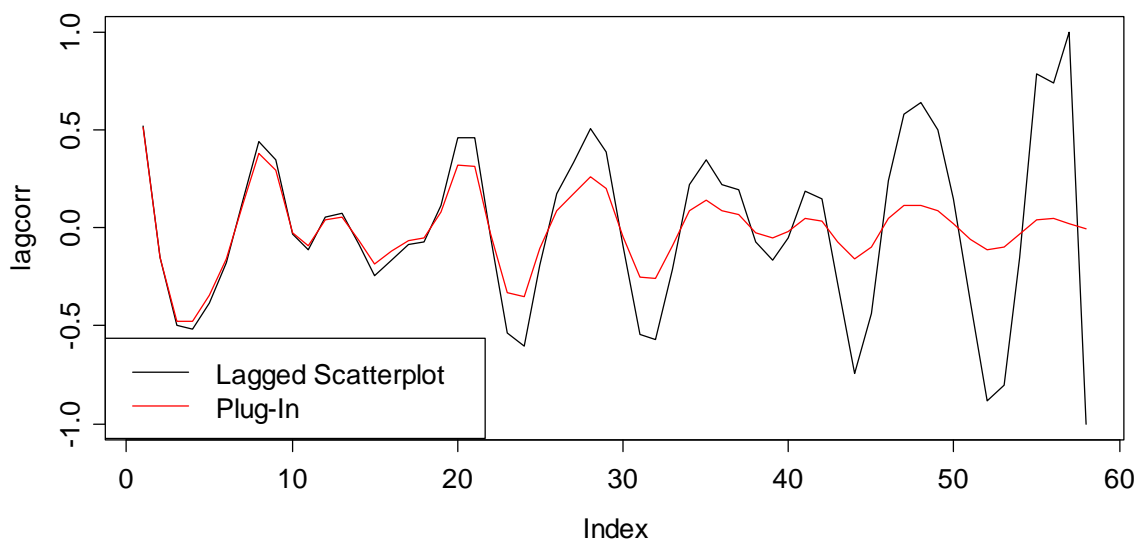
due to the built-in damping mechanism, i.e. the estimates for high lags are shrunk towards zero; it can be shown that it has lower mean squared error. This is because it produces results with much less (random) variability. It can also be shown that the plug-in estimates are consistent, i.e. the bias disappears asymptotically.

**ACF Estimation: Lagged Scatterplot vs. Plug-In**



Nevertheless, all our findings still suggest that it is a good idea to consider only a first portion of the estimated autocorrelations. A rule of the thumb suggests that  $10 \cdot \log_{10}(n)$  is a good threshold. For a series with 100 observations, the threshold becomes lag 20. A second rule operates with  $n/4$  as the maximum lag to which the autocorrelations are shown.

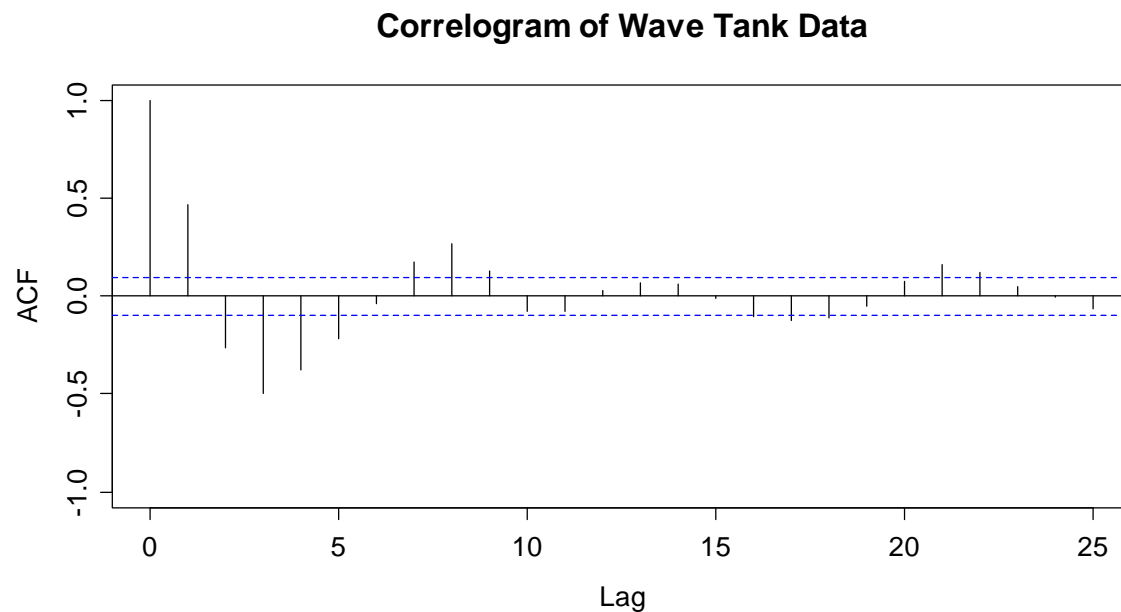
**ACF Estimation: Lagged Scatterplot vs. Plug-In**



### 4.4.3 Correlogram

Now, we know how to estimate the autocorrelation function (ACF) for any lag  $k$ . Here, we introduce the *correlogram*, the standard means of visualization for the ACF. We will then also study the properties of the ACF estimator. We employ `R` and obtain:

```
> acf(wave, ylim=c(-1,1))
```



It has become a widely accepted standard to use vertical spikes for displaying the estimated autocorrelations. Also note that the ACF starts with lag 0, at which it always takes the value 1. For better judgment, we also recommend setting the  $y$ -range to the interval  $[-1,1]$ . Apart from these technicalities, the ACF reflects the properties of the series. We also observe a cyclic behavior with a period of 8, as it is apparent in the time series plot of the original data. Moreover, the absolute value of the correlations attenuates with increasing lag. Next, we will discuss the interpretation of the correlogram.

#### Confidence Bands

It is obvious that even for an iid series without any serial correlation, and thus  $\rho(k) = 0$  for all  $k$ , the estimated autocorrelations  $\hat{\rho}(k)$  will generally not be zero. Hopefully, they will be close, but the question is how close. An answer is indicated by the confidence bands, i.e. the blue dashed lines in the plot above.

These so-called confidence bands are obtained from an asymptotic result: for long iid time series it can be shown that the  $\hat{\rho}(k)$  approximately follow a  $N(0,1/n)$  distribution. Thus, each  $\rho(k)$  lies within the interval of  $\pm 1.96/\sqrt{n}$  with a probability of approximately 95%. This leads us to the following statement that facilitates interpretation of the correlogram: “for any stationary time series, sample autocorrelation coefficients  $\hat{\rho}(k)$  that fall within the confidence band  $\pm 2/\sqrt{n}$  are

*considered to be different from 0 only by chance, while those outside the confidence band are considered to be truly different from 0 .”*

On the other hand, the above statement means that even for iid series, we expect 5% of the estimated ACF coefficients to exceed the confidence bounds; these correspond to type 1 errors. Please note again that the indicated bounds are asymptotic and derived from iid series. The properties of serially dependent series are much harder to derive.

### Ljung-Box Test

The Ljung-Box approach tests the null hypothesis that a number of autocorrelation coefficients are simultaneously equal to zero. Or, more colloquially, it evaluates whether there is any significant autocorrelation in a series. The test statistic is:

$$Q(h) = n \cdot (n+2) \cdot \sum_{k=1}^h \frac{\hat{\rho}_k^2}{n-k}$$

Here,  $n$  is the length of the time series,  $\hat{\rho}_k$  are the sample autocorrelation coefficients at lag  $k$  and  $h$  is the lag up to which the test is performed. It is typical to use  $h=1, 3, 5, 10$  or  $20$ . The test statistic asymptotically follows a  $\chi^2$  distribution with  $h$  degrees of freedom. As an example, we compute the test statistic and the respective p-value for the wave tank data with  $h=10$ .

```
> nn <- length(wave)
> qq <- nn*(nn+2)*sum((acf(wave)$acf[2:11]^2)/(nn-(1:10)))
> qq
[1] 344.0155
> 1-pchisq(qq, 10)
[1] 0
```

We observe that  $Q(10)=344.0155$  which is far in excess of what we would expect by chance on independent data. The critical value, i.e. the 95%-quantile of the  $\chi^2_{10}$  is at 18.3 and thus, the p-value is close to (but not exactly) zero. There is also a dedicated R function which can be used to perform Ljung-Box testing:

```
> Box.test(wave, lag=10, type="Ljung-Box")
```

```
Box-Ljung test
```

```
data: wave
```

```
X-squared = 344.0155, df = 10, p-value < 2.2e-16
```

The result is, of course, identical. Please be aware that the test is sometimes also referred to as Box-Ljung test. Also R is not very consistent in its nomenclature. However, the two are one and the same. Moreover, with a bit of experience the results of the Ljung-Box test can usually be guessed quite well from the correlogram by eyeballing.

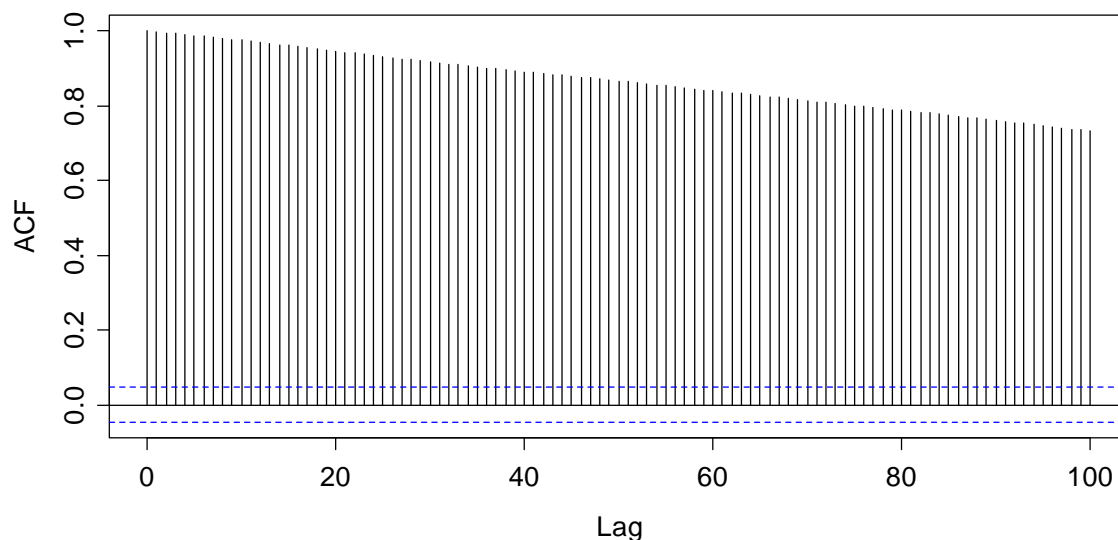


### ACF of Non-Stationary Series

Estimation of the ACF from an observed time series assumes that the underlying process is stationary. Only then we can treat pairs of observations at lag  $k$  as being probabilistically “equal” and compute sample covariance coefficients. Hence, while stationarity is at the root of ACF estimation, we can of course still apply the formulae given above to non-stationary series. The ACF then usually exhibits some typical patterns. This can serve as a second check for non-stationarity, i.e. helps to identify it, should it have gone unnoticed in the time series plot. We start by showing the correlogram for the SMI daily closing values from section 1.2.4. This series does not have seasonality, but a very clear trend.

```
> acf(smi, lag.max=100)
```

**Correlogram of SMI Daily Closing Values**



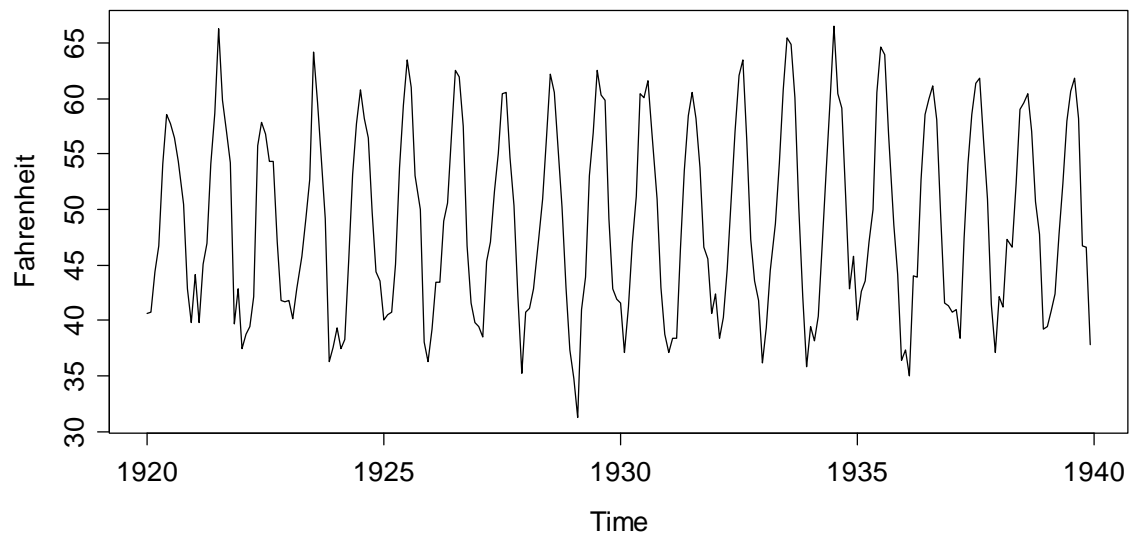
We observe that the ACF decays very slowly. The reason is that if a time series features a trend, the observations at consecutive observations will usually be on the same side of the series' global mean  $\bar{x}$ . This is why that for small to moderate lags  $k$ , most of the terms

$$(x_{s+k} - \bar{x})(x_s - \bar{x})$$

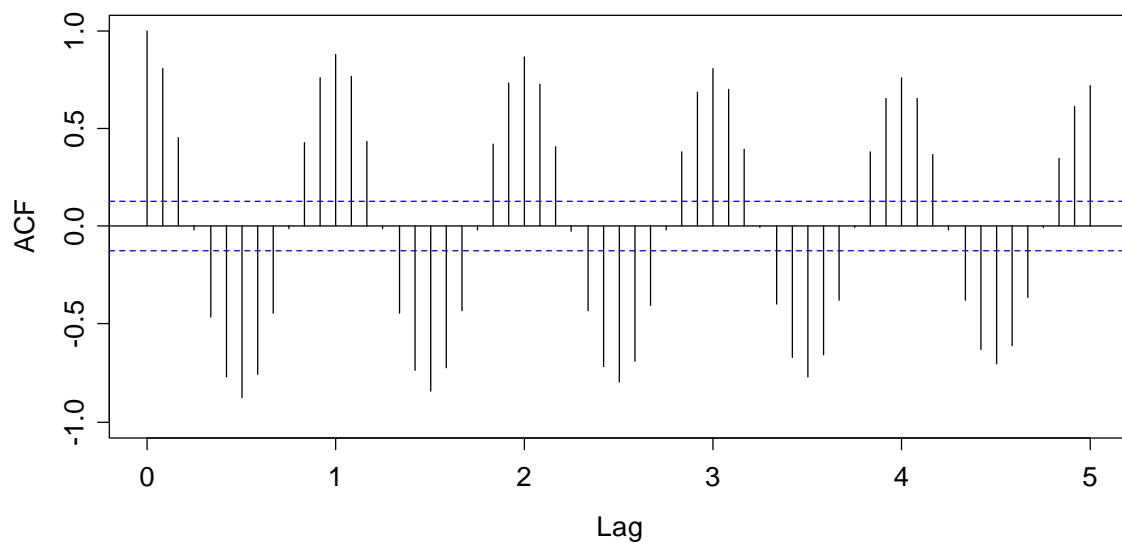
are positive. For this reason, the sample autocorrelation coefficient will be positive as well, and is most often also close to 1. Thus, a very slowly decaying ACF is an indicator for non-stationarity, i.e. a trend which was not removed before autocorrelations were estimated.

Next, we show an example of a series that has no trend, but a strongly recurring seasonal effect. We use **R**'s `data(nottem)`, a time series containing monthly average air temperatures at Nottingham Castle in England from 1920-1939. Time series plot and correlogram are as follows:

### Nottingham Monthly Average Temperature Data



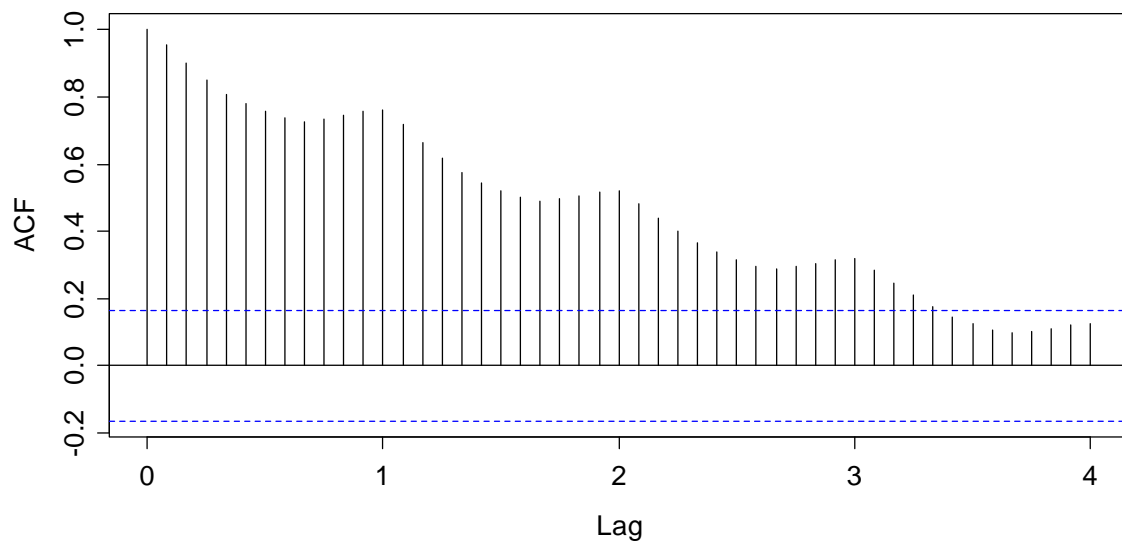
### Correlogram of Nottingham Temperature Data



The ACF is cyclic, and owing to the recurring seasonality, the envelope again decays very slowly. Also note that for periodic series,  $\mathbb{R}$  has periods rather than lags on the x-axis – often a matter of confusion. We conclude that a hardly, or very slowly decaying periodicity in the correlogram is an indication of a seasonal effect which was forgotten to be removed. Finally, we also show the correlogram for the logged air passenger bookings. This series exhibits both an increasing trend and a seasonal effect. The result is as follows:

```
> data(AirPassengers)
> txt <- "Correlogram of Logged Air Passenger Bookings"
> acf(log(AirPassengers), lag.max=48, main=txt)
```

### Correlogram of Logged Air Passenger Bookings

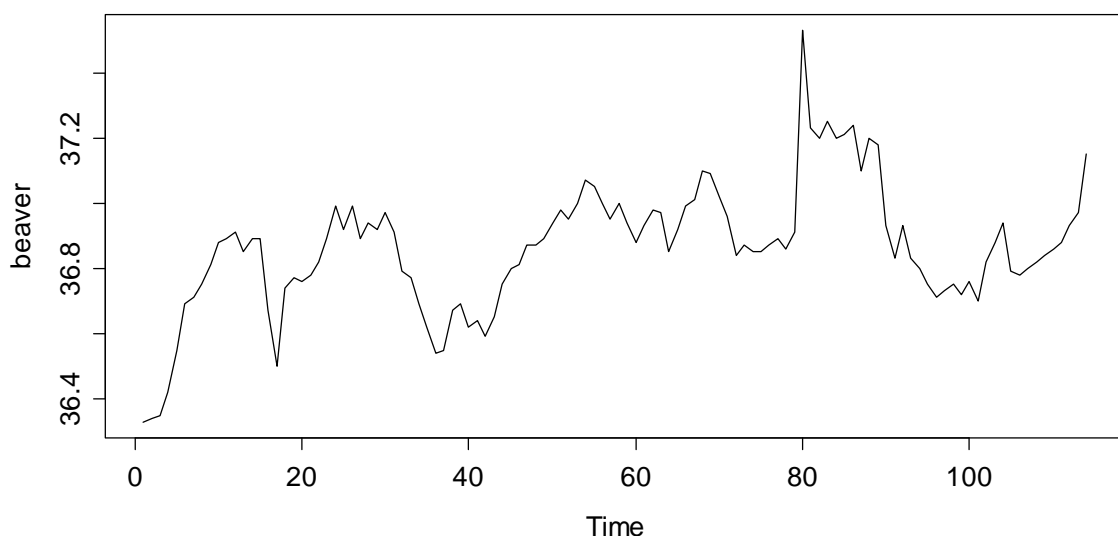


Here, the two effects described above are interspersed. We have a (here dominating) slow decay in the general level of the ACF, plus some periodicity. Again, this is an indication for a non-stationary series. It needs to be decomposed, before the serial correlation in the stationary remainder term can be studied.

### The ACF and Outliers

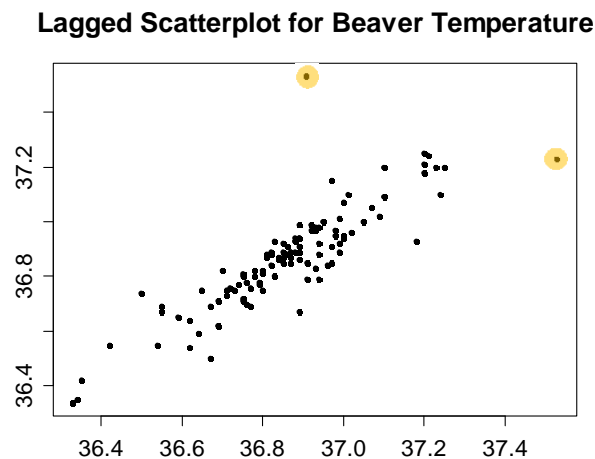
If a time series has an outlier, it will appear twice in any lagged scatterplot, and will thus potentially have “double” negative influence on the  $\hat{\rho}(k)$ . As an example, we consider variable `temp` from data frame `beaver1`, which can be found in `R`’s `data(beavers)`. This is the body temperature of a female beaver, measured by telemetry in 10 minute intervals. We first visualize the data with a time series plot.

### Beaver Body Temperature Data

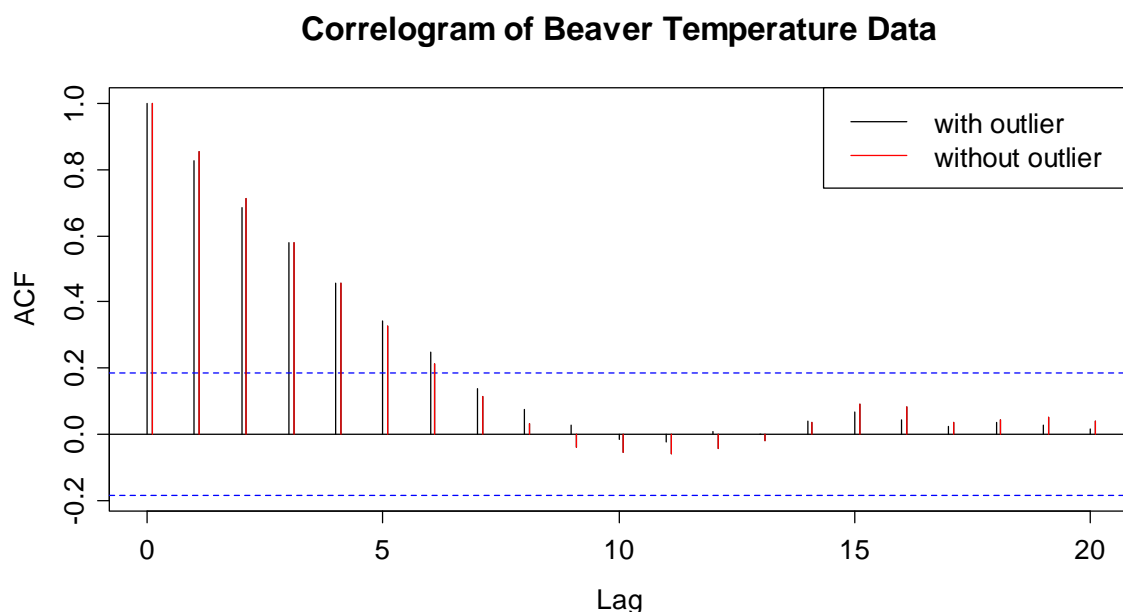


Observation 80 is a moderate, but distinct outlier. It is unclear to the author whether this actually is an error, or whether the reported value is correct. But because the purpose of this section is showing the potential influence of erroneous values, that is not important. Neither the Pearson correlation coefficient, nor the plug-in autocorrelation estimator is robust, thus the appearance of the correlogram can be altered quite strongly due to the presence of just one single outlier.

```
> plot(beaver[1:113], beaver[2:114], pch=20,)  
> title("Lagged Scatterplot for Beaver Temperature")
```



The two data points where the outlier is involved are highlighted. The Pearson correlation coefficients with and without these two observations are 0.86 and 0.91. Depending on the outliers severity, the difference can be much bigger. The next plot shows the entire correlogram for the beaver data, computed with (black) and without (red) the outlier. Also here, the difference may seem small and rather academic, but it could easily be severe if the outlier was just pronounced enough.



The question is, how do we handle missing values in time series? In principle, we cannot just omit them without breaking the time structure. And breaking it means going away from our paradigm of equally spaced points in time. A popular choice is thus replacing the missing value. This can be done with various degrees of sophistication:

- a) replacing the value with the global mean
- b) using a local mean, i.e. +/- 3 observations
- c) model based imputation by forecasting

The best strategy depends upon the case at hand. And in fact, there is a fourth alternative: while R's `acf()` function by default does not allow for missing values, it still offers the option to proceed without imputation. If argument is set as `na.action=na.pass`, the covariances are computed from the complete cases, and the correlogram is shown as usual. However, having missed values in the series has the consequence that the estimates produced may well not be a valid (i.e. positive definite) autocorrelation sequence, and may contain missing values. From a practical viewpoint, these drawbacks can often be neglected, though.

#### 4.4.4 Quality of ACF Estimates

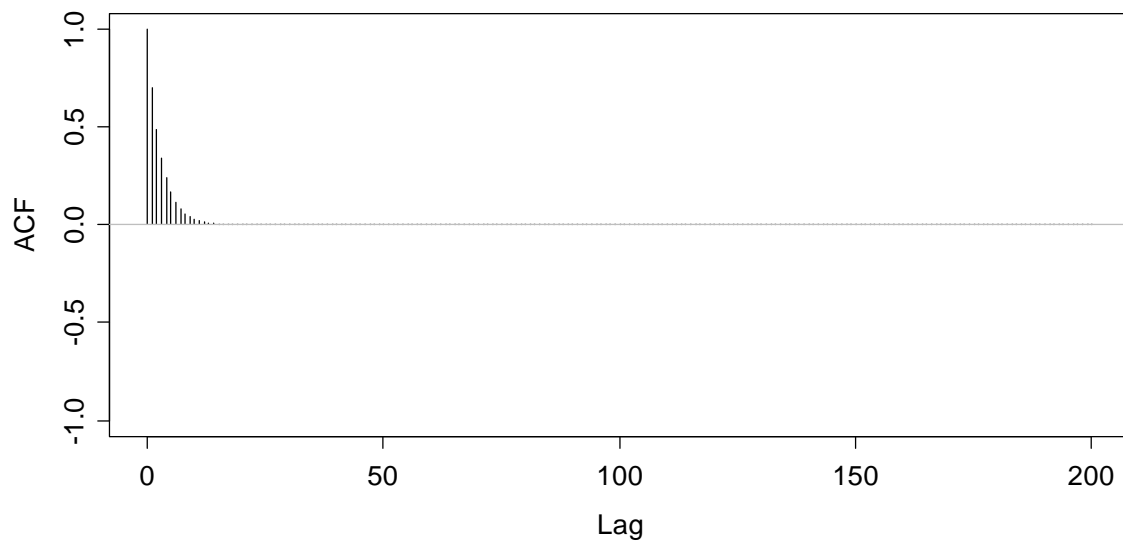
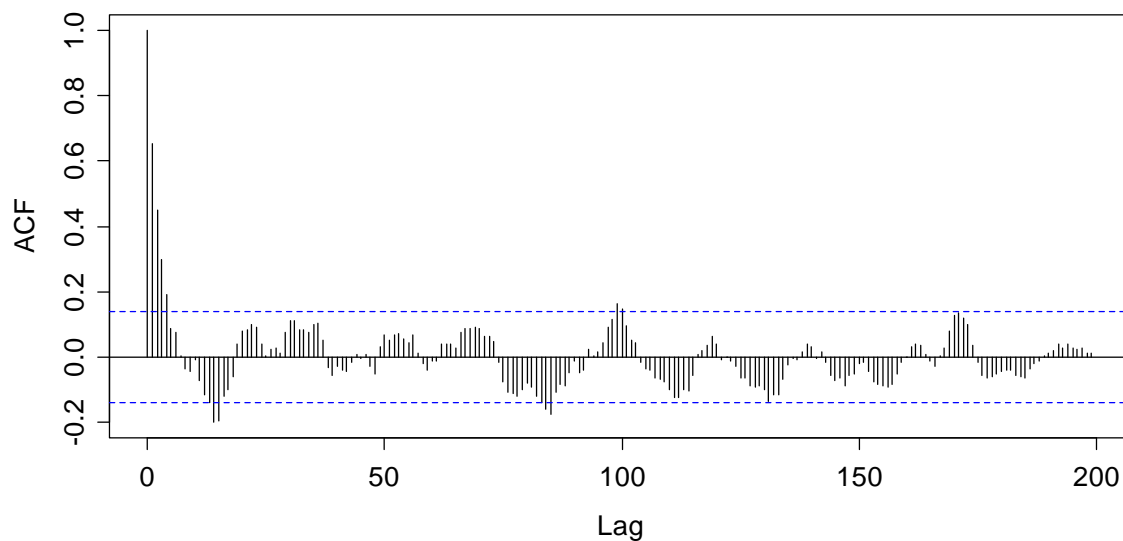
In this section we will deal with the quality of the information that is contained in the correlogram. We will not do this from a very theoretical viewpoint, but rather focus on the practical aspects. We have already learned that the ACF estimates are generally biased, i.e. shrunk towards zero for higher lags. This means that it is better to cut off the correlogram at a certain lag. Furthermore, non-stationarities in the series can hamper the interpretation of the correlogram and we have also seen that outliers can have a quite strong impact. But there are even more aspects in ACF estimation that are problematic...

##### The Compensation Issue

One can show that the sum of all autocorrelations which can be estimated from a time series realization, the sum over all  $\hat{\rho}(k)$  for lags  $k = 1, \dots, n-1$ , adds up to  $-1/2$ . Or, written as a formula:

$$\sum_{k=1}^{n-1} \hat{\rho}(k) = -\frac{1}{2}$$

We omit the proof here. It is clear that the above condition will lead to quite severe artifacts, especially when a time series process has only positive correlations. We here show both the true, theoretical ACF of an  $AR(1)$  process with  $\alpha_1 = 0.7$ , which, as we will see in section 5, has  $\rho(k) > 0$  for all  $k$ , and the sample correlogram for a realization of that process with a length 200 observations.

**True ACF of an AR(1) Process with  $\alpha=0.7$** **Correlogram for a Realization from an AR(1) Process**

The respective R-commands for producing these plots are as follows:

```
## True ACF
true.acf <- ARMAacf(ar=0.7, lag.max=200)
plot(0:200, true.acf, type="h", xlab="Lag", ylim=c(-1,1))
title("True ACF of an AR(1) Process with alpha=0.7")
abline(h=0, col="grey")

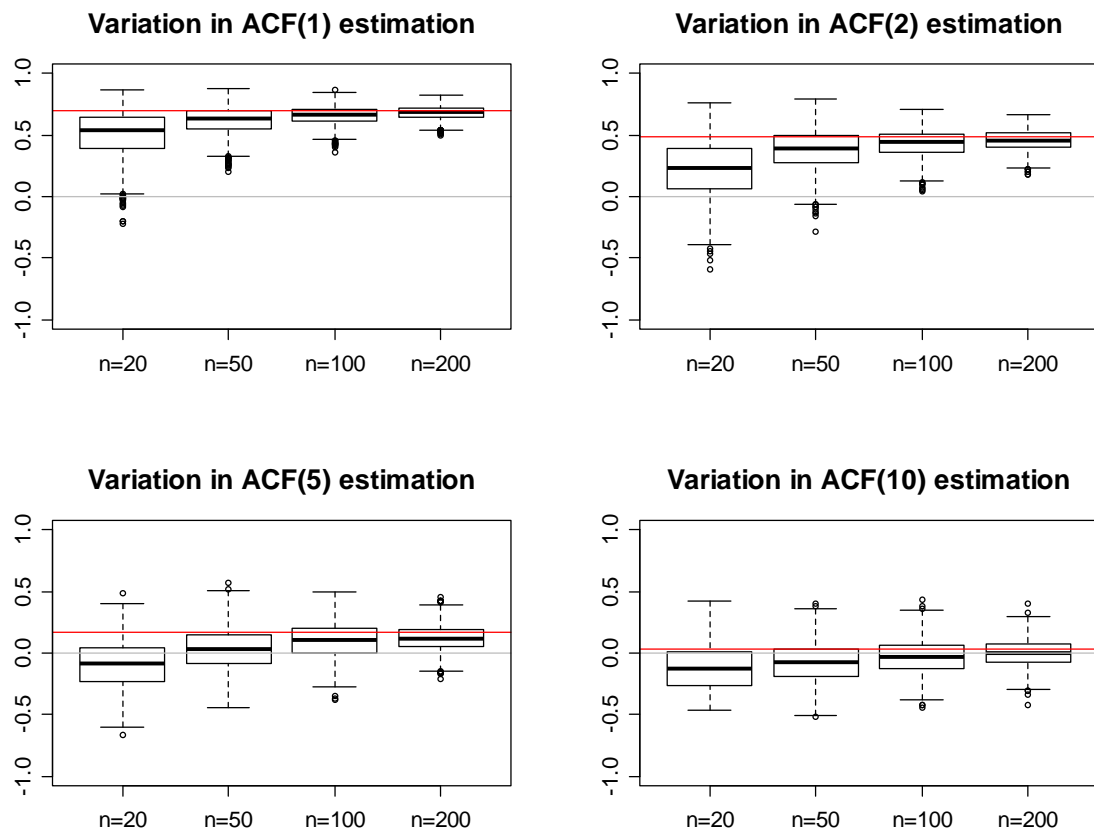
## Simulation and Generating the ACF
set.seed(25)
ts.simul <- arima.sim(list(ar=0.7), 200)
acf(ts.simul, lag=200, main="Correlogram ...")
```

What we observe is quite striking: only for the very first few lags, the sample ACF does match with its theoretical counterpart. As soon as we are beyond lag  $k = 6$ , the sample ACF turns negative. This is an artifact, because the sum of the estimated autocorrelations coefficients needs to add up to  $-1/2$ . Some of these spurious, negative correlation estimates are so big that they even exceed the confidence bounds – an observation that has to be well kept in mind if one analyzes and tries to interpret the correlogram.

### Simulation Study

Last but not least, we will run a small simulation study that visualizes bias and variance in the sample autocorrelation coefficients. We will again base this on the simple  $AR(1)$  process with coefficient  $\alpha_1 = 0.7$ . For further discussion of the process' properties, we refer to section 5. There, it will turn out that the  $k^{th}$  autocorrelation coefficient of such a process takes the value  $(0.7)^k$ , as visualized on the previous page.

For understanding the variability in  $\hat{\rho}(1)$ ,  $\hat{\rho}(2)$ ,  $\hat{\rho}(5)$  and  $\hat{\rho}(10)$ , we simulate from the aforementioned  $AR(1)$  process. We generate series of length  $n = 20$ ,  $n = 50$ ,  $n = 100$  and  $n = 200$ . We then obtain the correlogram, record the estimated autocorrelation coefficients and repeat this process 1000 times. This serves as a basis for displaying the variability in  $\hat{\rho}(1)$ ,  $\hat{\rho}(2)$ ,  $\hat{\rho}(5)$  and  $\hat{\rho}(10)$  with boxplots. They can be found below.



We observe that for “short” series with less than 100 observations, estimating the ACF is difficult: the  $\hat{\rho}(k)$  are strongly biased, and there is huge variability. Only for longer series, the consistency of the estimator “kicks in”, and yields estimates which are reasonably precise. For lag  $k = 10$ , on the other hand, we observe less bias, but the variability in the estimate remains large, even for “long” series.

We conclude this situation by summarizing: by now, we have provided quite a bit of evidence that the correlogram can be tricky to interpret at best, sometimes even misleading, or plain wrong. However, it is the best means we have for understanding the dependency in a time series. And we will base many if not most of our decisions in the modeling process on the correlogram. However, please be aware of the bias and the estimation variability there is.

## 4.5 Partial Autocorrelation

For the above  $AR(1)$  process, with its strong positive correlation at lag 1, it is somehow “evident” that the autocorrelation for lags 2 and higher will be positive as well – just by propagation: if A is highly correlated to B, and B is highly correlated to C, then A is usually highly correlated to C as well. It would now be very instructive to understand the direct relation between A and C, i.e. exploring what dependency there is in excess to the one associated to B. In a time series context, this is exactly what the partial autocorrelations do. The mathematical definition is the one of a conditional correlation:

$$\pi(k) = \text{Cor}(X_{t+k}, X_t \mid X_{t+1} = x_{t+1}, \dots, X_{t+k-1} = x_{t+k-1})$$

In other words, we can also say that the partial autocorrelation is the association between  $X_t$  and  $X_{t+k}$  with the linear dependence of  $X_{t+1}$  through  $X_{t+k-1}$  removed. Another instructive analogy can be drawn to linear regression. The autocorrelation coefficient  $\rho(k)$  measures the simple dependence between  $X_t$  and  $X_{t+k}$ , whereas the partial autocorrelation  $\pi(k)$  measures the contribution to the multiple dependence, with the involvement of all intermediate instances  $X_{t+1}, \dots, X_{t+k-1}$  as explanatory variables. There is a (theoretical) relation between the partial autocorrelations  $\pi(k)$  and the plain autocorrelations  $\rho(1), \dots, \rho(k)$ , i.e. they can be derived from each other, e.g.:

$$\pi(1) = \rho(1) \text{ and } \pi(2) = (\rho(2) - \rho(1)^2) / (1 - \rho(1)^2)$$

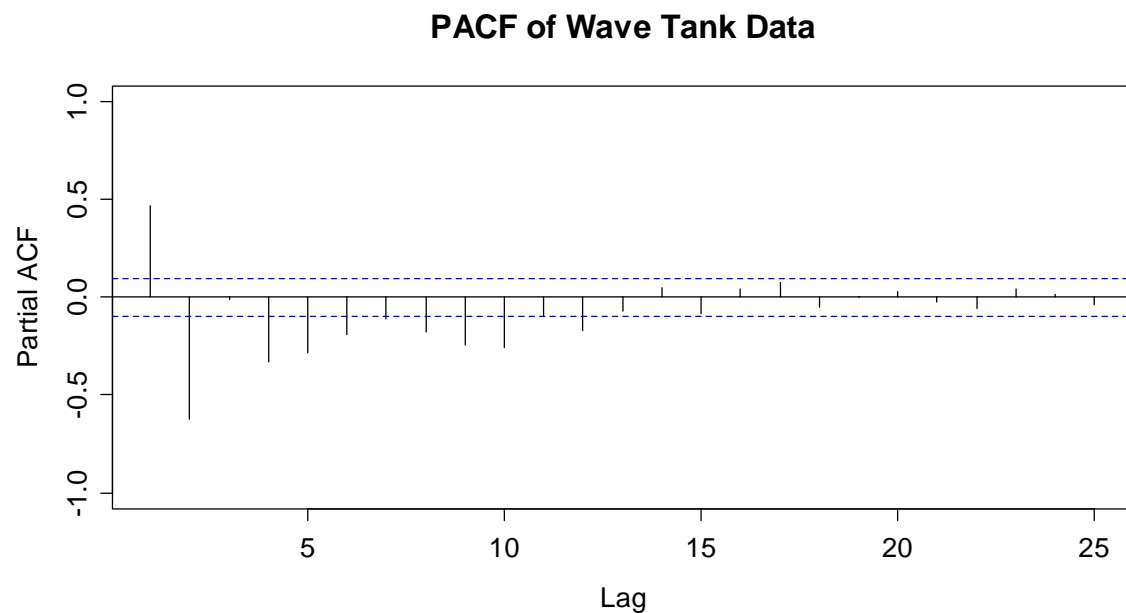
The formula for higher lags  $k$  exists, but get complicated rather quickly, so we do without displaying them. However, another absolutely central property of the partial autocorrelations  $\pi(p)$  is that the  $k^{\text{th}}$  coefficient of the  $AR(p)$  model, denoted as  $\alpha_p$ , is equal to  $\pi(p)$ . While there is an in depth discussion of  $AR(p)$  models in section 5, we here briefly sketch the idea, because it makes the above property seem rather logical. An autoregressive model of order  $p$ , i.e. an  $AR(p)$  is:

$$X_t = \alpha_1 X_{t-1} + \dots + \alpha_p X_{t-p} + E_t,$$



where  $E_t$  is a sequence of iid random variables. Making the above statement concrete, this means that in an  $AR(3)$  process, we have  $\pi(3) = \alpha_3$ , but generally  $\pi(2) \neq \alpha_2$  and  $\pi(1) \neq \alpha_1$ . Moreover, we have  $\pi(k) = 0$  for all  $k > p$ . These properties are used in R for estimating partial autocorrelation coefficients. Estimates  $\hat{\pi}(p)$  are generated by fitting autoregressive models of successively higher orders. The job is done with function `pacf()`: input/output are equal/similar to ACF estimation. In particular, the confidence bounds are also presented for the PACF. We conclude this section by showing the result for the wave tank data.

```
> pacf(wave, ylim=c(-1,1), main="PACF of Wave Tank Data")
```



We observe that  $\hat{\pi}(1) \approx 0.5$  and  $\hat{\pi}(2) \approx -0.6$ . Some further PACF coefficients up to lag 10 seem significantly different from zero, but are smaller. From what we see here, we could try to describe the wave tank data with an  $AR(2)$  model. The next section will explain why.



## 5 Stationary Time Series Models

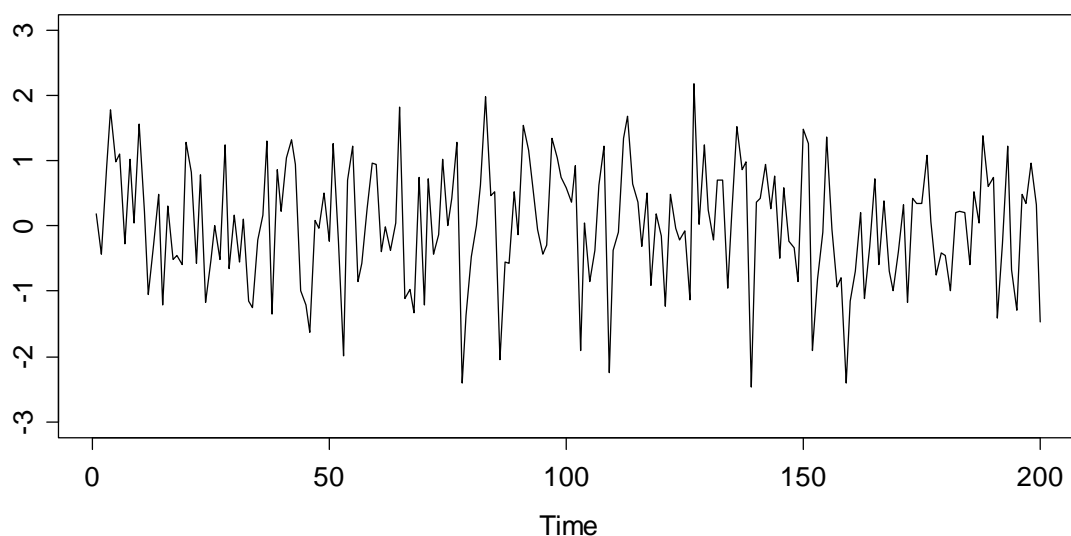
Rather than simply describing observed time series data, we now aim for fitting models. This will prove useful for a deeper understanding of the data, but is especially beneficial when forecasting is the main goal. We here focus on parametric models for stationary time series, namely the broad class of *autoregressive moving average (ARMA) processes* – these have shown great importance in modeling real-world data.

### 5.1 White Noise

As the most basic stochastic process, we introduce discrete White Noise. A time series  $(W_1, W_2, \dots, W_n)$  is called *White Noise* if the random variables  $W_1, W_2, \dots$  are independent and identically distributed with mean zero. This also implies that all random variables  $W_t$  have identical variance, and there are no autocorrelations and partial autocorrelations either:  $\rho(k)=0$  and  $\pi(k)=0$  for all lags  $k$ . If in addition, the variables also follow a Gaussian distribution, i.e.  $W_t \sim N(0, \sigma_w^2)$ , the series is called *Gaussian White Noise*.

Before we show a realization of a White Noise process, we state that the term “White Noise” was coined in an article on heat radiation published in Nature in April 1922. There, it was used to refer to series time series that contained all frequencies in equal proportions, analogous to white light. It is possible to show that iid sequences of random variables do contain all frequencies in equal proportions, and hence, here we are.

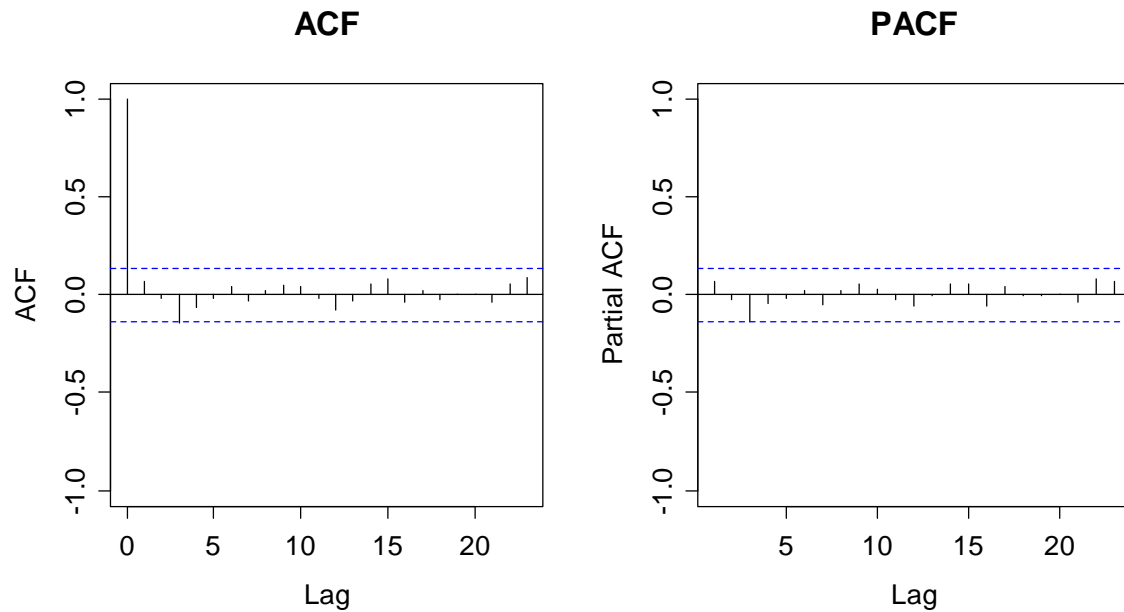
**Gaussian White Noise**



In **R**, it is easy to generate Gaussian White Noise, we just type:

```
> ts(rnorm(200, mean=0, sd=1))
```

Well, by giving more thought on how computers work, i.e. by relying on deterministic algorithms, it may seem implausible that they can really generate independent data. We do not embark into these discussions here, but treat the result of `rnorm()` as being “good enough” for a realization of a White Noise process. Here, we show ACF and PACF of the above series. As expected, there are no (strongly) significant estimates.



White Noise series are important, because they usually arise as residual series when fitting time series models. The correlogram generally provides enough evidence for attributing a series as White Noise, provided the series is of reasonable length – our studies in section 4.4 suggests that 100 or 200 is such a value. Please also note that while there is not much structure in Gaussian White Noise, it still has a parameter. It is the variance  $\sigma_w^2$ .

## 5.2 Estimating the Conditional Mean

Before we present some time series models, it is important to build some understanding of what we are actually doing. All the  $AR(p)$ ,  $MA(q)$  and  $ARMA(p,q)$  models that will be presented below are based on the assumption that the time series can be written as:

$$X_t = \mu_t + E_t.$$

Hereby,  $\mu_t$  is the conditional mean of the series, i.e.  $\mu_t = E[X_t | X_{t-1}, X_{t-2}, \dots]$  and  $E_t$  is a disturbance term. For all models in section 5, the disturbance term is assumed to be a White Noise innovation.

It is very important to notice that while stationary series feature a constant marginal expectation  $\mu$ , the conditional mean  $\mu_t$  is can be and often is non-constant and time-dependent. Or in other words, there is some short-term memory in the series. The  $ARMA(p, q)$  processes that will be discussed here in this section are built on the following notion:

$$\mu_t = f(X_{t-1}, X_{t-2}, \dots, X_{t-p}, E_{t-1}, E_{t-2}, \dots, E_{t-q}).$$

In words, the conditional mean is a function of past instances of the series as well as past innovations. We will see that usually, a selection of the involved terms is made, and that the function  $f(\cdot)$  is linear.

## 5.3 Autoregressive Models

### 5.3.1 Definition and Properties

The most natural formulation of a time series model is a linear regression approach on the past instances, i.e. a regression on the series itself. This coined the term *autoregressive*. In practice, such models prove to be very important; they are the most popular way of describing time series.

#### Model and Terms

An *autoregressive model* of order  $p$ , abbreviated as  $AR(p)$ , is based on a linear combination of past observations according to the following equation:

$$X_t = \alpha_1 X_{t-1} + \alpha_2 X_{t-2} + \dots + \alpha_p X_{t-p} + E_t.$$

Hereby, the disturbance term  $E_t$  comes from a White Noise process, i.e. is iid. Moreover, we require that it is an *innovation*, i.e. that it is stochastically independent of  $X_{t-1}, X_{t-2}, \dots$ . The term innovation is illustrative, because (under suitable conditions), it has the power to drive the series into a new direction, meaning that it is strong enough so that it can overplay the dependence of the series from its own past. An alternative notation for  $AR(p)$  models is possible with the backshift operator:

$$(1 - \alpha_1 B - \alpha_2 B^2 - \dots - \alpha_p B^p) X_t = E_t, \text{ or short } \Phi(B) X_t = E_t$$

Hereby,  $\Phi(B)$  is called the *characteristic polynomial*. It determines all the relevant properties of the process. The most important questions that we will deal with in this chapter are of course the choice of the order  $p$  and the estimation of the coefficients  $\alpha_1, \dots, \alpha_p$ . But first, a very important point:

- *$AR(p)$  models must only be fitted to stationary time series. Any potential trends and/or seasonal effects need to be removed first. We will also make sure that the  $AR(p)$  processes are stationary.*

When is an  $AR(p)$  stationary? Not always, but under some mild conditions. First of all, we study the unconditional expectation of an  $AR(p)$  process  $X_t$  which we assume to be stationary, hence  $E[X_t] = \mu$  for all  $t$ . When we take expectations on both sides of the model equation, we have:

$$\mu = E[X_t] = E[\alpha_1 X_{t-1} + \dots + \alpha_p X_{t-p} + E_t] = (\alpha_1 + \dots + \alpha_p) \cdot \mu + 0, \text{ hence } \mu = 0.$$

Thus, any stationary  $AR(p)$  process has a global mean of zero. But please be aware of the fact that the conditional mean is time dependent and generally different from zero.

$$\mu_t = E[X_t | X_{t-1}, \dots, X_{t-p}] = \alpha_1 x_{t-1} + \dots + \alpha_p x_{t-p}$$

The question remains if  $AR(p)$  processes are practically useful, because most of the real-world time series have a global mean  $\mu$  that is different from zero. However, that generally poses little difficulties if we add an additional parameter  $m$  to the model definition:

$$Y_t = m + X_t$$

In that case,  $Y_t$  is a *shifted*  $AR(p)$  process, i.e. it has all dependency properties from an  $AR(p)$ , but its mean is different from zero. In fact, all R methodology that exists for fitting  $AR(p)$ 's assumes the process  $Y_t$  and thus estimates a global mean  $m$  unless this is explicitly excluded. In practice, if one colloquially speaks of an  $AR(p)$ , mostly one thinks of  $Y_t$  rather than  $X_t$ .

However, for the stationarity of an  $AR(p)$ , some further conditions on the model coefficients  $\alpha_1, \dots, \alpha_p$  are required. The general derivation is quite complicated and will be omitted here. But for illustrative purpose, we assume a stationary  $AR(1)$  which has  $Var(X_t) = \sigma_X^2$  for all  $t$ . If we determine the centralized second moment on both sides of the model equation, we obtain:

$$\sigma_X^2 = Var(X_t) = Var(\alpha_1 X_{t-1} + E_t) = \alpha_1^2 \sigma_X^2 + \sigma_E^2, \text{ hence } \sigma_X^2 = \frac{\sigma_E^2}{1 - \alpha_1^2}.$$

From this we derive that an  $AR(1)$  can only be stationary if  $|\alpha_1| < 1$ . That limitation means that the dependence from the series' past must not be too strong, so that the memory fades out. If  $|\alpha_1| > 1$ , the process diverges. The general condition for  $AR(p)$  models is (as mentioned above) more difficult to derive. We require that:

*The (potentially complex) roots of the characteristic polynomial  $\Phi(B)$  must all exceed 1 in absolute value for an  $AR(p)$  process to be stationary.*

In R, there is function `polyroot()` for finding a polynomials roots. If we want to verify whether an  $AR(3)$  with  $\alpha_1 = 0.4$ ,  $\alpha_2 = -0.2$ ,  $\alpha_3 = 0.3$  is stationary, we type:

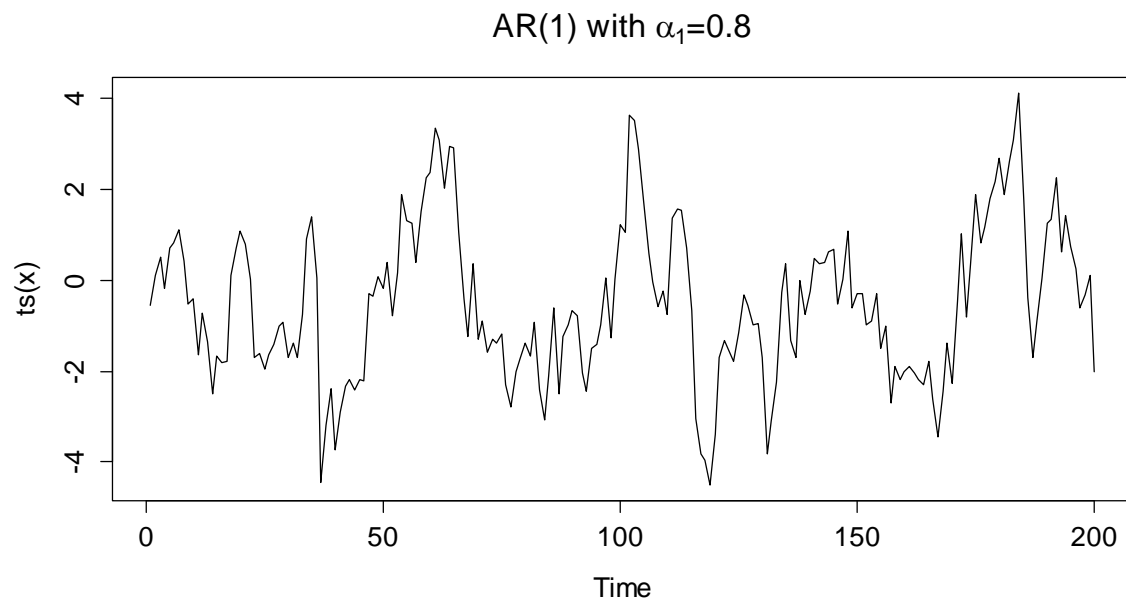
```
> abs(polyroot(c(1, 0.4, -0.2, 0.3)))
[1] 1.776075 1.056710 1.776075
```

Thus, the  $AR(3)$  we specified is stationary. We will proceed by studying the dependency in  $AR(p)$  processes. For illustration, we first simulate from an  $AR(1)$  with  $\alpha_1 = 0.8$ . The model equation is:

$$X_t = 0.8 \cdot X_{t-1} + E_t$$

So far, we had only required that  $E_t$  is a White Noise innovation, but not a distribution. We use the Gaussian in this example and set  $x_1 = E_1$  as the starting value.

```
> set.seed(24)
> E <- rnorm(200, 0, 1)
> x <- numeric()
> x[1] <- E[1]
> for(i in 2:200) x[i] <- 0.8*x[i-1] + E[i]
> plot(ts(x), main= "AR(1) with...")
```



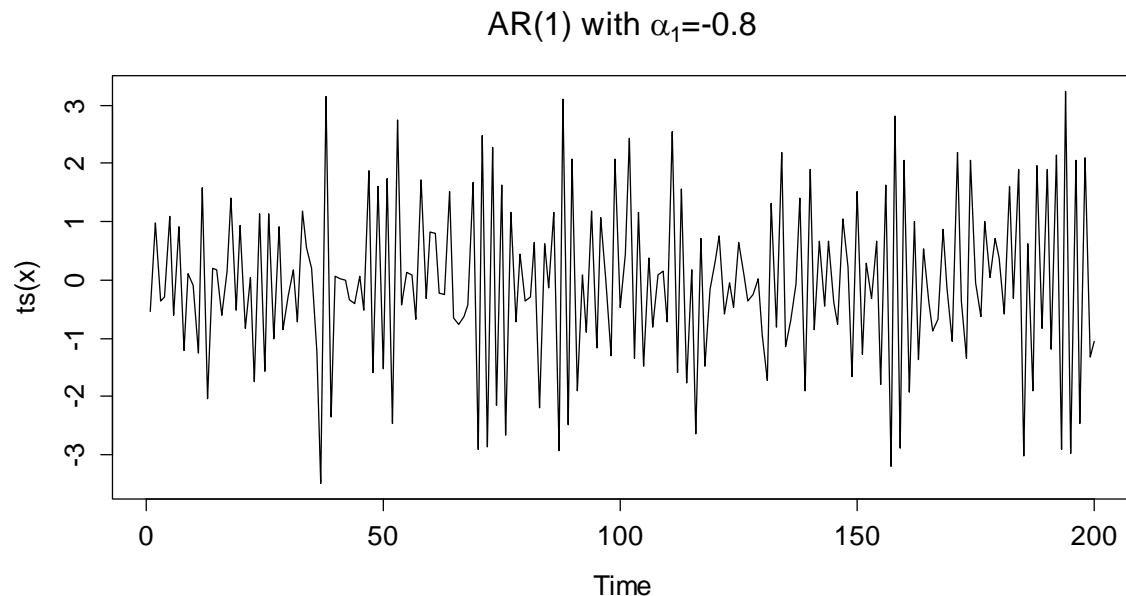
We observe some cycles with exclusively positive and others with only negative values. That is not surprising: if the series takes a large value, then the next one is determined as 0.8 times that large value plus the innovation. Thus, it is more likely that the following value has the same sign as its predecessor. On the other hand, the innovation is powerful enough so that jumping to the other side of the global mean zero is always a possibility. Given that behavior, it is evident that the autocorrelation at lag 1 is positive. We can compute it explicitly from the model equation:

$$\text{Cor}(X_t, X_{t-1}) = \text{Cor}(\alpha_1 X_{t-1} + E_t, X_{t-1}) = \alpha_1$$

Thus we have  $\rho(1) = 0.8$  here, or in general  $\rho(1) = \alpha_1$ . The correlation for higher lags can be determined similarly by repeated plug-in of the model equation. It is:

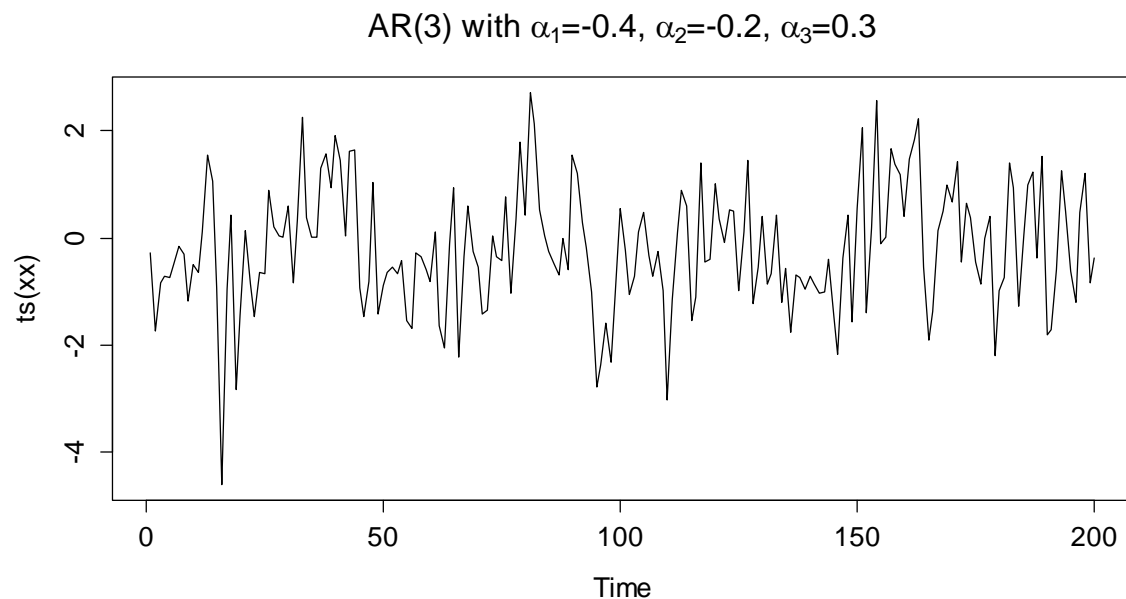
$$\rho(k) = \alpha_1^k.$$

Thus, for stationary  $AR(1)$  series, we have an exponential decay of the autocorrelation coefficients. Of course, it is also allowed to have a negative value for  $\alpha_1$ , as long as  $|\alpha_1| < 1$ . A realization of length 200 with  $\alpha_1 = -0.8$  is as follows:



The series shows an alternating behavior: the next value is more likely to lie on the opposite side of the global mean zero, but there are exceptions when the innovation takes a large value. The autocorrelation still follows  $\rho(k) = \alpha_1^k$ . It is also alternating between positive and negative values with an envelope that is exponentially decaying.

We will now focus on appearance and dependency of an  $AR(3)$  (with the coefficients from above). While we could still program the simulation code by ourselves, it is more convenient to use function `arma.sim()`.





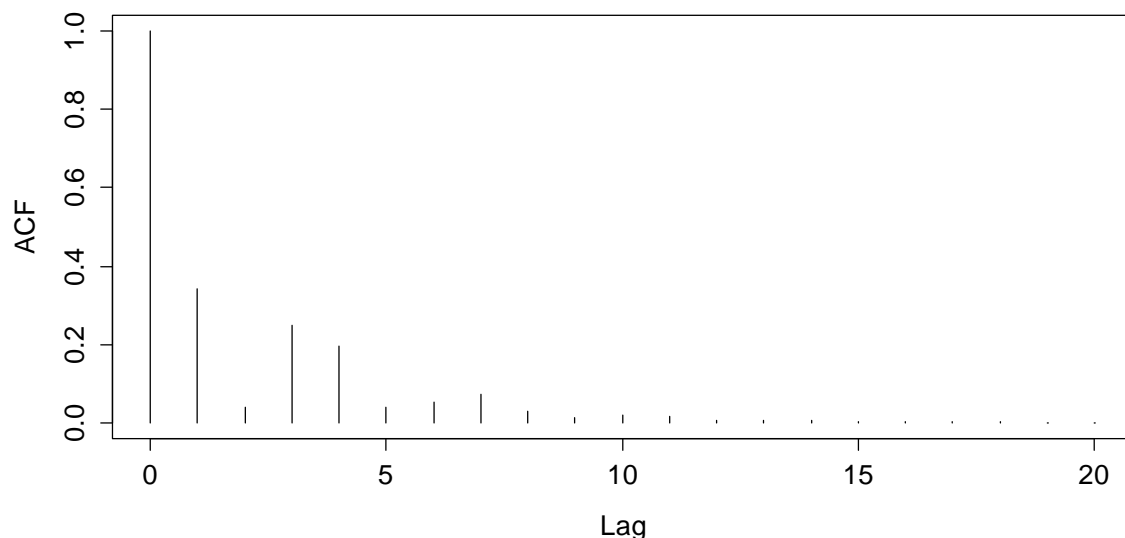
What is now the (theoretical) correlation in this  $AR(3)$ ? We apply the standard trick of plugging-in the model equation. This yields:

$$\begin{aligned}\rho(k) &= \text{Cor}(X_{t+k}, X_t) \\ &= \text{Cor}(\alpha_1 X_{t+k-1} + \dots + \alpha_p X_{t+k-p}, X_t) \\ &= \alpha_1 \rho(k-1) + \dots + \alpha_p \rho(k-p)\end{aligned}$$

with  $\rho(0)=1$  and  $\rho(-k)=\rho(k)$ . For  $k=1, \dots, p$  this results in a  $p \times p$  linear equation system called the *Yule-Walker equations*. It can be solved to obtain the autocorrelation coefficients which can finally be propagated for  $k=p+1, p+2, \dots$ . In R, there is function `armaACF()` that allows to determine the autocorrelation from autoregressive model coefficients.

```
> autocorr <- ARMAacf(ar=c(0.4, -0.2, 0.3), lag.max=20)
> plot(0:20, autocorr, type="h", xlab="Lag")
```

**Theoretical Autocorrelation for an AR(3)**

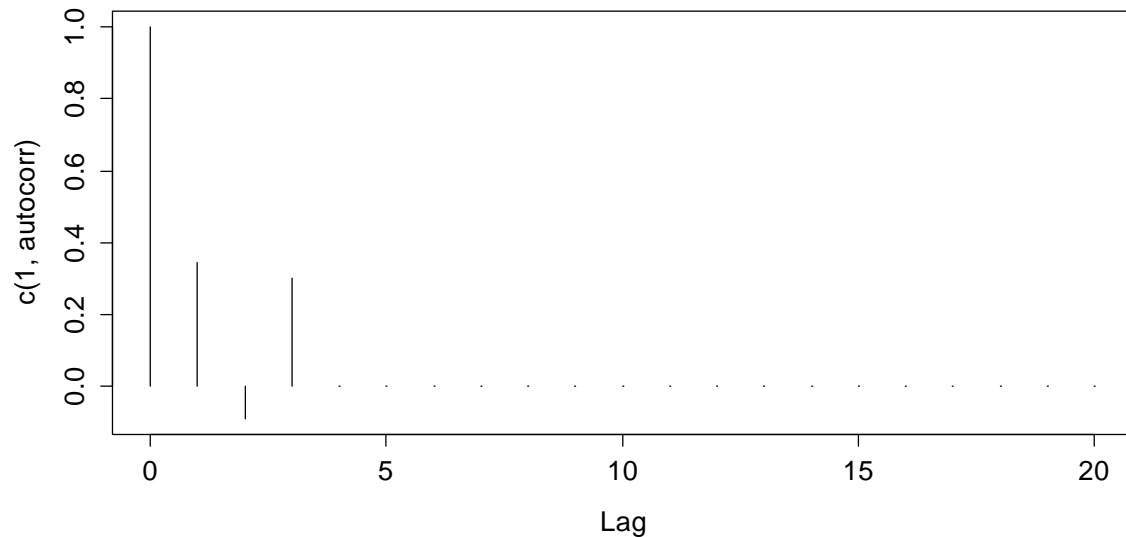


We observe that the theoretical correlogram shows a more complex structure than what could be achieved with an  $AR(1)$ . Nevertheless, one can still find an exponentially decaying envelope for the magnitude of the autocorrelations. That is a property which is common to all  $AR(p)$  models.

From the above, we can conclude that the autocorrelations are generally non-zero for all lags, even though in the underlying model,  $X_t$  only depends on the  $p$  previous values  $X_{t-1}, \dots, X_{t-p}$ . In section 4.5 we learned that the partial autocorrelation at lag  $k$  illustrates the dependence between  $X_t$  and  $X_{t+k}$  when the linear dependence on the intermittent terms was already taken into account. It is evident by definition that for any  $AR(p)$  process, we have  $\pi(k)=0$  for all  $k > p$ . This can and will serve as a useful indicator for deciding on the model order  $p$  if we are trying to identify the suitable model order when fitting real world data. In this section, we focus on the PACF for the above  $AR(3)$ .

```
> autocorr <- ARMAacf(ar=..., pacf=TRUE, lag.max=20)
> plot(0:20, autocorr, type="h", xlab="Lag")
```

### Theoretical Partial Autocorrelation for an AR(3)



As claimed previously, we indeed observe  $\rho(1) = \pi(1) = 0.343$  and  $\pi(3) = \alpha_3 = 0.3$ . All partial autocorrelations from  $\pi(4)$  on are exactly zero.

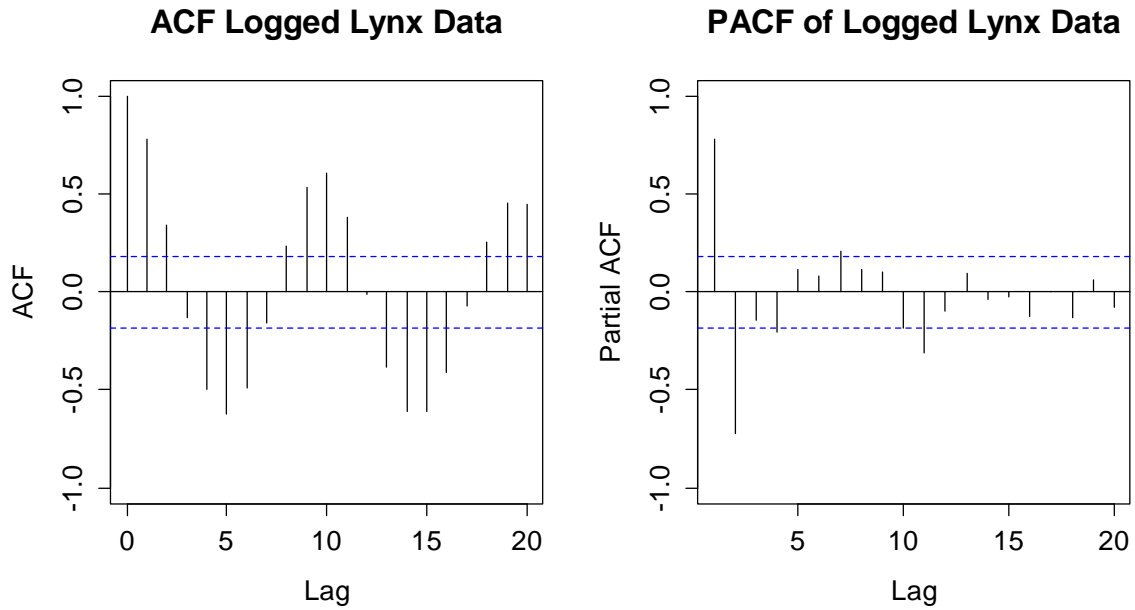
## 5.3.2 Fitting

Fitting an  $AR(p)$  model to data involves three main steps. First, the model and its order need to be identified. Second, the model parameters need to be estimated and third, the quality of the fitted model needs to be verified by residual analysis.

### Model Identification

The model identification step first requires verifying that the data show properties which make it plausible that they were generated from an  $AR(p)$  process. In particular, the time series we are aiming to model needs to be stationary, show an ACF with approximately exponentially decaying envelope and a PACF with a recognizable cut-off at some lag  $p$  smaller than about 5–10. If any of these three properties is strongly violated, it is unlikely that an  $AR(p)$  will yield a satisfactory fit, and there might be models which are better suited for the problem at hand.

The choice of the model order  $p$  then relies on the analysis of the sample PACF. Following the paradigm of parameter parsimony, we would first try the simplest model that seems plausible. This means choosing the smallest  $p$  at which we suspect a cut-off, i.e. the smallest after which none, or only few and weakly significant partial autocorrelations follow. We illustrate the concept with the logged Lynx data that were already discussed in section 1.2.2. We need to generate both ACF and PACF, which can be found on the next page.



There is no reason to doubt the stationarity of the Lynx series. Moreover, the ACF shows a cyclic behavior that has an exponentially decaying envelope. Now does the PACF show a cut-off? That is a bit less clear, and several orders  $p$  ( $= 2, 4, 7, 11$ ) come into question. However in summary, we conjecture that there are no strong objections against fitting an  $AR(p)$ . The choice of the order is debatable, but the parsimony paradigm tells us that we should try with the smallest candidate first, and that is  $p = 2$ .

### Parameter Estimation

Observed time series are rarely centered and thus, it is usually inappropriate to fit a pure  $AR(p)$  process. In fact, all **R** routines for fitting autoregressive models by default assume the shifted process  $Y_t = m + X_t$ . Hence, we have a regression-type equation with observations:

$$(Y_t - m) = \alpha_1(Y_{t-1} - m) + \dots + \alpha_p(Y_{t-p} - m) + E_t \text{ for } t = p+1, \dots, n.$$

The goal here is to estimate the parameters  $m, \alpha_1, \dots, \alpha_p$  such that the data are *fitted well*. There are several concepts that define *well fitting*. These include ordinary least squares estimation (OLS), Burg's algorithm (Burg), the Yule-Walker approach (YW) and maximum likelihood estimation (MLE). Already at this point we note that while the four methods have fundamental individuality, they are asymptotically equivalent (under some mild assumptions) and yield results that mostly only differ slightly in practice. Still, it is worthwhile to study all the concepts.

### OLS

The OLS approach is based on the notion with the centering; the above equation defines a multiple linear regression problem without intercept. The goodness-of-fit criterion is  $(x_t - \hat{x}_t)^2$  resp.  $(y_t - \hat{y}_t)^2$ , the two quantities are equal. The first step with this approach is to center the data, which is based on subtracting the global mean:

Estimate  $\hat{m} = \bar{y} = \sum_{t=1}^n y_t$  and then compute  $x_t = y_t - \hat{m}$  for all  $t = 1, \dots, n$ .

On the  $x_t$ , an OLS (auto)regression without intercept is performed. Note that this regression is (technically) conditional on the first  $p$  observations  $x_1, \dots, x_p$ , which are only used as predictors, but not as response terms. In other words, the goodness-of-fit of the model is only evaluated for the last  $n-p$  observations. The following code chunk implements the procedure for the logged lynx data:

```
> llc      <- log(lynx)-mean(log(lynx))
> resp     <- llc[3:114]
> pred1     <- llc[2:113]
> pred2     <- llc[1:112]
> fit.ols  <- lm(resp ~ -1 + pred1 + pred2)
> summary(fit.ols)
```

Coefficients:

	Estimate	Std. Error	t value	Pr(> t )	
pred1	1.38435	0.06359	21.77	<2e-16	***
pred2	-0.74793	0.06364	-11.75	<2e-16	***

---

Residual standard error: 0.528 on 110 degrees of freedom  
 Multiple R-squared: 0.8341, Adjusted R-squared: 0.8311  
 F-statistic: 276.5 on 2 and 110 DF, p-value: < 2.2e-16

We can extract  $\hat{m}=6.686$ ,  $\hat{\alpha}_1=1.384$ ,  $\hat{\alpha}_2=-0.748$  and  $\hat{\sigma}_E=0.528$ . But while this is an instructive way of estimating  $AR(p)$  models, it is a bit cumbersome and time consuming. Not surprisingly, there are procedures that are dedicated to fitting such models in R. We here display the use of function `ar.ols()`. To replicate the hand-produced result, we type:

```
> f.ar.ols <- ar.ols(log(lynx), aic=F, intercept=F, order=2)
> f.ar.ols
```

Coefficients:

	1	2
	1.3844	-0.7479

Order selected 2 sigma^2 estimated as 0.2738

Note that for producing the result, we need to avoid AIC-based model fitting with `aic=FALSE`. The shift  $m$  is automatically estimated, and thus we need to exclude an intercept term in the regression model using `intercept=FALSE`. We observe that the estimated  $AR$ -coefficients  $\hat{\alpha}_1, \hat{\alpha}_2$  take exactly the same values as with the hand-woven procedure above. The estimated shift  $\hat{m}$  can be extracted via

```
> fit.ar.ols$x.mean
[1] 6.685933
```

and corresponds to the global mean of the series. Finally, the estimate for the innovation variance requires some prudence. The `lm()` summary output yields an

estimate of  $\sigma_E$  that was computed as  $RSS/(n-p)$ , whereas the value in the `ar.ols()` output is an estimate of  $\sigma_E^2$  that was computed as  $RSS/n$ . The former is intended to be an unbiased estimate (though it should use the denominator  $n-p-1$  due to the estimation of the shift  $m$ ), and the latter is the MLE-estimator for the innovation variance. In practice, the numerical difference between the two is neglectable for any series that has reasonable length for fitting an  $AR$  model.

```
> sum(na.omit(fit.ar.ols$resid)^2)/112
[1] 0.2737594
```

### Burg's Algorithm

While the OLS approach works, its downside is the asymmetry: the first  $p$  terms are never evaluated as responses. That is cured by Burg's Algorithm, an alternative approach for estimating  $AR(p)$  models. It is based on the notion that any  $AR(p)$  process is also an  $AR(p)$  if the time is run in reverse order. Under this property, minimizing the forward and backward 1-step squared prediction errors makes sense:

$$\sum_{t=p+1}^n \left\{ \left( X_t - \sum_{k=1}^p \alpha_k X_{t-k} \right)^2 + \left( X_{t-p} - \sum_{k=1}^p \alpha_k X_{t-p+k} \right)^2 \right\}$$

In contrast to OLS, there is no explicit solution and numerical optimization is required. This is done with a recursive method called the Durbin-Levison algorithm. We do not explain its details here, but refer to the R implementation `ar.burg()`.

```
> f.ar.burg <- ar.burg(log(lynx), aic=FALSE, order.max=2)
> f.ar.burg
```

Call:

```
ar.burg.default(x = log(lynx), aic = FALSE, order.max = 2)
```

Coefficients:

```
      1      2
1.3831 -0.7461
```

Order selected 2 sigma^2 estimated as 0.2707

```
> f.ar.burg$x.mean
[1] 6.685933
> sum(na.omit(f.ar.burg$resid)^2)/112
[1] 0.2737614
```

There are a few interesting points which require commenting. First and foremost, Burg's algorithm also uses the arithmetic mean to estimate the global mean  $\hat{m}$ . The fitting procedure is then done on the centered observations  $x_t$ . On a side remark, note that assuming centered observations is possible. If argument `demean=FALSE` is set, the global mean is assumed to be zero and not estimated.

The two coefficients  $\hat{\alpha}_1, \hat{\alpha}_2$  take some slightly different values than with OLS estimation. While often, the difference between the two methods is practically neglectable, it is nowadays generally accepted that the Burg solution is better for finite samples. Asymptotically, the two methods are equivalent. Finally, we observe that the `ar.burg()` output specifies  $\hat{\sigma}_E^2 = 0.2707$ . This is different from the MLE estimate of 0.27376 on the residuals. The explanation is that for Burg's Algorithm, the innovation variance is estimated from the Durbin-Levinson updates; see the R help file for further reference.

### Yule-Walker Equations

A third option for estimating  $AR(p)$  models is to plugging-in the sample ACF into the Yule-Walker equations. In section 5.3.1 we had learned that there is a  $p \times p$  linear equation system  $|\rho(k) = \alpha_1 \rho(k-1) + \dots + \alpha_p \rho(k-p)|$  for  $k = 1, \dots, p$ . Hence we can and will explicitly determine  $\hat{\rho}(0), \dots, \hat{\rho}(k)$  and then solve the linear equation system for the coefficients  $\alpha_1, \dots, \alpha_p$ . The procedure is implemented in R function `ar.yw()`.

```
> f.ar.yw <- ar.yw(log(lynx), aic=FALSE, order.max=2)
> f.ar.yw
```

```
Call: ar.yw.default(x=log(lynx), aic=FALSE, order.max=2)
```

```
Coefficients:
```

```
      1      2
1.3504 -0.7200
```

```
Order selected 2  sigma^2 estimated as  0.3109
```

Again, the two coefficients  $\hat{\alpha}_1, \hat{\alpha}_2$  take some slightly different values than compared to the two methods before. Mostly this difference is practically neglectable and Yule-Walker is asymptotically equivalent to OLS and Burg. Nevertheless, for finite samples, the estimates from the Yule-Walker method are often worse in the sense that their (Gaussian) likelihood is lower. Thus, we recommend to prefer Burg's algorithm. We conclude this section by noting that the Yule-Walker method also involves estimating the global mean  $m$  with the arithmetic mean as the first step. The innovation variance is estimated from the fitted coefficients and the autocovariance of the series and thus again takes a different value than before.

### Maximum-Likelihood Estimation (MLE)

The MLE is based on determining the model coefficients such that the likelihood given the data is maximized, i.e. the density function takes its maximal value under the present observations. This requires assuming a distribution for the  $AR(p)$  process, which comes quite naturally if one assumes that for the innovations, we have  $E_t \sim N(0, \sigma_E^2)$ , i.e. they are *iid* Gaussian random variables. With some theory (which we omit), one can then show that an  $AR(p)$  process  $X_1, \dots, X_n$  is a random vector with a multivariate Gaussian distribution.

MLE then provides a simultaneous estimation of the shift  $m$ , the innovation variance  $\sigma_E^2$  and the model coefficients  $\alpha_1, \dots, \alpha_p$ . The criterion that is optimized can, in a simplified version, be written as:

$$L(\alpha, m, \sigma_E^2) \propto \exp\left(-\frac{1}{2\sigma_E^2} \sum_{t=1}^n (x_t - \hat{x}_t)^2\right)$$

The details are quite complex and several constants are part of the equation, too. But we here note that the MLE derived from the Gaussian distribution is based on minimizing the sum of squared errors and thus equivalent to the OLS approach. Due to the simultaneous estimation of model parameters and innovation variance, a recursive algorithm is required. There is an implementation in R:

```
> f.ar.mle

Call: arima(x = log(lynx), order = c(2, 0, 0))

Coefficients:
      ar1      ar2  intercept
  1.3776 -0.7399    6.6863
s.e.  0.0614   0.0612    0.1349

sigma^2 = 0.2708:  log likelihood = -88.58,  aic = 185.15
```

We observe estimates which are again slightly different from the ones computed previously. Again, those differences are mostly neglectable for practical data analysis. What is known from theory is that the MLE is (under mild assumptions) asymptotically normal with minimum variance among all asymptotically normal estimators. Note that the MLE based on Gaussian distribution still works reasonably well if that assumption is not met, as long as we do not have strongly skewed data (apply a transformation in that case) or extreme outliers.

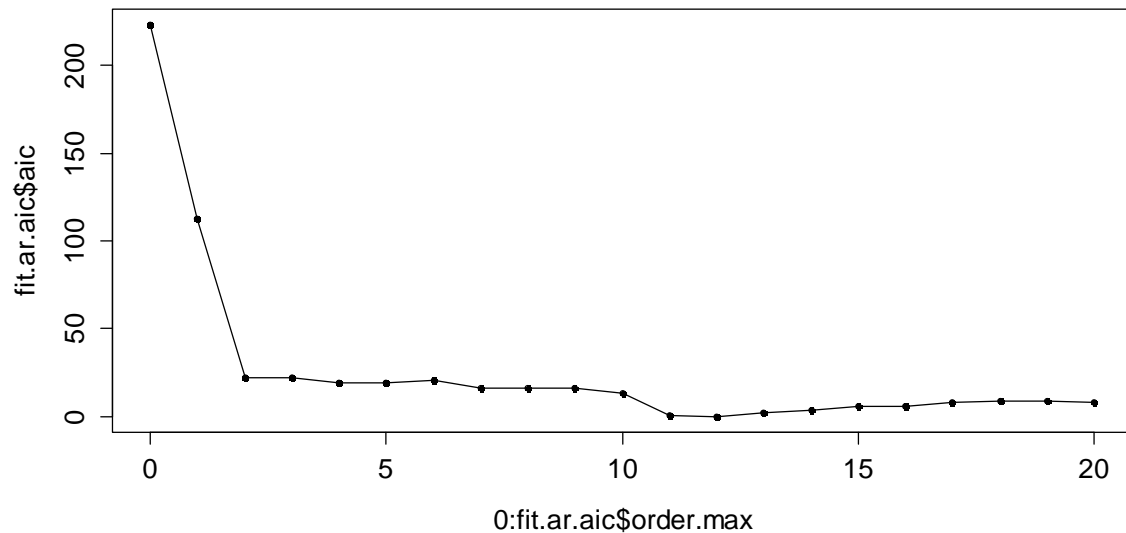
### Practical Aspects

We presented four different methods for fitting  $AR(p)$  models. How to make a choice in practice? We explained that all methods are asymptotically equivalent and even on finite samples; the differences among them are little. Also, all methods are non-robust with respect to outliers and perform best on data which are approximately Gaussian. There is one practical aspect linked to the fitting routines that are available in R, though. Function `arima()` yields standard errors for  $m$  and  $\alpha_1, \dots, \alpha_p$ . Approximate 95% confidence intervals can be obtained by taking the point estimate  $\pm$  twice the standard error. Hence, statements about the significance of the estimates can be made.

On the other hand, `ar.ols()`, `ar.yw()` und `ar.burg()` do not provide standard errors, but allow for convenient determination of the model order  $p$  with the AIC statistic. While we still recommend investigating on the suitable order by analyzing ACF and PACF, the parsimony paradigm and inspecting residual plots, using AIC as a second opinion is still recommended. It works as follows:

```
> fit.aic <- ar.burg(log(lynx))
> plot(0:fit.aic$order.max, fit.aic$aic)
```

**AIC-Values for AR(p)-Models on the Logged Lynx Data**



We observe that already  $p = 2$  yields a good AIC value. Then there is little further improvement until  $p = 11$ , and a just slightly lower value is found at  $p = 12$ . Hence, we will evaluate  $p = 2$  and  $p = 11$  as two competing models with some further tools in the next section.

### 5.3.3 Residual Analysis

When comparing different models, a simple approach is to plot the original series along with the fitted model values. However, one has to keep in mind that this is an insample analysis, i.e. the bigger model has an advantage which does not necessarily persist once analyzes out-of-sample data. Please note that the residuals are estimates of the innovations  $E_t$ . Thus, a good model yields residuals that resemble a White Noise process. We require mean zero, constant variance and no autocorrelation. If these properties are not met, the model is not adequate.

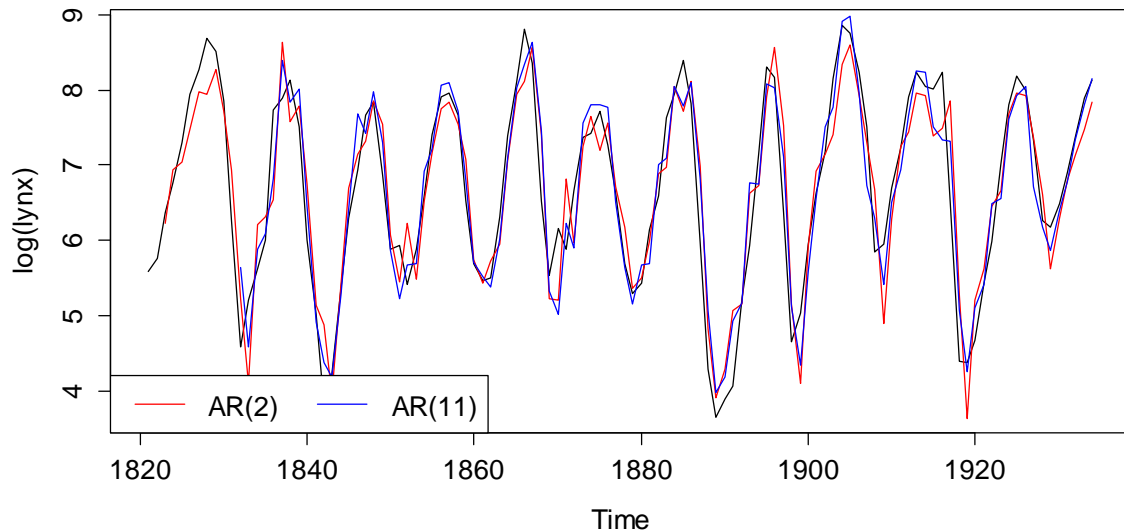
```
> fit.ar02 <- ar.burg(log(lynx), aic=FALSE, order.max=2)
> fit.ar11 <- ar.burg(log(lynx), aic=FALSE, order.max=11)
> plot(log(lynx), main="Logged Lynx Data with ...")
> lines(log(lynx)-fit.ar02$resid, col="red")
> lines(log(lynx)-fit.ar11$resid, col="blue")
```

The output is displayed on the next page. While some differences are visible, it is not easy to judge from the fitted values which of the two models is preferable. A better focus on the quality of the fit is obtained when the residuals and their dependance are inspected with time series plots as well as ACF/PACF correlograms. The graphical output is again displayed on the next page. We observe that the  $AR(2)$  residuals are not iid. Hence they do not form a White



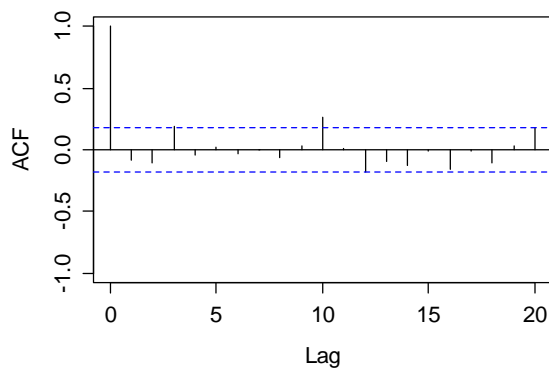
Noise process and thus, we conclude that the  $AR(11)$  model yields a better description of the logged lynx data.

**Logged Lynx Data with AR(2) and AR(11)**

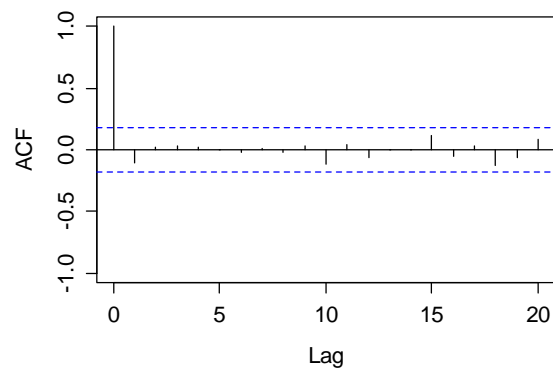


```
> acf(fit.ar02$resid, na.action=na.pass, ylim=c(-1,1))
> pacf(fit.ar02$resid, na.action=na.pass, ylim=c(-1,1))
> acf(fit.ar11$resid, na.action=na.pass, ylim=c(-1,1))
> pacf(fit.ar11$resid, na.action=na.pass, ylim=c(-1,1))
```

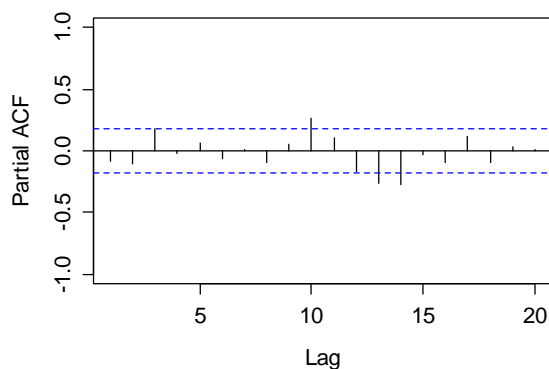
**ACF of AR(2)**



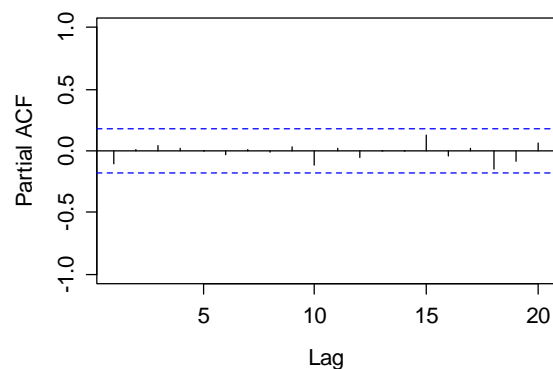
**ACF of AR(11)**



**PACF of AR(2)**

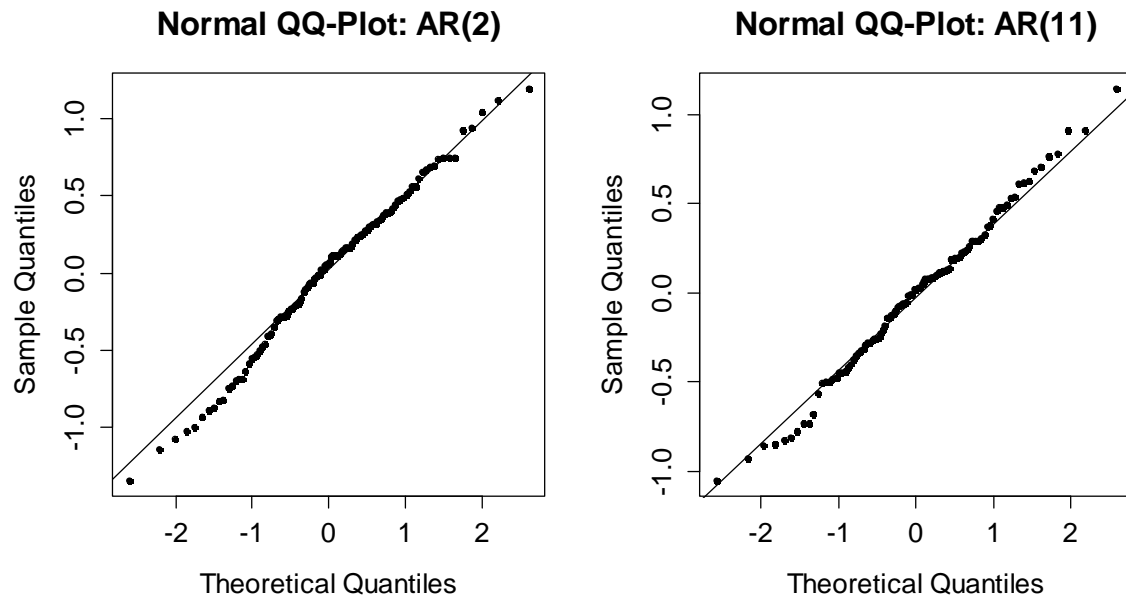


**PACF of AR(11)**



Because our estimation routines to some extent rely on the Gaussian distribution, it is always worthwhile to generate a Normal QQ-Plot for verifying this. Here, we obtain:

```
> par(mfrow=c(1,2))
> qqnorm(as.numeric(fit.ar02$resid))
> qqline(as.numeric(fit.ar02$resid))
> qqnorm(as.numeric(fit.ar11$resid))
> qqline(as.numeric(fit.ar11$resid))
```



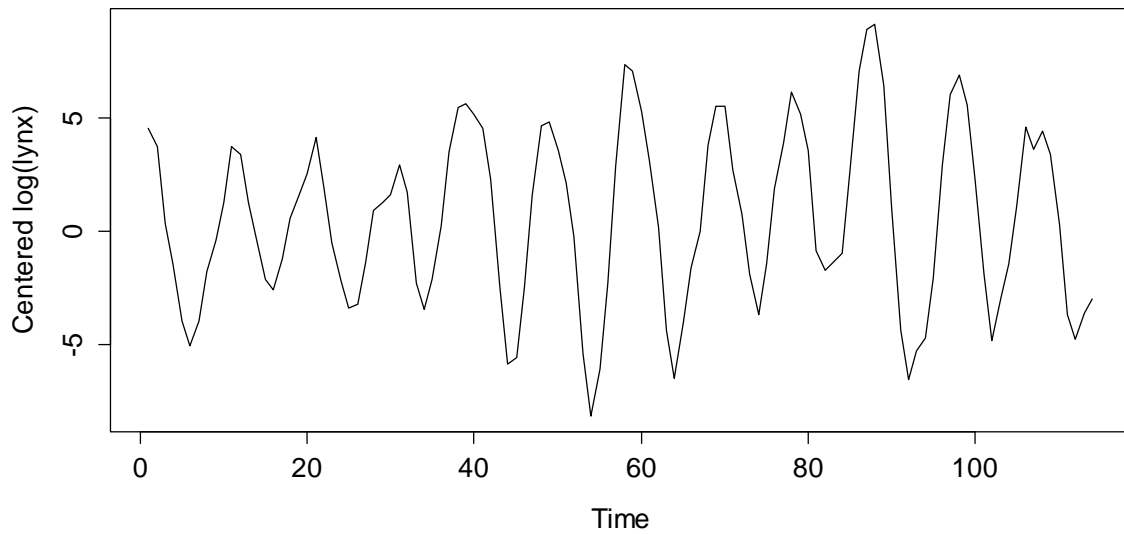
Neither of the two plots (which are very similar) does indicate any problems. If the residuals' distribution looks non-normal, a log-transformation might be worth a consideration, as it often improves the situation.

### Simulation from the Fitted Model

If there are competing models and none of the other criteria dictate which one to use, another option is to generate realizations from the fitted process using R's function `arima.sim()`. It usually pays off to generate multiple realizations from each fitted model. By eyeballing, one then tries to judge which model yields data that resemble the true observations best. We here do the following:

```
> ## Repeat these commands a number of times
> plot(arima.sim(n=114, list(ar=fit.ar02$ar)))
> plot(arima.sim(n=114, list(ar=fit.ar11$ar)))
```

A realization from the fitted  $AR(11)$  can be seen on the next side. In summary, the simulations from this bigger model look more realistic than the ones from the  $AR(2)$ . The clearest answer about the model which is preferable here comes from the ACF/PACF correlograms, though. We conclude this section about model fitting by saying that the logged lynx data are best modeled with the  $AR(11)$ .

**Simulated Series from the Fitted AR(11)**

## 5.4 Moving Average Models

Here, we discuss moving average models. They are an extension of the White Noise process, i.e.  $X_t$  is as a linear combination of the current plus a few of the most recent innovation terms. As we will see, this leads to a time series process that is always stationary, but not iid. Furthermore, we will see that in many respects, moving average models are complementary to autoregressive models.

### 5.4.1 Definition and Properties

As we had mentioned above, a *moving average process of order  $q$* , or abbreviated, an  $MA(q)$  model for a series  $X_t$  is a linear combination of the current innovation term  $E_t$ , plus the  $q$  most recent ones  $E_{t-1}, \dots, E_{t-q}$ . The model equation is:

$$X_t = E_t + \beta_1 \cdot E_{t-1} + \dots + \beta_q \cdot E_{t-q}$$

We require that  $E_t$  is an innovation, which means independent and identically distributed, and also independent of any  $X_s$  where  $s < t$ . For simple notation, we can make use of the backshift operator and rewrite the model:

$$X_t = (1 + \beta_1 B + \dots + \beta_q B^q) E_t = \Theta(B) E_t$$

We call  $\Theta(B)$  the characteristic polynomial of the  $MA(q)$  process and obviously, it defines all properties of the series. As a remark, please note that a number of other textbooks define the  $MA(q)$  process with negative signs for the  $\beta_j$ . While this is mathematically equivalent, we prefer our notation with the '+' signs, as it matches the way how things are implemented in **R**. We turn our sights towards the motivation for the moving average process.

### What is the rationale for the $MA(q)$ process?

Firstly, they have been applied successfully in many applied fields, particularly in econometrics. Time series such as economic indicators are affected by a variety of random events such as strikes, government decision, referendums, shortages of key commodities, et cetera. Such events will not only have an immediate effect on the indicator, but may also affect its value (to a lesser extent) in several of the consecutive periods. Thus, it is plausible that moving average processes appear in practice. Moreover, some of their theoretical properties are in a nice way complementary to the ones of autoregressive processes. This will become clear if we study the moments and stationarity of the  $MA$  process.

### Moments and Dependence

A first, straightforward but very important result is that any  $MA(q)$  process  $X_t$ , as a linear combination of innovation terms, has zero mean and constant variance:

$$E[X_t] = 0 \text{ for all } t, \text{ and } Var(X_t) = \sigma_E^2 \cdot \left(1 + \sum_{j=1}^q \beta_j^2\right) = const$$

Please note that in practice, we can always enhance  $MA(q)$ 's by adding a constant  $m$  that accounts for non-zero expectation of a time series, i.e. we can consider the shifted  $MA(q)$  process

$$Y_t = m + X_t.$$

Hence, the zero mean property does not affect the possible field of practical application. Now, if we could additionally show that the autocovariance in  $MA$  processes is independent of the time  $t$ , we had already proven their stationarity. This is indeed the case. We start by considering a  $MA(1)$  with  $X_t = E_t + \beta_1 E_{t-1}$

$$\gamma(1) = Cov(X_t, X_{t-1}) = Cov(E_t + \beta_1 E_{t-1}, E_{t-1} + \beta_1 E_{t-2}) = \beta_1 \sigma_E^2.$$

For any lag  $k$  exceeding the order  $q=1$ , we use the same trick of plugging-in the model equation and directly obtain a perhaps somewhat surprising result:

$$\gamma(k) = Cov(X_t, X_{t-k}) = 0 \text{ for all } k > q = 1.$$

Thus, there is no more unconditional serial dependence in lags  $>1$ . For the autocorrelation of a  $MA(1)$  process, we have:

$$\rho(1) = \frac{\gamma(1)}{\gamma(0)} = \frac{\beta_1}{1 + \beta_1^2} \text{ and } \rho(k) = 0 \text{ for all } k > q = 1.$$

From this we conclude that  $\rho(1) \leq 0.5$ , no matter what the choice for  $\beta_1$  is. Thus if in practice we observe a series where the first-order autocorrelation coefficient clearly exceeds this value, we have counterevidence to a  $MA(1)$  process.

Furthermore, we have shown that any  $MA(1)$  has zero mean, constant variance and an ACF that only depends on the lag  $k$ , hence it is stationary. Note that the stationarity does (in contrast to  $AR$  processes) not depend on the choice of the parameter  $\beta_1$ . The stationarity property can be generalized to  $MA(q)$  processes. Using some calculations and  $\beta_0 = 1$ , we obtain:

$$\rho(k) = \begin{cases} \sum_{j=0}^{q-k} \beta_j \beta_{j+k} / \sum_{j=0}^q \beta_j^2 & \text{for } k = 1, \dots, q \\ 0 & \text{for } k > q \end{cases}$$

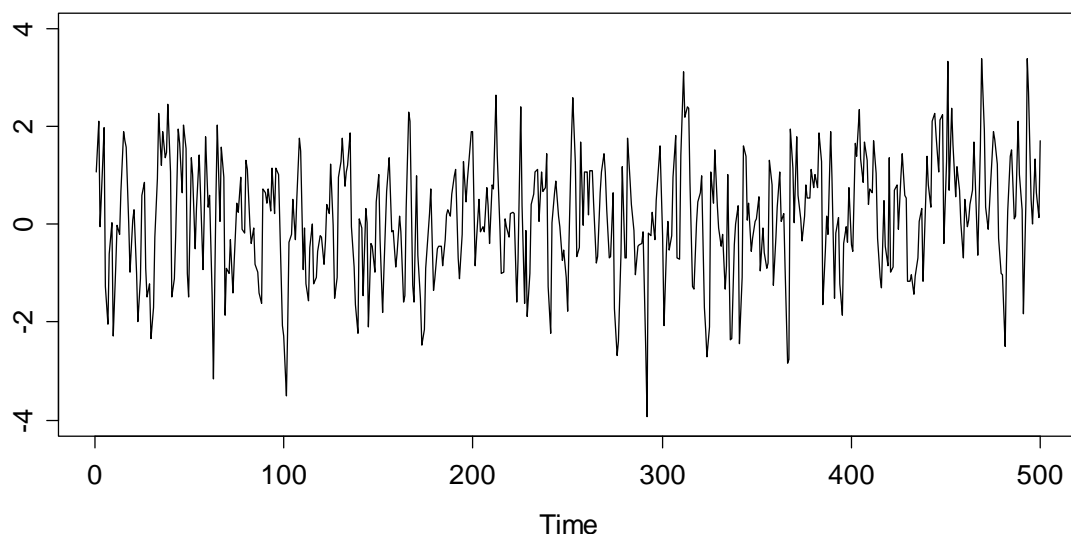
Hence,  $\rho(k)$  is independent of the time  $t$  for any  $MA(q)$  process, irrespective of the order  $q$ . The main results which can be derived from this property is that  $MA(q)$  processes are *always stationary, independent of  $\beta_1, \dots, \beta_q$* . Moreover, we learn from the above that the autocorrelation is zero for all orders  $k > q$ . And there obviously is a relation between the model parameters and the autocorrelation, although it gets quite complex for higher orders. While this formula may be employed for finding the true ACF of a given  $MA(q)$ , the most convenient way of doing this in practice remains with the `R` function `ARMAacf()`.

### Example of a $MA(1)$

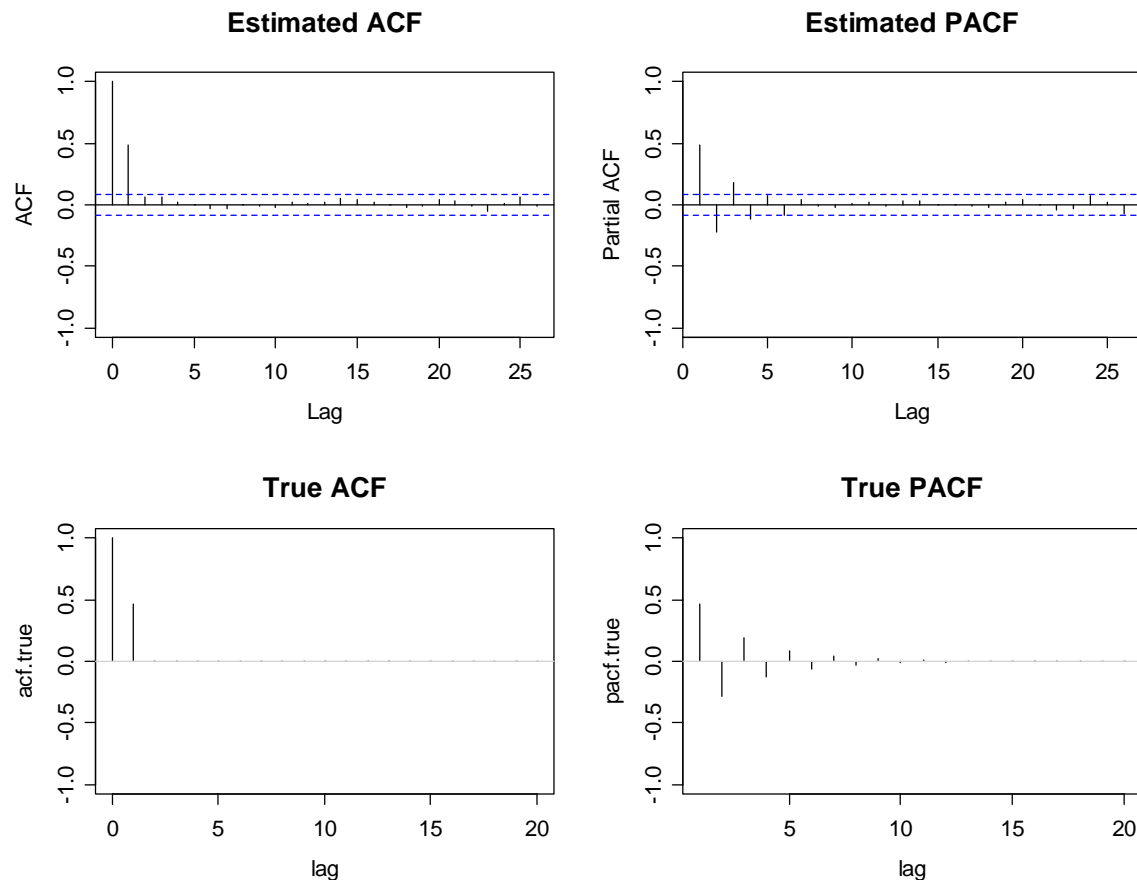
For illustration, we generate a realization consisting of 500 observations, from a  $MA(1)$  process with  $\beta_1 = 0.7$ , and display time series plot, along with both estimated and true ACF/PACF.

```
> set.seed(21)
> ts.mal <- arima.sim(list(ma=0.7), n=500)
>
> plot(ts.mal, ylab="", ylim=c(-4,4))
> title("Simulation from a MA(1) Process")
```

**Simulation from a  $MA(1)$  Process**



```
> acf.true <- ARMAacf(ma=0.7, lag.max=20)
> pacf.true <- ARMAacf(ma=0.7, pacf=TRUE, lag.max=20)
```



We observe that the estimates are pretty accurate: the ACF has a clear cut-off, whereas the PACF seems to feature some alternating behavior with an exponential decay in absolute value. This behavior is typical: the PACF of any  $MA(q)$  process shows an exponential decay, while the ACF has a cut-off. In this respect,  $MA(q)$  processes are in full contrast to the  $AR(p)$ 's, i.e. the appearance of ACF and PACF is swapped.

### Invertibility

It is easy to show that the first autocorrelation coefficient  $\rho(1)$  of an  $MA(1)$  process can be written in standard form, or also as follows:

$$\rho(1) = \frac{\beta_1}{1 + \beta_1^2} = \frac{1/\beta_1}{1 + (1/\beta_1)^2}$$

Apparently, any  $MA(1)$  process with coefficient  $\beta_1$  has exactly the same ACF as the one with  $1/\beta_1$ . Thus, the two processes  $X_t = E_t + 0.5E_{t-1}$  and  $U_t = E_t + 2E_{t-1}$  have the same dependency structure. Or in other words, given some ACF, we cannot identify the generating  $MA$  process uniquely. This problem of ambiguity leads to the concept of *invertibility*. Now, if we express the processes  $X_t$  and  $U_t$  in terms of  $X_{t-1}, X_{t-2}, \dots$  resp.  $U_{t-1}, U_{t-2}, \dots$ , we find by successive substitution:

$$E_t = X_t - \beta_1 X_{t-1} + \beta_1^2 X_{t-2} - \dots$$

$$E_t = U_t - (1/\beta_1)U_{t-1} + (1/\beta_1^2)U_{t-2} - \dots$$

Hence, if we rewrite the  $MA(1)$  as an  $AR(\infty)$ , only one of the processes will converge. That is the one where  $|\beta_1| < 1$ , and it will be called *invertible*. It is important to know that invertibility of  $MA$  processes is central when it comes to fitting them to data, because parameter estimation is based on rewriting them in the form of an  $AR(\infty)$ .

For higher-order  $MA(q)$  processes, the property of invertibility is equally central. If it is met, the series can be rewritten in form of an  $AR(\infty)$  and it is guaranteed that there is a unique  $MA$  process for any given ACF. Invertibility of a  $MA(q)$  is met if the roots of the characteristic polynomial  $\Theta(B)$  all lie outside of the unit circle. As was explained earlier in chapter 5.3.1, we can verify this using the `R` function `polyroot()`. Please note that the estimation procedure described below will always result in coefficients  $\hat{\beta}_1, \dots, \hat{\beta}_q$  that define an invertible  $MA(q)$  process.

## 5.4.2 Fitting

The process of fitting  $MA(q)$  models to data is more difficult than for  $AR(p)$ , as there are no (efficient) explicit estimators and numerical optimization is mandatory. Perhaps the simplest idea for estimating the parameters is to exploit the relation between the model parameters and the autocorrelation coefficients, i.e.:

$$\rho(k) = \begin{cases} \sum_{j=0}^{q-k} \beta_j \beta_{j+k} / \sum_{j=0}^q \beta_j^2 & \text{for } k = 1, \dots, q \\ 0 & \text{for } k > q \end{cases}$$

Hence in case of a  $MA(1)$ , we would determine  $\hat{\beta}_1$  by plugging-in  $\hat{\rho}(1)$  into the equation  $\rho(1) = \beta_1 / (1 + \beta_1^2)$ . This can be seen as an analogon to the Yule-Walker approach in  $AR$  modelling. Unfortunately, the plug-in idea yields an inefficient estimator and is not a viable option for practical work.

### Conditional Sum of Squares

Another appealing idea would be to use some (adapted) least squares procedure for determining the parameters. A fundamental requirement for doing so is that we can express the sum of squared residuals  $\sum E_t^2$  in terms of the observations  $X_1, \dots, X_n$  and the parameters  $\beta_1, \dots, \beta_q$  only, and do not have to rely on the unobservable  $E_1, \dots, E_n$  directly. This is (up to the choice of some initial values) possible for all invertible  $MA(q)$  processes. For simplicity, we restrict our illustration to the  $MA(1)$  case, where we can replace any innovation term  $E_t$  by:

$$E_t = X_t - \beta_1 X_{t-1} + \beta_1^2 X_{t-2} + \dots + (-\beta_1)^{t-1} X_1 + \beta_1^t E_0$$

By doing so, we managed to express the innovation/residual at time  $t$  as a function of the model parameter  $\beta_1$  and a combination of the current and past observations of the series. What is also remaining is the (hypothetical) initial innovation term  $E_0$ . Conditional on the assumption  $E_0 = 0$ , we can indeed rewrite the residuals sum of squares  $\sum E_t^2$  of any  $MA(1)$  using  $X_1, \dots, X_n$  and  $\beta_1$  only. However, there is no closed form solution for the minimization of  $\sum E_t^2$ , since powers of the parameter  $\beta_1$  appear; but the problem can be tackled using numerical optimization. This approach is known as the Conditional Sum of Squares (CSS) method. It works similarly for higher orders  $q$ , i.e. fundamentally relies on the invertibility of the  $MA(q)$  and assumes that  $E_t = 0$  for all  $t = -\infty, \dots, 0$ . In R, the method is implemented in function `arima()` if argument `method="CSS"` is set.

### Maximum-Likelihood Estimation

As can be seen from the R help file, the Conditional Sum of Squares method is only secondary to `method="CSS-ML"` in the R function `arima()`. This means that it is preferable to use CSS only to obtain a first estimate of the coefficients  $\beta_1, \dots, \beta_q$ . They are then used as starting values for a Maximum-Likelihood estimation, which is based on the assumption of Gaussian innovations  $E_t$ . It is pretty obvious that  $X_t = E_t + \beta_1 E_{t-1} + \dots + \beta_q E_{t-q}$ , as a linear combination of normally distributed random variables, follows a Gaussian too. By taking the covariance terms into account, we obtain a multivariate Gaussian for the time series vector:

$$X = (X_1, \dots, X_n) \sim N(0, V), \text{ resp. } Y = (Y_1, \dots, Y_n) \sim N(m \cdot \mathbf{1}, V).$$

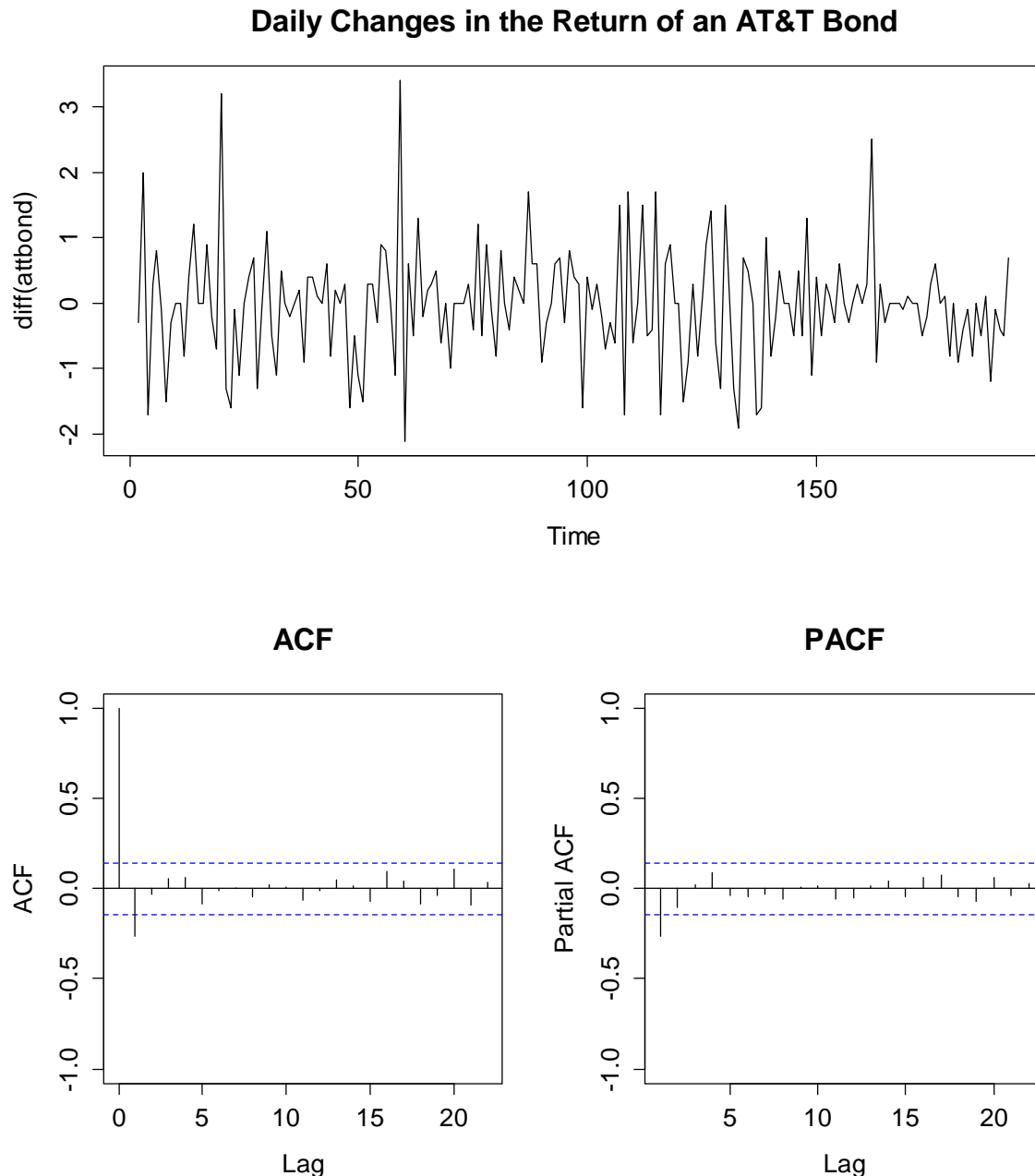
MLE then relies on determining the parameters  $m$  (if a shifted  $MA(q)$  is estimated),  $\beta_1, \dots, \beta_q$  and  $\sigma_E^2$  simultaneously by maximizing the probability density function of the above multivariate Gaussian with assuming the data  $x_1, \dots, x_n$  as given quantities. This is a quite complex non-linear problem which needs to be solved numerically. A good implementation is found in R's `arima()`.

The benefit of MLE is that (under mild and in practice usually fulfilled conditions) certain optimality conditions are guaranteed. It is well known that the estimates are asymptotically normal with minimum variance among all asymptotically normal estimators. Additionally, it is pretty easy to derive standard errors for the estimates, which further facilitates their interpretation. And even though MLE is based on assuming Gaussian innovations, it still produces reasonable results if the deviations from that model are not too strong. Be especially wary in case of extremely skewed data or massive outliers. In such cases, applying a log-transformation before the modelling/estimation starts is a wise idea.

### 5.4.3 Example: Return of AT&T Bonds

As an example, we consider the daily changes in the return of an AT&T bond from April 1975 to December 1975, which makes for a total of 192 observations. The data are displayed along with their ACF and PACF on the next page.





The series seems to originate from a stationary process. There are no very clear cycles visible, hence it is hard to say anything about correlation and dependency, and it is impossible to identify the stochastic process behind the generation of these data from a time series plot alone. Using the ACF and PACF as a visual aid, we observe a pretty clear cut-off situation in the ACF at lag 1 which lets us assume that a  $MA(1)$  might be suitable. That opinion is undermined by the fact that the PACF drops off to small values quickly, i.e. we can attribute some exponential decay to it for lags 1 and 2.

Our next goal is now to fit the  $MA(1)$  to the data. As explained above, the simplest solution would be to determine  $\hat{\rho}(1) = -0.266$  and derive  $\hat{\beta}_1$  from  $\rho(1) = \beta_1 / (1 + \beta_1^2)$ . This yields two solutions, namely  $\hat{\beta}_1 = -0.28807$  and  $\hat{\beta}_1 = -3.47132$ . Only one of these (the former) defines an invertible  $MA(1)$ , hence we would stick to that

solution. A better alternative is to use the CSS approach for parameter estimation. The code for doing so is as follows:

```
> arima(diff(attbond), order=c(0,0,1), method="CSS")

Call:
arima(x = diff(attbond), order = c(0, 0, 1), method = "CSS")

Coefficients:
          ma1  intercept
      -0.2877   -0.0246
s.e.    0.0671    0.0426

sigma^2 estimated as 0.6795:  part log likelihood = -234.11
```

Even more elegant and theoretically sound is the MLE. We can also perform this in **R** using function `arima()`. It yields a very similar but not identical result:

```
> arima(diff(attbond), order=c(0,0,1))

Call:
arima(x = diff(attbond), order = c(0, 0, 1))

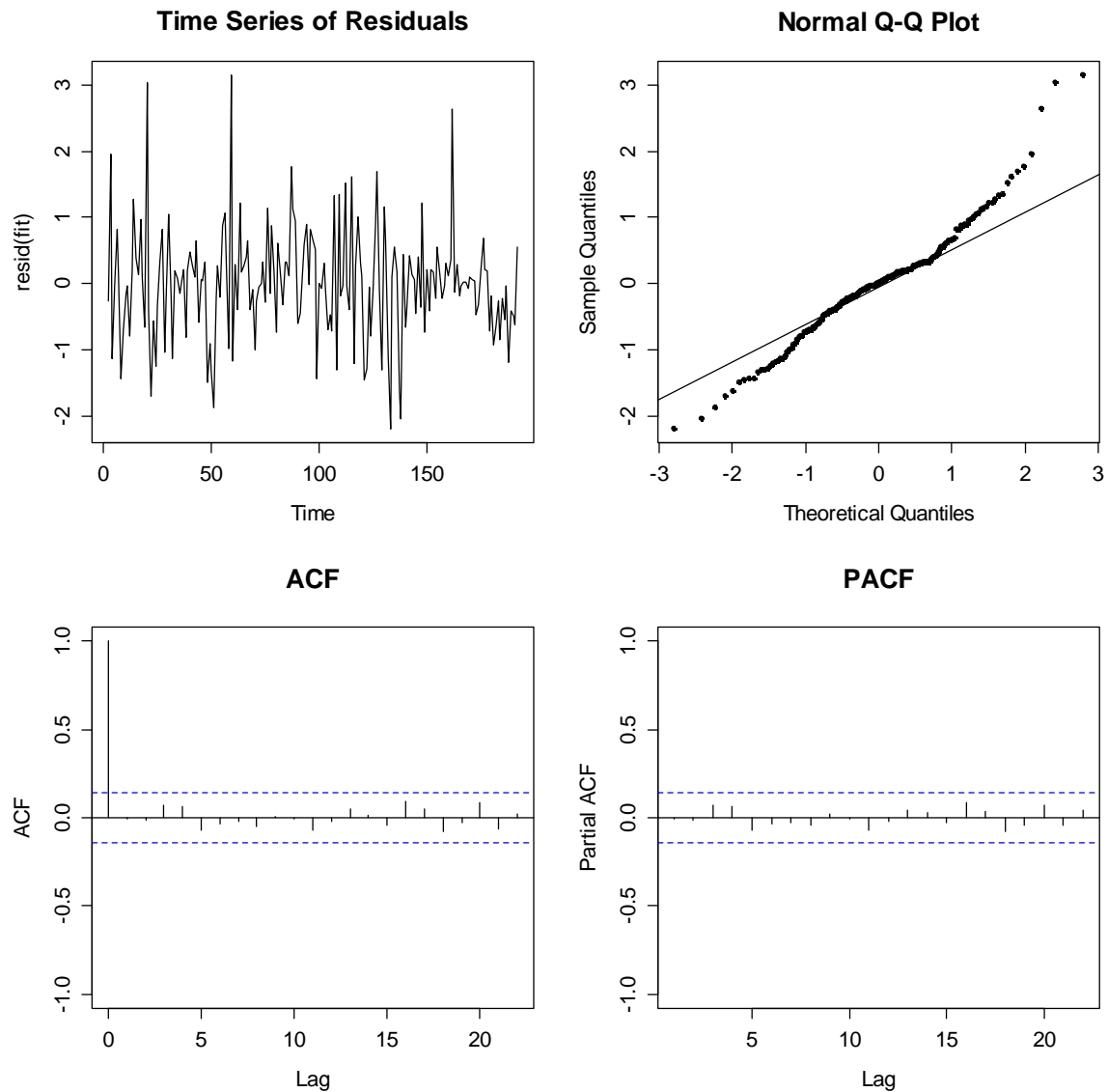
Coefficients:
          ma1  intercept
      -0.2865   -0.0247
s.e.    0.0671    0.0426

sigma^2 = 0.6795: log likelihood = -234.16, aic = 474.31
```

Please note that the application of the three estimation procedures here was just for illustrative purposes, and to show the (slight) differences that manifest themselves when different estimators are employed. In any practical work, you can easily restrict yourself to the application of the `arima()` procedure using the default fitting by `method="CSS-ML"`.

For verifying the quality of the fit, a residual analysis is mandatory. The residuals of the  $MA(1)$  are estimates of the innovations  $E_t$ . The model can be seen as adequate if the residuals reflect the main properties of the innovations. Namely, they should be stationary and free of any dependency, as well as approximately Gaussian. We can verify this by producing a time series plot of the residuals, along with their ACF and PACF, and a Normal QQ-Plot. Sometimes, it is also instructive to plot the fitted values into the original data, or to simulate from the fitted process, since this further helps verifying that the fit is good.

```
> par(mfrow=c(2,2))
> fit <- arima(diff(attbond), order=c(0,0,1))
> plot(resid(fit))
> qqnorm(resid(fit)); qqline(resid(fit))
> acf(resid(fit)); pacf(resid(fit))
```



There are no (partial) autocorrelations that exceed the confidence bounds, hence we can safely conjecture that the residuals are not correlated and hence, all the dependency signal has been captured by the  $MA(1)$ . When inspecting the time series of the residuals, it seems stationary. However, what catches the attention is the presence of three positive outliers and the fact that the residuals are generally long-tailed. We might try to overcome this problem by a log-transformation, but this is left to the reader.

## 5.5 ARMA(p,q) Models

Here, we discuss models that feature both dependency on previous observations  $X_{t-1}, X_{t-2}, \dots$  as well as previous innovations terms  $E_{t-1}, E_{t-2}, \dots$ . Thus, they are a hybrid between  $AR(p)$  and  $MA(q)$  models, and aptly named  $ARMA(p, q)$ . Their importance lies in the fact that it is possible to model a far wider spectrum of dependency structures, and that they are parsimonious: often, an  $ARMA(p, q)$  requires (far) fewer parameters than pure  $AR$  or  $MA$  processes would.

### 5.5.1 Definition and Properties

The formal definition of an  $ARMA(p, q)$  process is as follows:

$$X_t = \alpha_1 X_{t-1} + \dots + \alpha_p X_{t-p} + E_t + \beta_1 E_{t-1} + \dots + \beta_q E_{t-q}$$

As before, we assume that  $E_t$  is causal and White Noise, i.e. an innovation with mean  $E[E_t] = 0$  and finite variance  $Var(E_t) = \sigma_E^2$ . It is much more convenient to use the characteristic polynomials  $\Phi(\cdot)$  for the  $AR$  part, and  $\Theta(\cdot)$  for the  $MA$  part, because this allows for a very compact notation:

$$\Phi(B)X_t = \Theta(B)E_t.$$

It is obvious that all relevant properties of an  $ARMA(p, q)$  process lie in the characteristic polynomials. If the roots of  $\Phi(\cdot)$  are outside of the unit circle, the process will be stationary and have mean zero. On the other hand, if the roots of  $\Theta(\cdot)$  are outside of the unit circle, the process is invertible. Both properties are important for practical application. If they are met, we can rewrite any  $ARMA(p, q)$  in the form of a  $AR(\infty)$  or an  $MA(\infty)$ . This explains why fitting an  $ARMA(p, q)$  can in practice often be replaced by fitting  $AR$ - or  $MA$ -models with high orders (although it is not a good idea to do so!). As has been argued above, any stationary  $ARMA(p, q)$  has mean zero, i.e.  $E[X_t] = 0$ . Thus, in practice we will often consider shifted  $ARMA$ -processes that are of the form:

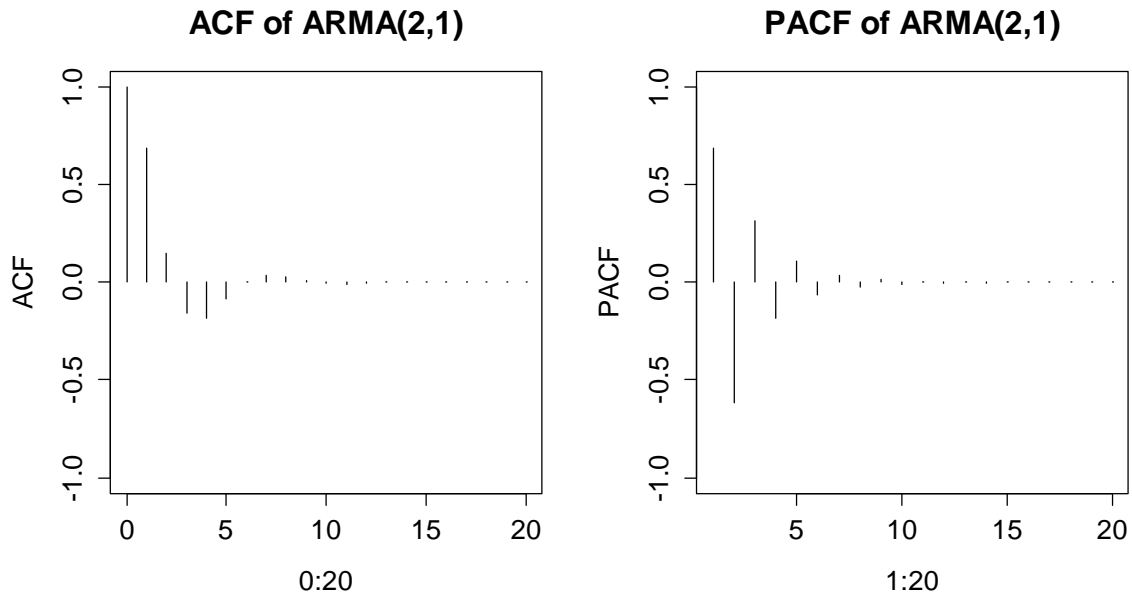
$$Y_t = m + X_t, \text{ where } X_t \text{ is an } ARMA(p, q).$$

In principle, it is straightforward to derive the ACF of an  $ARMA(p, q)$ , though algebraically a bit tedious. Given the applied focus of this scriptum, we do without and focus on the results and consequences instead. We illustrate the typical behavior of the  $ARMA$  autocorrelations on the basis of an example. Namely, we consider the  $ARMA(2, 1)$  defined by:

$$X_t - 0.8X_{t-1} + 0.4X_{t-2} = E_t + 0.6E_{t-1}$$

On the next page, we exhibit the (theoretical) ACF and PACF. It is typical that neither the ACF nor the PACF cut-off strictly at a certain lag. Instead, they both show some infinite behavior, i.e. an exponential decay in the magnitude of the coefficients. However, superimposed on that is a sudden drop-off in both ACF and PACF. In our example, it is after lag 1 in the ACF, as induced by the moving average order  $q = 1$ . In the PACF, the drop-off happens after lag 2, which is the logical consequence of the autoregressive order of  $p = 2$ . The general behavior of the ACF and PACF is summarized in the table below.

Model	ACF	PACF
$AR(p)$	infinite / exp. decay	cut-off at lag $p$
$MA(q)$	cut-off at lag $q$	infinite / exp. decay
$ARMA(p, q)$	infinite / mix of decay & cut-off	infinite / mix of decay & cut-off



It is important to know that with  $ARMA(p, q)$  processes, a wealth of autocorrelation structures can be generated. As to how visible the two cut-offs in ACF and PACF are, resp. whether the cut-off or the decay is dominating, depends on the model's coefficients. There are  $ARMA$ 's where the  $AR$  part is dominating, there are others where the  $MA$  is stronger, and of course they can also be on an equal footing.

### 5.5.2 Fitting

The above properties of ACF and PACF can be exploited for choosing the type and order of a time series model. In particular, if neither the ACF nor the PACF shows a pronounced cut-off, where after some low lag (i.e.  $p$  or  $q < 10$ ) all the following correlations are non-significantly different from zero, then it is usually wise to choose an  $ARMA(p, q)$ . For determining the order  $(p, q)$ , we search for the superimposed cut-off in the ACF (for  $q$ ), respectively PACF (for  $p$ ). The drop-off is not always easy to identify in practice. In "difficult" situations, it has also proven beneficial to support the choice of the right order with the AIC criterion. We could for example perform a grid search on all possible  $ARMA(p, q)$  models which do not use more than 5 parameters, i.e.  $p + q < 5$ . This can readily be done in  $\mathbf{R}$  by programming a `for()` loop.

It is very important to know that  $ARMA$  models are parsimonious, i.e. they usually do not require high orders  $p$  and  $q$ . In particular, they work well with far fewer parameters than pure  $AR$  or  $MA$  models would. Or in other words: often it is possible to fit high-order  $AR(p)$ 's or  $MA(q)$ 's instead of a low-order  $ARMA(p, q)$ . That property does not come as a surprise: as we conjectured above, any stationary and invertible  $ARMA$  can be represented in the form of an  $AR(\infty)$  or an  $MA(\infty)$ . However, this is not a good idea in practice: estimating parameters "costs money", i.e. will lead to less precise estimates. Thus, a low-order  $ARMA(p, q)$  is always to be preferred over a high-order  $AR(p)$  or  $MA(q)$ .

For estimating the coefficients, we are again confronted with the fact that there are no explicit estimators available. This is due to the *MA* component in the model which involves innovation terms that are unobservable. By rearranging terms in the model equation, we can again represent any  $ARMA(p, q)$  in a form where it only depends on the observed  $X_t$ , the coefficients  $\alpha_1, \dots, \alpha_p; \beta_1, \dots, \beta_q$  and some previous innovations  $E_t$  with  $t < 1$ . If these latter terms are all set to zero, we can determine the optimal set of model coefficients by minimizing the sum of squared residuals (i.e. innovations) with a numerical method. This is the CSS approach that was already mentioned in 5.4.2 and is implemented in function `arma()` when `method="CSS"`. By default however, these CSS estimates are only used as starting values for a MLE. If Gaussian innovations are assumed, then the joint distribution of any  $ARMA(p, q)$  process vector  $X = (X_1, \dots, X_n)$  has a multivariate normal distribution.

$$X = (X_1, \dots, X_n) \sim N(0, V), \text{ resp. } Y = (Y_1, \dots, Y_n) \sim N(m \cdot \underline{1}, V).$$

MLE then relies on determining the parameters  $m$  (if a shifted  $ARMA(p, q)$  is estimated),  $\alpha_1, \dots, \alpha_p; \beta_1, \dots, \beta_q$  and  $\sigma_E^2$  simultaneously by maximizing the probability density function of the above multivariate Gaussian with assuming the data  $x_1, \dots, x_n$  as given quantities. This is a quite complex non-linear problem which needs to be solved numerically. A good implementation is found in **R**'s `arma()`. As was stated previously, the benefit of MLE is that (under mild and mostly met conditions) some optimality is guaranteed. In particular, the estimates are asymptotically normal with minimum variance among all asymptotically normal estimators. Another benefit is provided by the standard errors which allow for judging the precision of the estimates.

## 6 SARIMA and GARCH Models

As we have discovered previously, many time series are non-stationary due to deterministic trends and/or seasonal effects. While we have learned to remove these and then explain the remainder with some time series models, there are other models that can directly incorporate trend and seasonality. While they usually lack some transparency for the decomposition, their all-in-one approach allows for convenient forecasting, and also AIC-based decisions for choosing the right amount of trend and seasonality modeling become feasible.

Time series from financial or economic background often show serial correlation in the conditional variance, i.e. are conditionally heteroskedastic. This means that they exhibit periods of high and low volatility. Understanding the behavior of such series pays off, and the usual approach is to set up autoregressive models for the conditional variance. These are the famous ARCH models, which we will discuss along with their generalized variant, the GARCH class.

### 6.1 ARIMA Models

ARIMA models are aimed at describing series which exhibit a deterministic trend that can be removed by differencing; and where these differences can be described by an  $ARMA(p, q)$  model. Thus, the definition of an  $ARIMA(p, d, q)$  process arises naturally:

**Definition:** A series  $X_t$  follows an  $ARIMA(p, d, q)$  model if the  $d$ th order difference of  $X_t$  is an  $ARMA(p, q)$  process. If we introduce

$$Y_t = (1 - B)^d X_t,$$

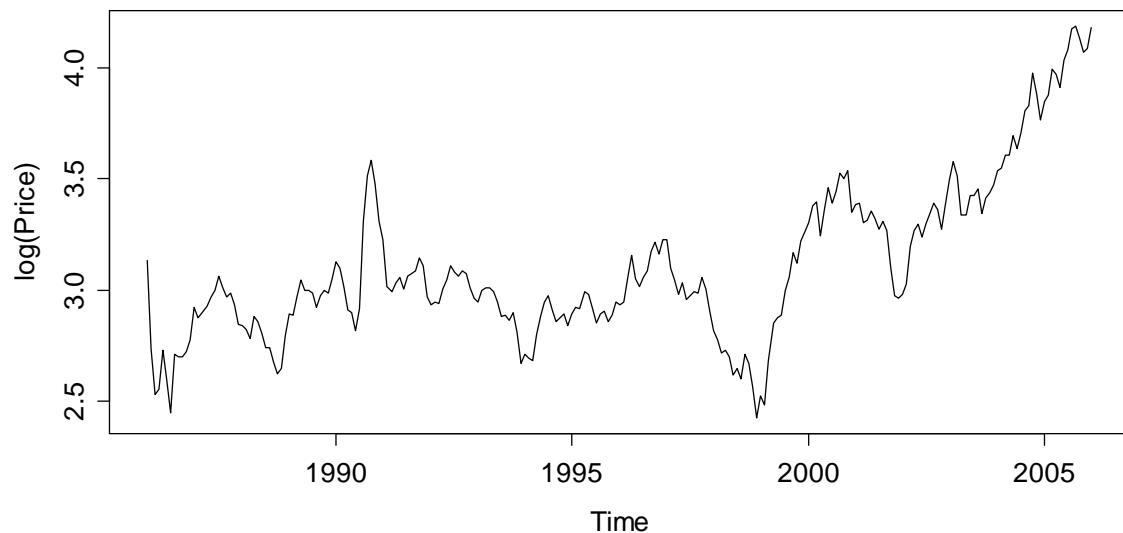
where  $B$  is the backshift operator, then we can write the  $ARIMA$  process using the characteristics polynomials, i.e.  $\Theta(\cdot)$  that accounts for the  $AR$ , and  $\Phi(\cdot)$  that stands for the  $MA$  part.

$$\begin{aligned}\Phi(B)Y_t &= \Theta(B)E_t \\ \Phi(B)(1-B)^d X_t &= \Theta(B)E_t\end{aligned}$$

Such series do appear in practice, as our example of the monthly prices for a barrel of crude oil (in US\$) from January 1986 to January 2006 shows. To stabilize the variance, we decide to log-transform the data, and model these.

```
> library(TSA)
> data(oil.price)
> lop <- log(oil.price)
> plot(lop, ylab="log(Price)")
> title("Logged Monthly Price for a Crude Oil Barrel")
```

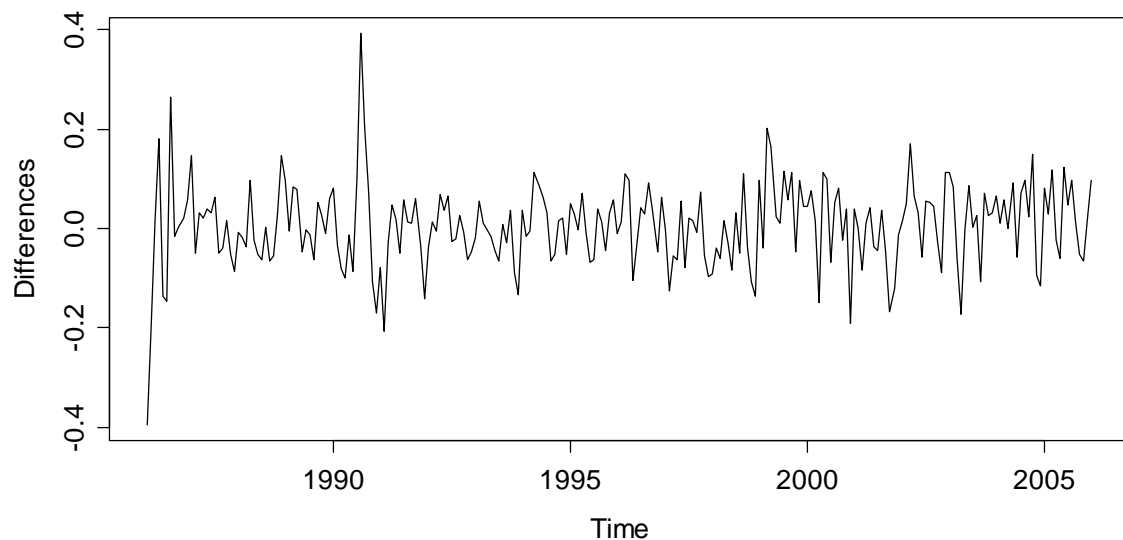
### Logged Monthly Price for a Crude Oil Barrel



The series does not exhibit any apparent seasonality, but there is a clear trend, so that it is non-stationary. We try first-order (i.e.  $d = 1$ ) differencing, and then check whether the result is stationary.

```
> dlop <- diff(lop)
> plot(dlop, ylab="Differences")
> title("Differences of Logged Monthly Crude Oil Prices")
```

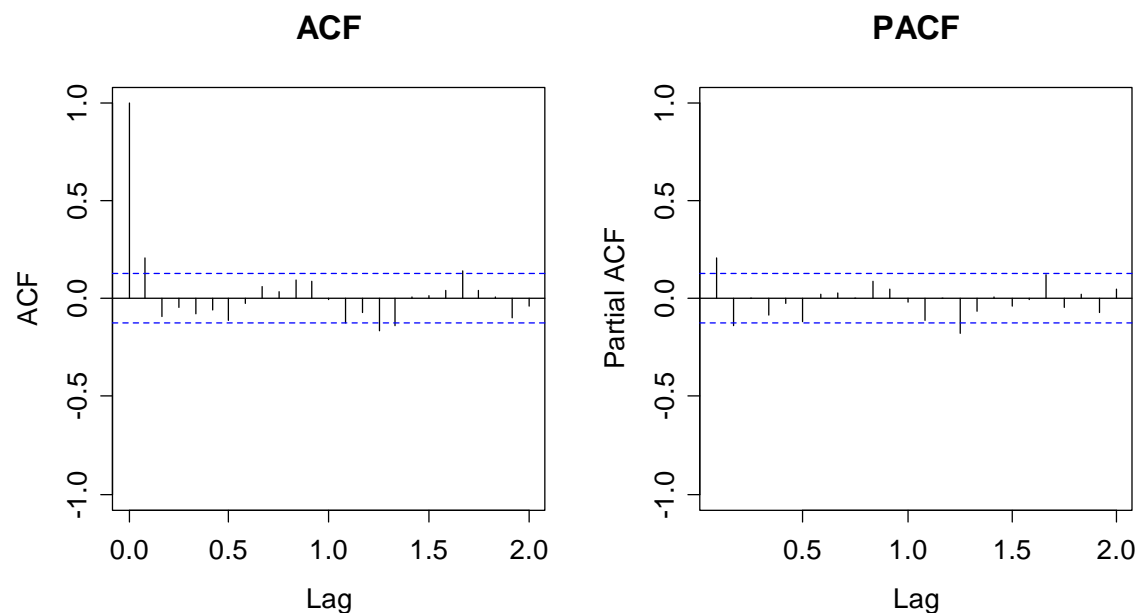
### Differences of Logged Monthly Crude Oil Prices



The trend was successfully removed by taking differences. ACF and PACF show that the result is serially correlated. There may be a drop-off in the ACF at lag 1, and in the PACF at either lag 1 or 2, suggesting an  $ARIMA(1,1,1)$  or an  $ARIMA(2,1,1)$  for the logged oil prices. However, the best performing model is somewhat surprisingly an  $ARIMA(1,1,2)$ , for which we show the results.



```
> par(mfrow=c(1,2))
> acf(dlop, main="ACF", ylim=c(-1,1), lag.max=24)
> pacf(dlop, main="ACF", ylim=c(-1,1), lag.max=24)
```



The fitting can be done with the `arima()` procedure that (by default) estimates the coefficients using Maximum Likelihood with starting values obtained from the Conditional Sum of Squares method. We can either let the procedure do the differencing:

```
> arima(lop, order=c(1,1,2))
```

Call:

```
arima(x = lop, order = c(1, 1, 2))
```

Coefficients:

	ar1	ma1	ma2
	0.8429	-0.5730	-0.3104
s.e.	0.1548	0.1594	0.0675

```
sigma^2 = 0.006598: log likelihood = 261.88, aic = -515.75
```

Or, we can use the differenced series `dlop` as input and fit an  $ARMA(1,2)$ . However, we need to tell `R` to not include an intercept – this is not necessary when the trend was removed by taking differences. The command is:

```
> arima(dlop, order=c(1,0,2), include.mean=FALSE)
```

The output from this is exactly the same as above. The next step is to perform residual analysis – if the model is appropriate, they must look like White Noise. This is (data not shown here) more or less the case. For decisions on the correct model order, also the AIC statistics can provide valuable information.

We finish this section by making some considerations on the model equation. We have:

$$\begin{aligned} Y_t &= 0.84 \cdot Y_{t-1} + E_t - 0.57 \cdot E_{t-1} - 0.31 \cdot E_{t-2} \\ X_t - X_{t-1} &= 0.84 \cdot (X_{t-1} - X_{t-2}) + E_t - 0.57 \cdot E_{t-1} - 0.31 \cdot E_{t-2} \\ X_t &= 1.84 \cdot X_{t-1} - 0.84 \cdot X_{t-2} + E_t - 0.57 \cdot E_{t-1} - 0.31 \cdot E_{t-2} \end{aligned}$$

Thus, the  $ARIMA(1,1,2)$  can be rewritten as a non-stationary  $ARMA(2,2)$ . The non-stationarity is due to the roots of the AR characteristic polynomial, which are within the unit circle. Finally, we give some recipe for fitting  $ARIMA$  models:

- 1) Choose the appropriate order of differencing, usually  $d = 1$  or (in rare cases)  $d = 2$ , such that the result is a stationary series.
- 2) Analyze ACF and PACF of the differenced series. If the stylized facts of an  $ARMA$  process are present, decide for the orders  $p$  and  $q$ .
- 3) Fit the model using the `arima()` procedure. This can be done on the original series by setting  $d$  accordingly, or on the differences, by setting  $d = 0$  and argument `include.mean=FALSE`.
- 4) Analyze the residuals; these must look like White Noise. If several competing models are appropriate, use AIC to decide for the winner.

The fitted  $ARIMA$  model can then be used to generate forecasts including prediction intervals. This will, however, only be discussed in section 8.

## 6.2 SARIMA Models

After becoming acquainted with the  $ARIMA$  models, it is quite natural to ask for an extension to seasonal series; especially, because we learned that differencing at a lag equal to the period  $s$  does remove seasonal effects, too. Suppose we have a series  $X_t$  with monthly data. Then, series

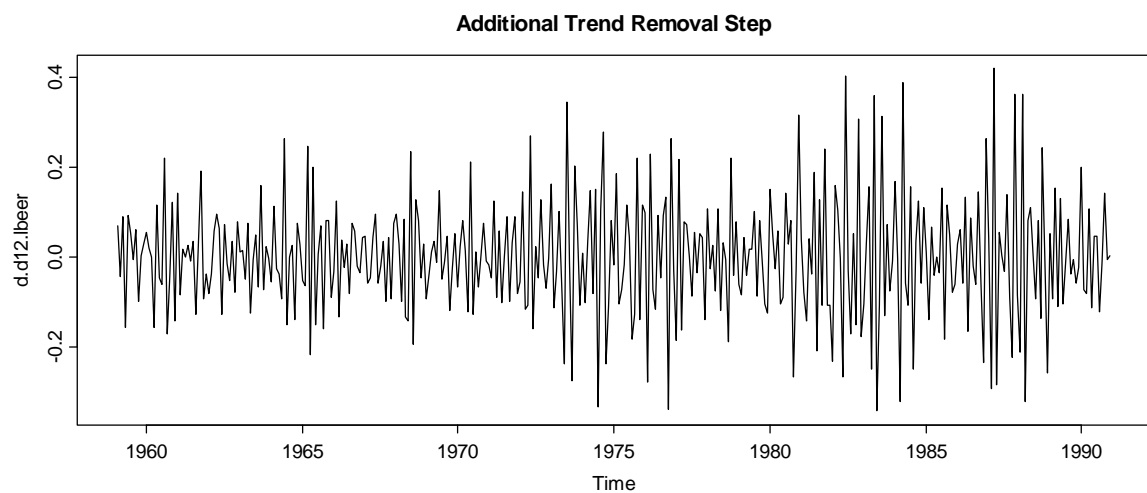
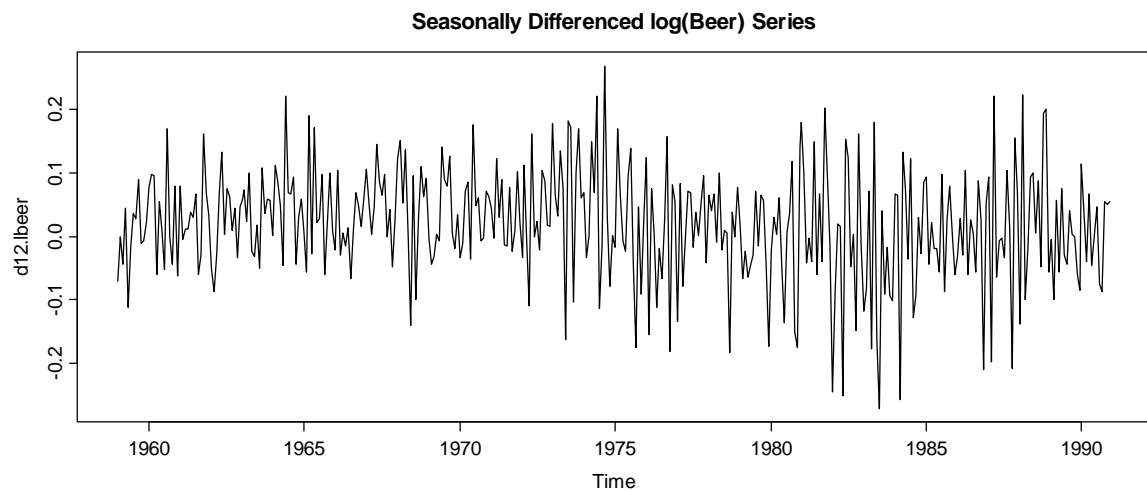
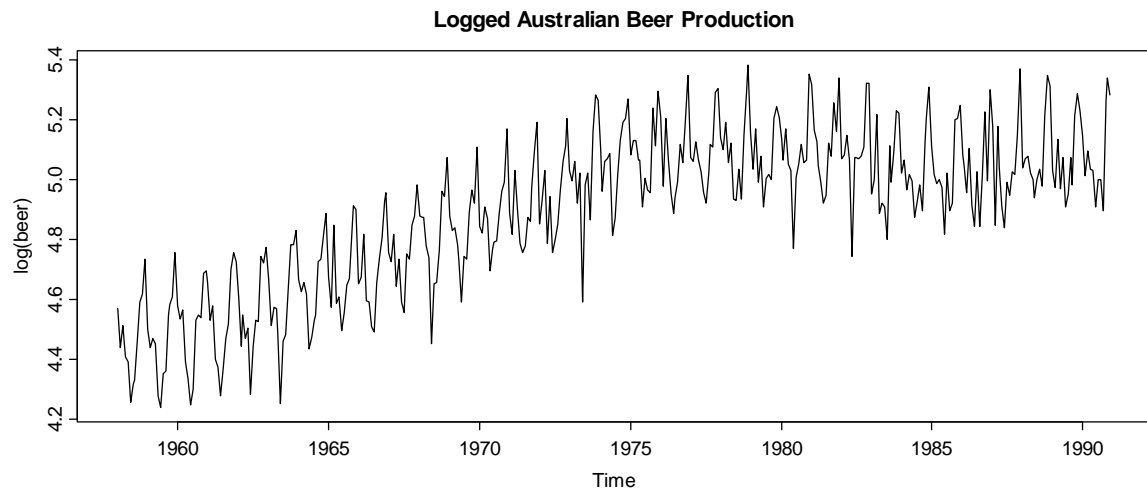
$$Y_t = X_t - X_{t-12} = (1 - B^{12})X_t$$

has the seasonality removed. However, it is quite often the case that the result has not yet constant mean, and thus, some further differencing at lag 1 is required to achieve stationarity:

$$Z_t = Y_t - Y_{t-1} = (1 - B)Y_t = (1 - B)(1 - B^{12})X_t = X_t - X_{t-1} - X_{t-12} + X_{t-13}$$

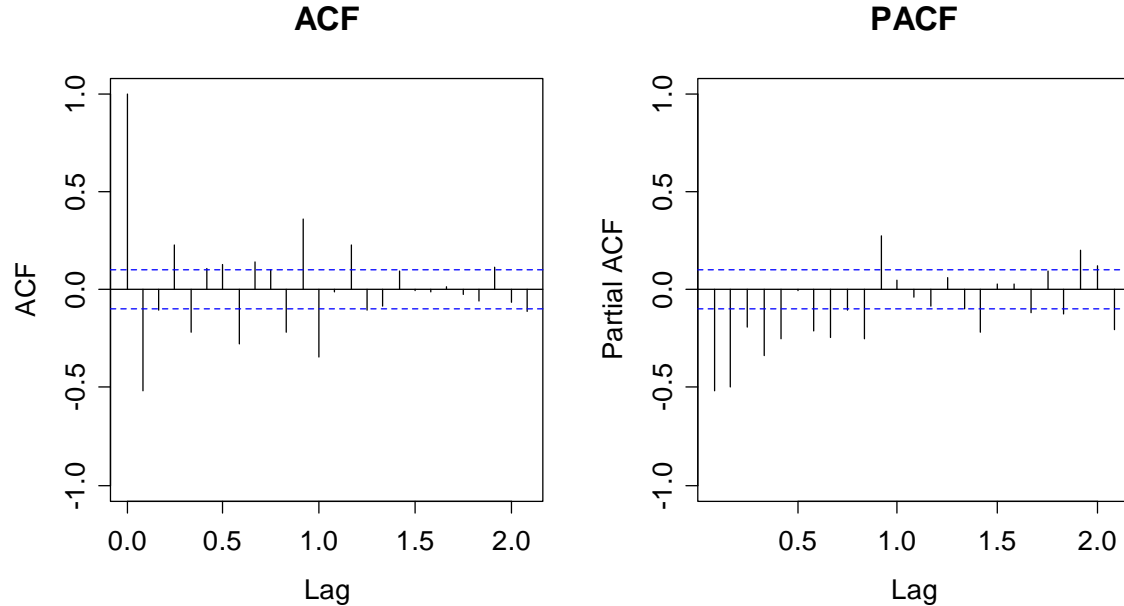
We illustrate this using the Australian beer production series that we had already considered in section 4. It has monthly data that range from January 1958 to December 1990. Again, a log-transformation to stabilize the variance is indicated. On the next page, we display the original series  $X_t$ , the seasonally differenced series  $Y_t$  and finally the seasonal-trend differenced series  $Z_t$ .

```
> www <- "http://staff.elena.aut.ac.nz/Paul-Cowpertwait/ts/"
> dat <- read.table(paste(www,"cbe.dat",sep="", header=T)
> beer      <- ts(dat$beer, start=1958, freq=12)
> d12.lbeer <- diff(log(beer), lag=12)
> d.d12.lbeer <- diff(d12.lbeer)
> plot(log(beer))
> plot(d12.lbeer)
> plot(d.d12.lbeer))
```



While the two series  $X_t$  and  $Y_t$  are non-stationary, the last one,  $Z_t$  may be, although it is a bit debatable whether the assumption of constant variation is violated or not. We proceed by analyzing ACF and PACF of series  $Z_t$ .

```
> par(mfrow=c(1,2))
> acf(d.d12.lbeer, ylim=c(-1,1))
> pacf(d.d12.lbeer, ylim=c(-1,1), main="PACF")
```



There is very clear evidence that series  $Z_t$  is serially dependent, and we could try an  $ARMA(p,q)$  to model this dependence. As for the choice of the order, this is not simple on the basis of the above correlograms. They suggest that high values for  $p$  and  $q$  are required, and model fitting with subsequent residual analysis and AIC inspection confirm this:  $p=14$  and  $q=11$  yield a good result.

It is (not so much in the above, but generally when analyzing data of this type) quite striking that the ACF and PACF coefficients have large values at multiples of the period  $s$ . This is very typical behavior for seasonally differenced series, in fact it originates from the evolution of resp. changes in the seasonality over the years. A simple model accounting for this is the so-called *airline model*:

$$\begin{aligned} Z_t &= (1 + \beta_1 B)(1 + \xi_1 B^{12})E_t \\ &= (1 + \beta_1 B + \xi_1 B^{12} + \beta_1 \xi_1 B^{13})E_t \\ &= E_t + \beta_1 E_{t-1} + \xi_1 E_{t-12} + \beta_1 \xi_1 E_{t-13} \end{aligned}$$

This is a MA(13) model, where many of the coefficients are equal to 0. Because it was made up of an MA(1) with  $B$  as an operator in the characteristic polynomial, and another one with  $B^s$  as the operator, we call this a SARIMA(0,1,1)(0,1,1)<sup>12</sup>. This idea can be generalized: we fit AR and MA parts with both  $B$  and  $B^s$  as operators in the characteristic polynomials, which again results in a high order  $ARMA$  model for  $Z_t$ .

**Definition:** A series  $X_t$  follows a  $SARIMA(p,d,q)(P,D,Q)^s$  process if the following equation holds:

$$\Phi(B)\Phi_s(B^s)Z_t = \Theta(B)\Theta_s(B^s)E_t,$$

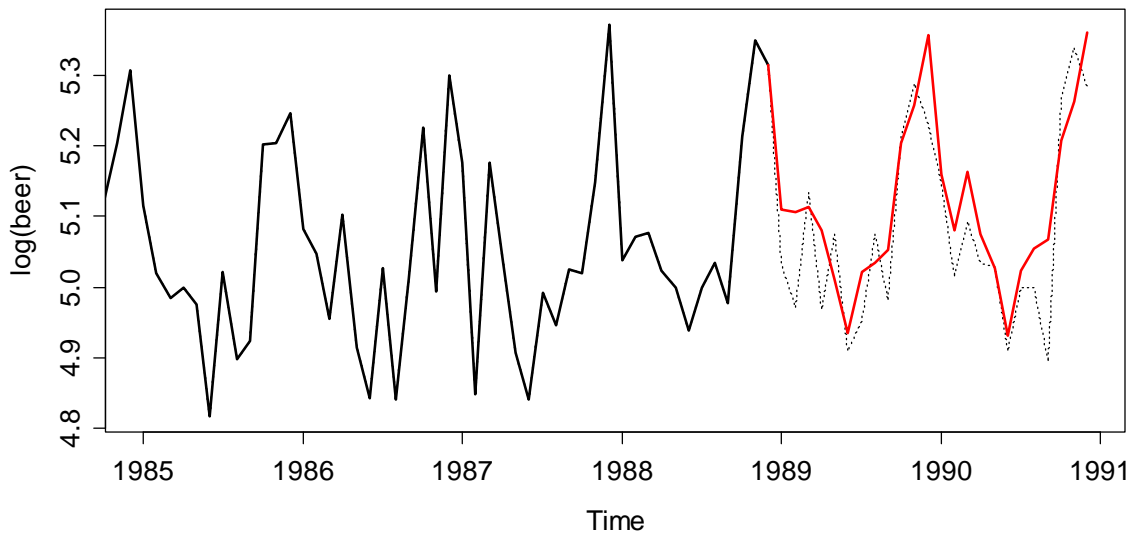
where series  $Z_t$  originated from  $X_t$  after appropriate seasonal and trend differencing, i.e.  $Z_t = (1-B)^d(1-B^s)^D$ .

Fortunately, it turns out that usually  $d = D = 1$  is enough. As for the model orders  $p, q, P, Q$ , the choice can be made on the basis of ACF and PACF, by searching for cut-offs. Mostly, these are far from evident, and thus, an often applied alternative is to consider all models with  $p, q, P, Q \leq 2$  and doing an AIC-based grid search.

For our example, the  $SARIMA(2,1,2)(2,1,2)^{12}$  has the lowest value and also shows satisfactory residuals, although it seems to perform slightly less well than the  $SARIMA(14,1,11)(0,1,0)^{12}$ . The R-command for the former is:

```
> fit <- arima(log(beer), order=c(2,1,2), seasonal=c(2,1,2))
```

**Forecast of log(beer) with SARIMA(2,1,2)(2,1,2)**



As it was mentioned in the introduction to this section, one of the main advantages of *ARIMA* and *SARIMA* models is that they allow for quick and convenient forecasting. While this will be discussed in depth later in section 8, we here provide a first example to show the potential.

From the logged beer production data, the last 2 years were omitted before the *SARIMA* model was fitted to the (shortened) series. On the basis of this model, a 2-year-forecast was computed, which is displayed by the red line in the plot above. The original data are shown as a solid (insample, 1958-1988) line, respectively as a dotted (out-of-sample, 1989-1990) line. We see that the forecast is reasonably accurate.

To facilitate the fitting of *SARIMA* models, we finish this chapter by providing some guidelines:

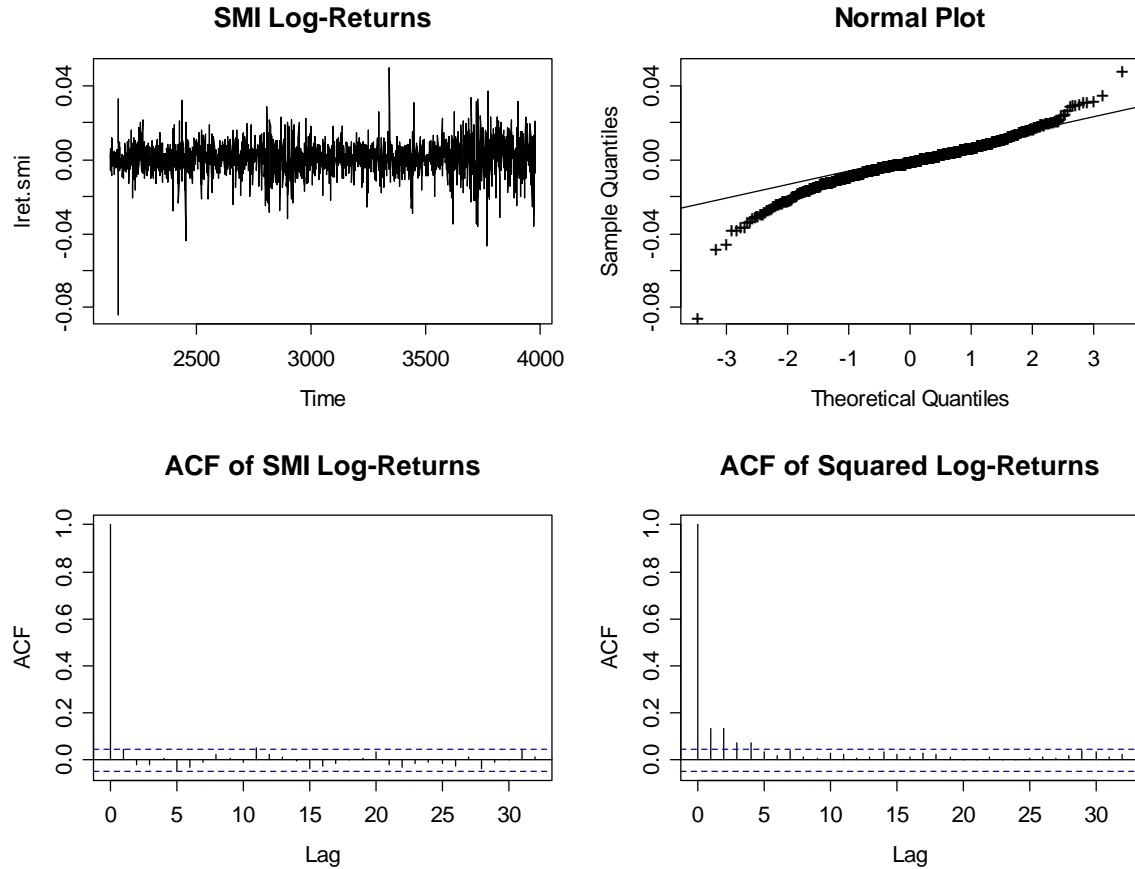
- 1) Perform seasonal differencing on the data. The lag  $s$  is determined by the periodicity of the data, for the order, in most cases  $D = 1$  is sufficient.
- 2) Do a time series plot of the output of the above step. Decide whether it is stationary, or whether additional differencing at lag 1 is required to remove a potential trend. If not, then  $d = 0$ , and proceed. If yes,  $d = 1$  is enough for most series.
- 3) From the output of step 2, i.e. series  $Z_t$ , generate ACF and PACF plots to study the dependency structure. Look for coefficients/cut-offs at low lags that indicate the direct, short-term dependency and determine orders  $p$  and  $q$ . Then, inspect coefficients/cut-offs at multiples of the period  $s$ , which imply seasonal dependency and determine  $P$  and  $Q$ .
- 4) Fit the model using procedure `arima()`. In contrast to *ARIMA* fitting, this is now exclusively done on the original series, with setting the two arguments `order=c(p,d,q)` and `seasonal=c(P,D,Q)` accordingly.
- 5) Check the accuracy of the fitted model by residual analysis. These must look like White Noise. If thus far, there is ambiguity in the model order, AIC analysis can serve to come to a final decision.

Next, we turn our attention to series that have neither trend nor seasonality, but show serial dependence in the conditional variance.

## 6.3 ARCH/GARCH Models

In this chapter, we consider the SMI log-returns that were already presented in section 1.2.4. By closer inspection of the time series plot, we observe some long-tailedness, and also, the series exhibits periods of increased variability, which is usually termed volatility in the (financial) literature. We had previously observed series with non-constant variation, such as the oil prices and beer production in the previous sections. Such series, where the variance increases with increasing level of the series, are called *heteroskedastic*, and can often be stabilized using a log-transformation.

However, that matter is different with the SMI log-returns: here, there are periods of increased volatility, and thus the conditional variance of the series is serially correlated, a phenomenon that is called *conditional heteroskedasticity*. This is not a violation of the stationarity assumption, but some special treatment for this type of series is required. Furthermore, the ACF of such series typically does not differ significantly from White Noise. Still, the data are not *iid*, which can be shown with the ACF of the squared observations. With the plots on the next page, we illustrate the presence of these stylized facts for the SMI log-returns:



### 6.3.1 The ARCH and GARCH Models

In order to account for volatility, we require a model that reflects the dependency in the conditional variance. We operate under the assumption that:

$$X_t = \mu_t + E_t,$$

where the disturbance term  $E_t$  can be rewritten as  $\sigma_t W_t$ :  $X_t = \mu_t + \sigma_t W_t$ . Here,  $W_t$  is a White Noise innovation and  $\sigma_t = \text{Var}(X_t | X_{t-1}, X_{t-2}, \dots)$  is the conditional variance that is assumed to be non-constant. Finally  $\mu_t = E[X_t | X_{t-1}, X_{t-2}, \dots]$  is the conditional expectation as before. It is perfectly allowed to have both dependence in the conditional mean and variance, and hence a mixture of *ARMA* and *GARCH* processes. However, for simplicity we assume throughout this section that both the conditional and the global mean are zero:  $\mu = \mu_t = 0$  and thus  $X_t = \sigma_t W_t$ .

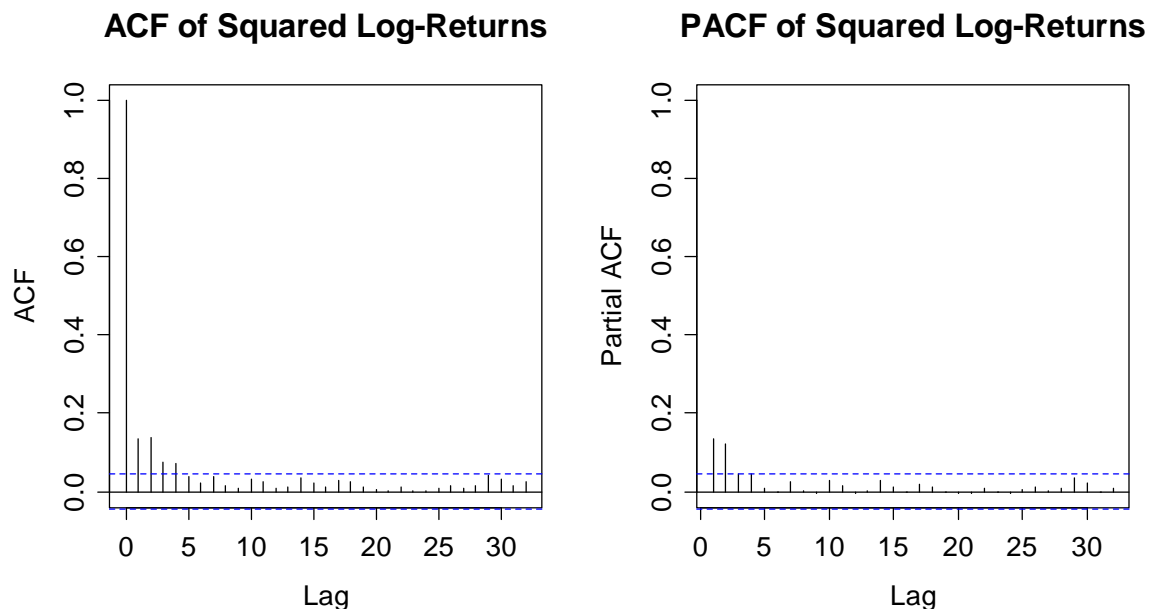
The most simple and intuitive way of doing this is to use an autoregressive model for the variance process. Thus, a series  $E_t$  is first-order autoregressive conditional heteroskedastic, denoted as *ARCH*(1), if:

$$E_t = W_t \sqrt{\alpha_0 + \alpha_1 E_{t-1}^2}.$$

Here,  $W_t$  is a White Noise process with mean zero and unit variance. The two parameters  $\alpha_0, \alpha_1$  are the model coefficients. An  $ARCH(1)$  process shows volatility, as can easily be derived:

$$\begin{aligned} \text{Var}(E_t) &= E[E_t^2] \\ &= E[W_t^2]E[\alpha_0 + \alpha_1 E_{t-1}^2] \\ &= E[\alpha_0 + \alpha_1 E_{t-1}^2] \\ &= \alpha_0 + \alpha_1 \cdot \text{Var}(E_{t-1}) \end{aligned}$$

Note that this derivation is based on  $E[W_t^2]=1$  and  $E[E_t]=E[W_t]=0$ . As we had aimed for, the variance of an  $ARCH(1)$  process behaves just like an  $AR(1)$  model. Hence, the decay in the autocorrelations of the squared residuals should indicate whether an  $ARCH(1)$  is appropriate or not.



In our case, the analysis of ACF and PACF of the squared log-returns suggests that the variance may be well described by an  $AR(2)$  process. This is not what we had discussed, but an extension exists. An  $ARCH(p)$  process is defined by:

$$E_t = W_t \sqrt{\alpha_0 + \sum_{i=1}^p \alpha_i E_{t-i}^2}$$

Fitting in **R** can be done using procedure `garch()`. This is a more flexible tool, which also allows for fitting GARCH processes, as discussed below. The command in our case is as follows:

```
> fit <- garch(lret.smi, order = c(0,2), trace=FALSE); fit
Call: garch(x = lret.smi, order = c(0, 2), trace = FALSE)
Coefficient(s):
      a0      a1      a2
6.568e-05 1.309e-01 1.074e-01
```



For verifying appropriate fit of the  $ARCH(2)$ , we need to check the residuals of the fitted model. This includes inspecting ACF and PACF for both the “normal” and the squared residuals. We here do without showing plots, but the  $ARCH(2)$  is OK.

A nearby question is whether we can also use an  $ARMA(p, q)$  process for describing the dependence in the variance of the process. The answer is yes. This is what a  $GARCH(p, q)$  model does. A series  $E_t = W_t \sqrt{H_t}$  is  $GARCH(p, q)$  if:

$$H_t = \alpha_0 + \sum_{i=1}^q \alpha_i E_{t-i}^2 + \sum_{j=1}^p \beta_j H_{t-j}$$

### 6.3.2 Use of GARCH Models

GARCH models are useless for the prediction of the level of a series, i.e. for the SMI log-returns, they do not provide any idea whether the stocks' value will increase or decrease on the next day. However, they allow for a more precise understanding in the (up or down) changes that might be expected during the next day(s). This allows stockholders to adjust their position, so that they do not take any undue risks.



# 7 Time Series Regression

## 7.1 What Is the Problem?

It is often the case that we aim for describing some time series  $Y_t$  with a linear combination of some explanatory series  $x_{t1}, \dots, x_{tp}$ . As we will see below, the predictors can either be true covariates, or terms that are derived from time, as for example linear trends or seasonal effects. We employ the universally known linear model for linking the response series with the predictors:

$$Y_t = \beta_0 + \beta_1 x_{t1} + \dots + \beta_p x_{tp} + E_t$$

The regression coefficients  $\beta_1, \dots, \beta_p$  are usually estimated with the least squares algorithm, for which an error term with zero expectation, constant variation and no correlation is assumed. However, if response and predictors are time series with autocorrelation, the last condition often turns out to be violated, though this is not always the case.

Now, if we are facing a (time series) regression problem *with* correlated errors, the estimates  $\hat{\beta}_j$  will remain being unbiased, but the least squares algorithm is no longer efficient. Or in other words: more precisely working estimators exist. Even more problematic are the standard errors of the regression coefficients  $\hat{\beta}_j$ : they are often grossly wrong in case of correlated errors. As they are routinely underestimated, inference on the predictors often yields spurious significance, i.e. one is prone to false conclusions from the analysis.

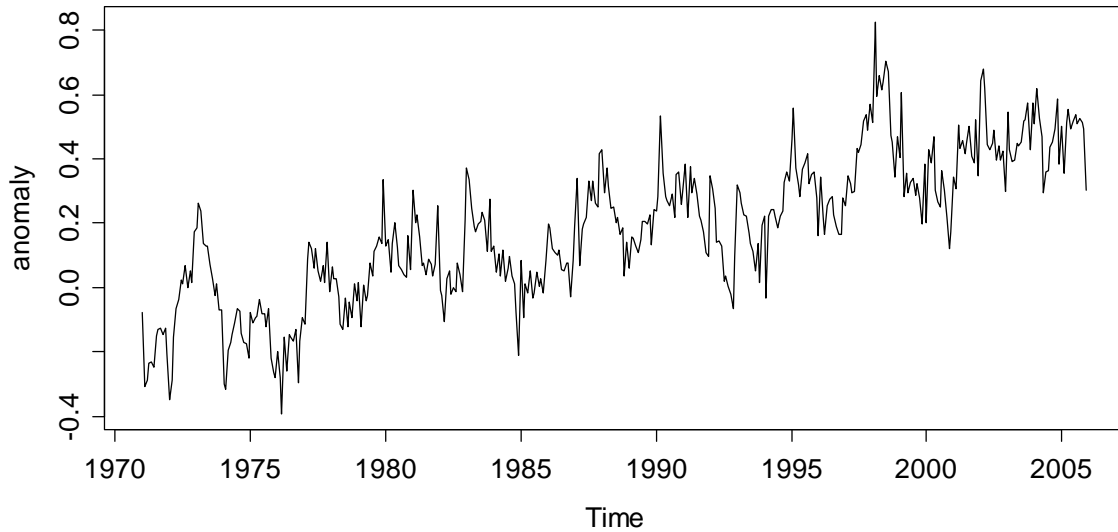
Thus, there is a need for more general linear regression procedures that can deal with serially correlated errors, and fortunately, they exist. We will here discuss the simple, iterative Cochrane-Orcutt procedure, and the Generalized Least Squares method, which marks a theoretically sound approach to regression with correlated errors. But first, we present some time series regression problems to illustrating what we are dealing with.

### Example 1: Global Temperature

In climate change studies time series with global temperature values are analyzed. The scale of measurement is anomalies, i.e. the difference between the monthly global mean temperature versus the overall mean between 1961 and 1990. The data can be obtained at <http://www.cru.uea.ac.uk/cru/data>. For illustrative purposes, we here restrict to a period from 1971 to 2005 which corresponds to a series of 420 records. For a time series plot, see the next page.

```
> ## Time Series Plot
> my.temp <- window(global, c(1971,1), c(2005,12))
> plot(my.temp, ylab="anomaly")
> title("Global Temperature Anomalies")
```

### Global Temperature Anomalies



There is a clear trend which seems to be linear. Despite being monthly measured, the data show no evident seasonality. This is not overly surprising, since we are considering a global mean, i.e. the season should not make for a big difference. But on the other hand, because the landmass is not uniformly distributed over both halves of the globe, it could still be present. It is natural to try a season-trend-decomposition for this series. We will employ a parametric model featuring a linear trend plus a seasonal factor.

$$Y_t = \beta_0 + \beta_1 \cdot t + \beta_2 \cdot 1_{\text{month}=\text{"Feb"}} + \dots + \beta_{12} \cdot 1_{\text{month}=\text{"Dec"}} + E_t,$$

where  $t = 1, \dots, 420$  and  $1_{\text{month}=\text{"Feb"}}$  is a dummy variable that takes the value 1 if an observation is from month February, and zero else. Clearly, this is a time series regression model. The response  $Y_t$  is the global temperature anomalies, and even the predictors, i.e. the time and the dummies, can be seen as time series, even if simple ones.

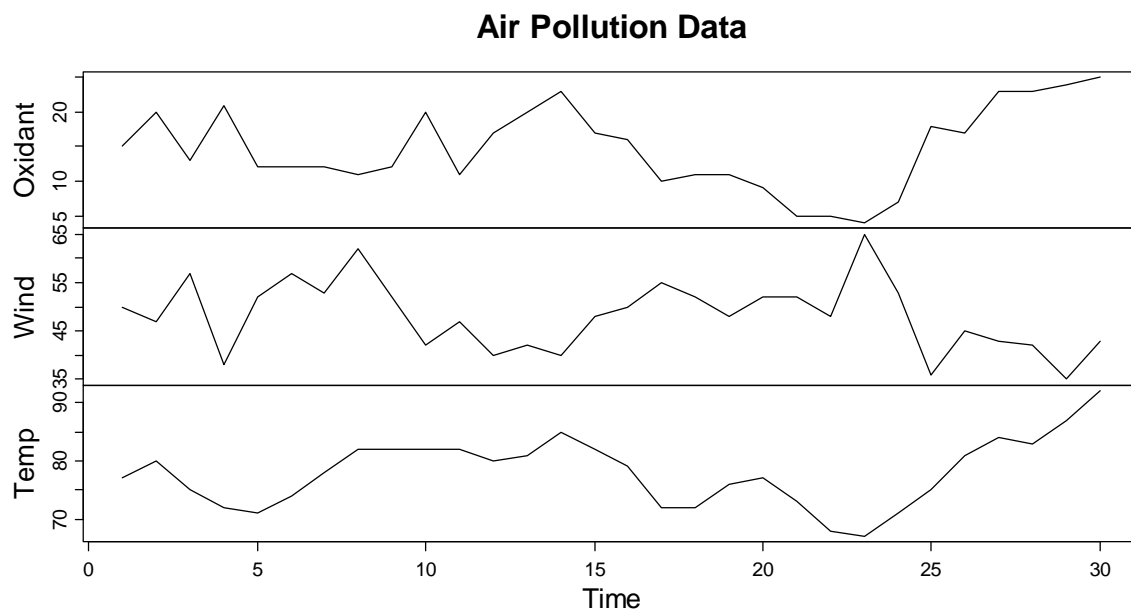
As we have seen previously, the goal with such parametric decomposition models is to obtain a stationary remainder term  $E_t$ . But stationary does not necessarily mean White Noise, and in practice it often turns out that  $E_t$  shows some serial correlation. Thus, if the regression coefficients are obtained from the least squares algorithm, we apparently feature some violated assumption.

This violation can be problematic, even in an applied setting: a question of utter importance with the above series is whether trend and seasonal effect are significantly present. It would be nice to answer such questions using the inference approaches (tests and confidence intervals) that linear regression provides. However, for obtaining reliable inference results, we need to account for the correlation among the errors. We will show this below, after introducing some more examples and theory.

## Example 2: Air Pollution

In this second example, we consider a time series that is stationary, and where the regression aims at understanding the series, rather than decomposing it into some deterministic and random components. We examine the dependence of a photochemical pollutant (morning maximal value) on the two meteorological variables wind and temperature. The series, which constitute of 30 observations taken on consecutive days, come from the Los Angeles basin. They are not publicly available, but can be obtained from the lecturer upon request.

```
> ## Importing the data
> tmp <- read.table("pollute.dat", header=TRUE)
> dat <- ts.union(Oxidant=ts(tmp$Oxidant), Wind=ts(tmp$Wind),
                  Temp=ts(tmp$Temp))
> ## Visualizing the data
> plot(dat, main="Air Pollution Data")
```



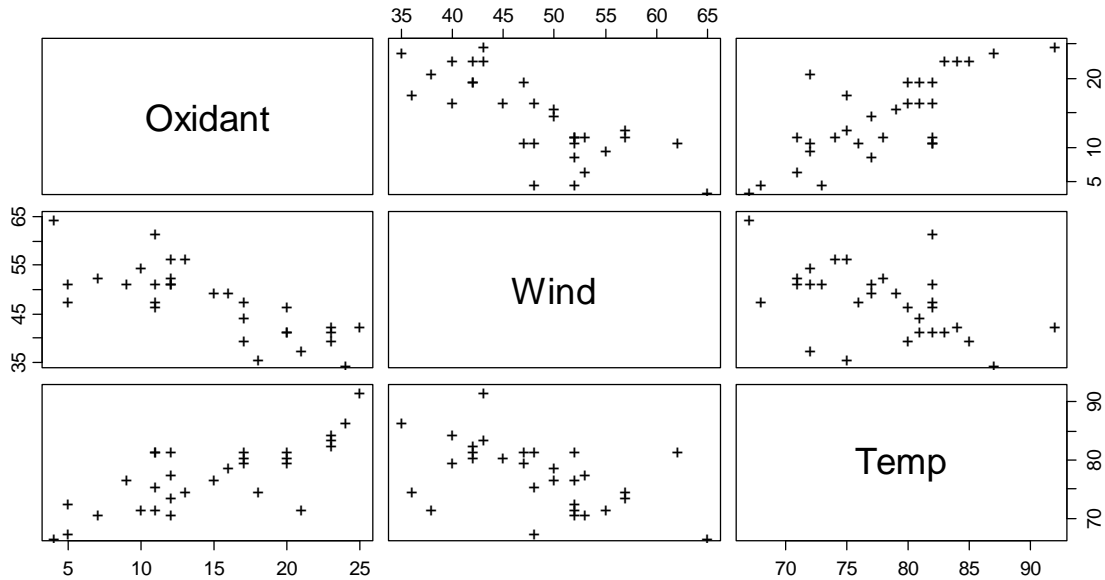
There is no counterevidence to stationarity for all three series. What could be the goal here? Well, we aim for enhancing the understanding of how the pollution depends on the meteorology, i.e. what influence wind and temperature have on the oxidant values. We can naturally formulate the relation with a linear regression model:

$$Y_t = \beta_0 + \beta_1 x_{t1} + \beta_2 x_{t2} + E_t.$$

In this model, the response  $Y_t$  is the oxidant, and as predictors we have  $x_{t1}$ , wind, and  $x_{t2}$ , the temperature. For the index, we have  $t = 1, \dots, 30$ , and obviously, this is a time series regression model.

For gaining some more insight with these data, it is also instructive to visualize the data using a pairs plot, as shown on the next page. There, a strong, positive linear

association is recognizable between pollutant and the temperature. In contrast, there is a negative linear relation between pollutant and wind. Lastly, between the predictors wind and temperature, there is not much of a correlation. This data structure is not surprising because wind causes a stronger movement of the air and thus the pollutant is "better" distributed. Also, the wind causes some cooling.



For achieving our practical goals with this dataset, we require precise and unbiased estimates of the regression coefficients  $\beta_1$  and  $\beta_2$ . Moreover, we might like to give some statements about the significance of the predictors, and thus, we require some sound standard errors for the estimates. However, also with these data, it is well conceivable that the error term  $E_t$  will be serially correlated. Thus again, we will require some procedure that can account for this.

### Time Series Regression Model

The two examples have shown that time series regression models do appear when decomposing series, but can also be important when we try to understand the relation between response and predictors with measurements that were taken sequentially. Generally, with the model

$$Y_t = \beta_0 + \beta_1 x_{t1} + \dots + \beta_p x_{tp} + E_t$$

we assume that the influence of the series  $x_{t1}, \dots, x_{tp}$  on the response  $Y_t$  is simultaneous. Nevertheless, lagged variables are also allowed, i.e. we can also use terms such as  $x_{(t-k);j}$  with  $k > 0$  as predictors. While this generalization can be easily built into our model, one quickly obtains models with many unknown parameters. Thus, when exploring the dependence of a response series to lags of some predictor series, there are better approaches than regression. In particular, this is the cross correlations and the transfer function model, which will be exhibited in later chapters of this scriptum.

In fact, there are not many restrictions for the time series regression model. As we have seen, it is perfectly valid to have non-stationary series as either the response or as predictors. However, it is crucial that there is no feedback from  $Y_t$  to the  $x_{tj}$ . Additionally, the error  $E_t$  must be independent of the explanatory variables, but it may exhibit serial correlation.

## 7.2 Finding Correlated Errors

When dealing with a time series regression problem, we first always assume uncorrelated errors and start out with an ordinary least squares regression. Based on its residuals, the assumption can be verified, and if necessary, action can be taken. For identifying correlation among the residuals, we analyze their time series plot, ACF and PACF.

### Example 1: Global Temperature

Our goal is the decomposition of the global temperature series into a linear trend plus some seasonal factor. First and foremost, we prepare the data:

```
> num.temp <- as.numeric(my.temp)
> num.time <- as.numeric(time(my.temp))
> mn01      <- c("Jan", "Feb", "Mar", "Apr", "May", "Jun")
> mn02      <- c("Jul", "Aug", "Sep", "Oct", "Nov", "Dec")
> month     <- factor(cycle(my.temp), labels=c(mn01, mn02))
> dat       <- data.frame(temp=num.temp, time=num.time, month)
```

The regression model is the estimated with  $\mathbf{R}$ 's function `lm()`. The summary function returns estimates, standard errors plus the results from some hypothesis tests. It is important to notice that all of these results are in question should the errors turn out to be correlated.

```
> fit.lm <- lm(temp ~ time + season, data=dat)
> summary(fit.lm)
```

Call:

```
lm(formula = temp ~ time + season, data = dat)
```

Residuals:

	Min	1Q	Median	3Q	Max
	-0.36554	-0.07972	-0.00235	0.07497	0.43348

Coefficients:

	Estimate	Std. Error	t value	Pr(> t )	
(Intercept)	-3.603e+01	1.211e+00	-29.757	<2e-16	***
time	1.822e-02	6.089e-04	29.927	<2e-16	***
seasonFeb	6.539e-03	3.013e-02	0.217	0.8283	
seasonMar	-1.004e-02	3.013e-02	-0.333	0.7392	
seasonApr	-1.473e-02	3.013e-02	-0.489	0.6252	
seasonMay	-3.433e-02	3.013e-02	-1.139	0.2552	

```

seasonJun    -2.628e-02  3.013e-02  -0.872   0.3836
seasonJul    -2.663e-02  3.013e-02  -0.884   0.3774
seasonAug    -2.409e-02  3.013e-02  -0.799   0.4245
seasonSep    -3.883e-02  3.013e-02  -1.289   0.1982
seasonOct    -5.212e-02  3.013e-02  -1.730   0.0844 .
seasonNov    -6.633e-02  3.013e-02  -2.201   0.0283 *
seasonDec    -4.485e-02  3.013e-02  -1.488   0.1374
---

```

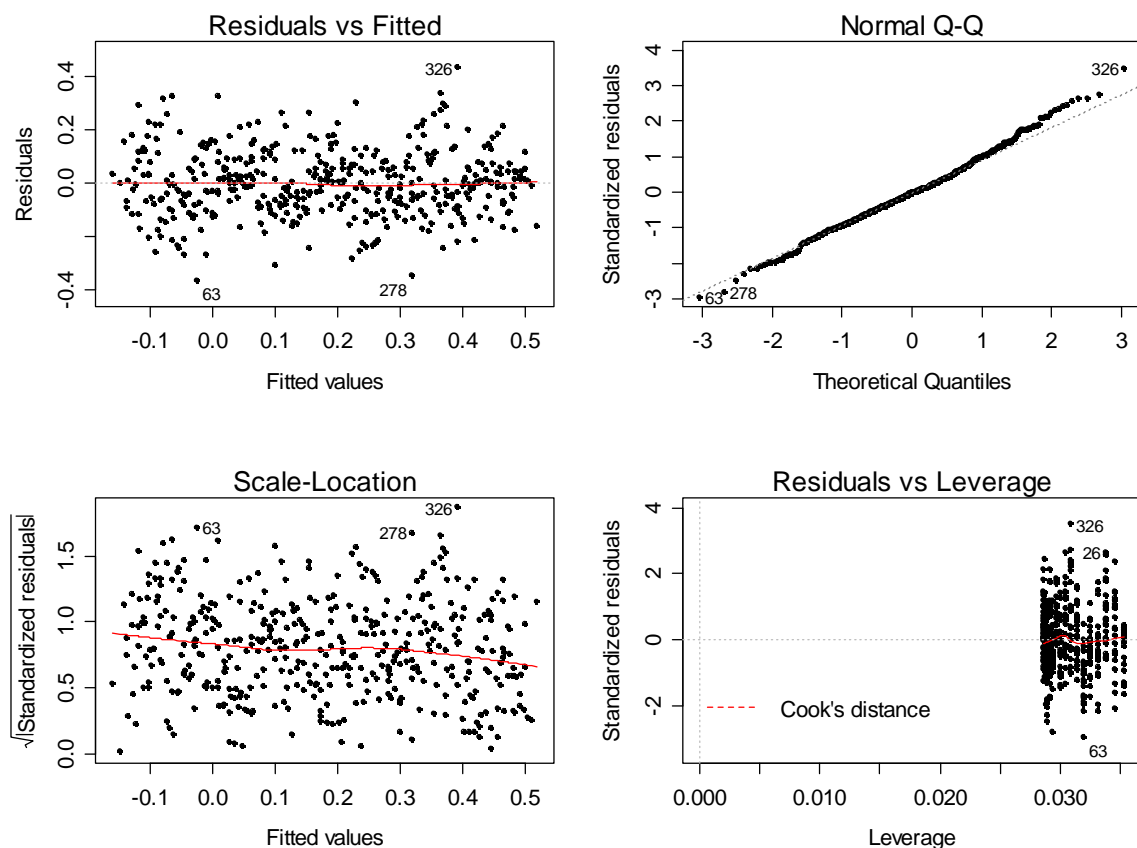
Residual standard error: 0.126 on 407 degrees of freedom  
Multiple R-squared: 0.6891, Adjusted R-squared: 0.68  
F-statistic: 75.18 on 12 and 407 DF, p-value: < 2.2e-16

As the next step, we need to perform some residual diagnostics. The `plot()` function, applied to a regression fit, serves as a check for zero expectation, constant variation and normality of the errors, and can give hints on potentially problematic leverage points.

```

> par(mfrow=c(2,2))
> plot(fit.lm, pch=20)

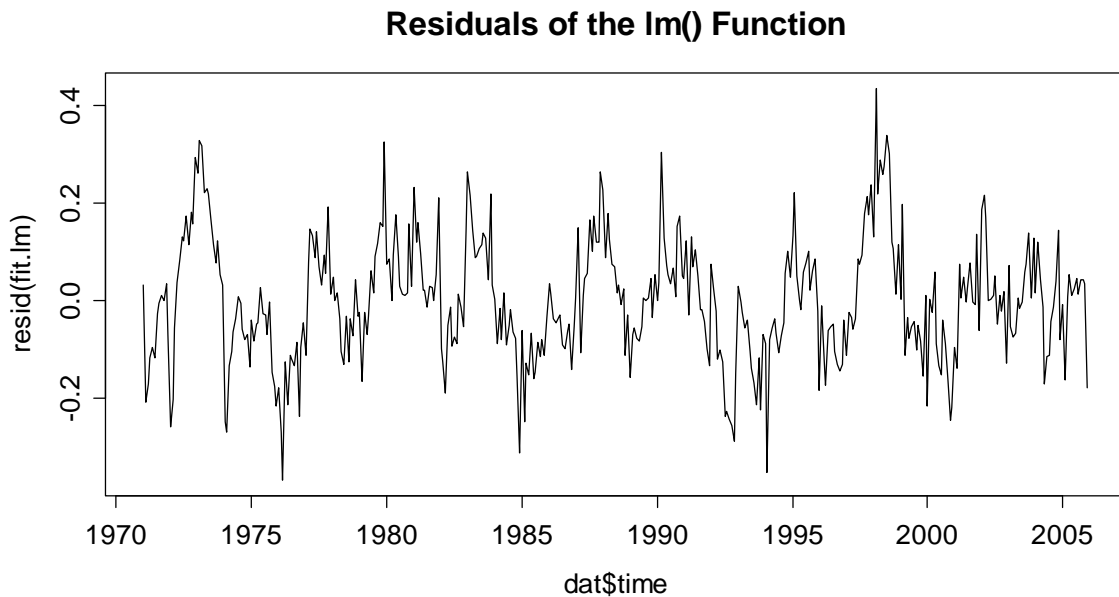
```



Except for some very slightly long tailed errors, which do not require any action, the residual plots look fine. What has not yet been verified is whether there is any serial correlation among the residuals. If we wish to see a time series plot, the following commands are useful:

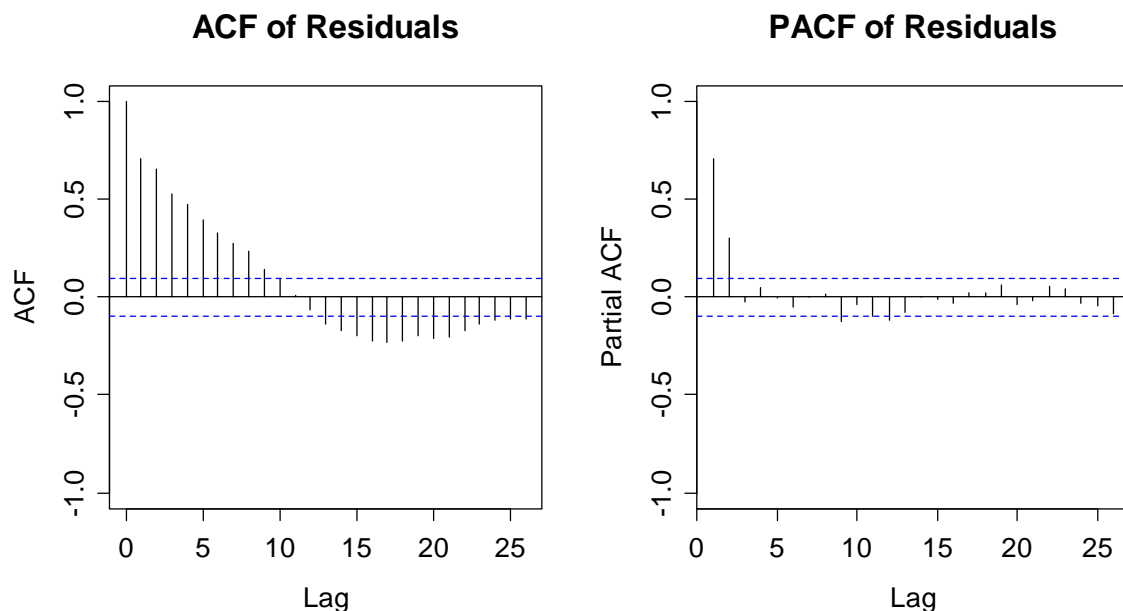


```
> plot(dat$time, resid(fit.lm), type="l")
```



It is fairly obvious from the time series plot that the residuals are correlated. Our main tool for describing the dependency structure is the ACF and PACF plots, however. These are as follows:

```
> par(mfrow=c(1,2))
> acf(resid(fit.lm), main="ACF of Residuals")
> pacf(resid(fit.lm), main="PACF of Residuals")
```



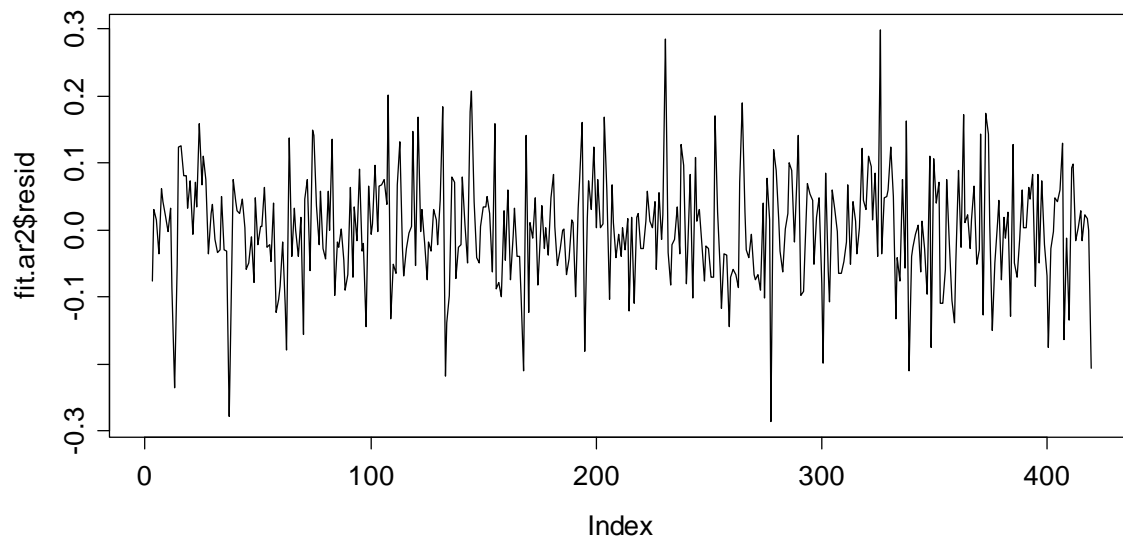
The ACF shows a rather slow exponential decay, whereas the PACF shows a clear cut-off at lag 2. With these stylized facts, it might well be that an  $AR(2)$

model is a good description for the dependency among the residuals. We verify this:

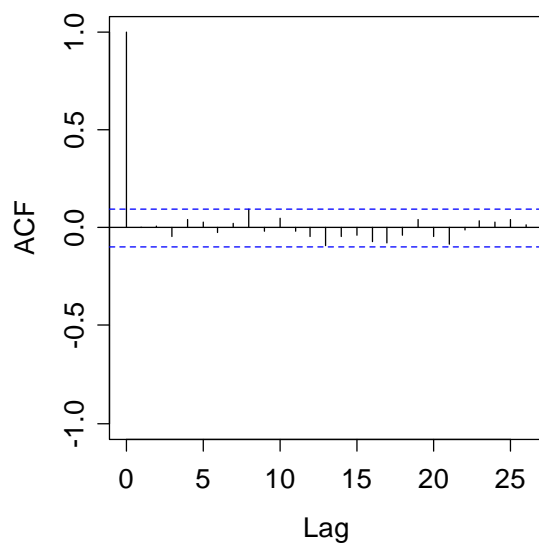
```
> fit.ar2 <- ar.burg(resid(fit.lm)); fit.ar2
Call: ar.burg.default(x = resid(fit.lm))
Coefficients:
      1      2
0.4945 0.3036
Order selected 2  sigma^2 estimated as 0.00693
```

When using Burg's algorithm for parameter estimation and doing model selection by AIC, order 2 also turns out to be optimal. For verifying an adequate fit, we visualize the residuals from the  $AR(2)$  model. These need to look like White Noise.

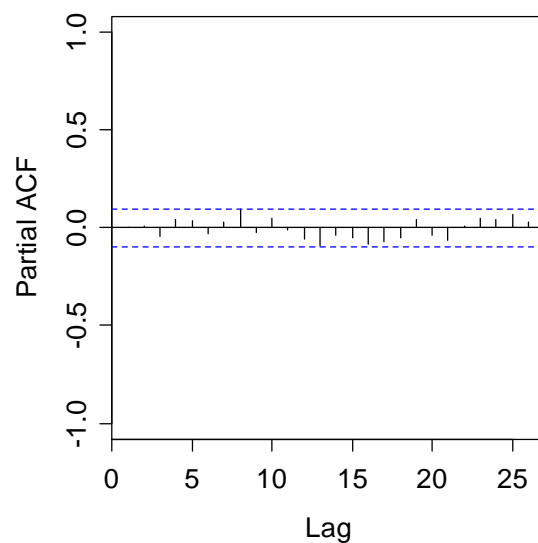
**Residuals of AR(2)**



**ACF of AR(2) Residuals**



**ACF of AR(2) Residuals**



There is no contradiction to the White Noise hypothesis for the residuals from the  $AR(2)$  model. Thus, we can summarize as follows: the regression model that was used for decomposing the global temperature series into a linear trend and a seasonal factor exhibit correlated errors that seem to originate from an  $AR(2)$  model. Theory tells us that the point estimates for the regression coefficients are still unbiased, but they are no longer efficient. Moreover, the standard errors for these coefficients can be grossly wrong. Thus, we need to be careful with the regression summary approach that was displayed above. And since our goal is inferring significance of trend and seasonality, we need to come up with some better suited method.

### Example 2: Air Pollution

Now, we are dealing with the air pollution data. Again, we begin our regression analysis using the standard assumption of uncorrelated errors. Thus, we start out by applying the `lm()` function and printing the `summary()`.

```
> fit.lm <- lm(Oxidant ~ Wind + Temp, data=dat)
> summary(fit.lm)
```

Call:

```
lm(formula = Oxidant ~ Wind + Temp, data = dat)
```

Residuals:

	Min	1Q	Median	3Q	Max
	-6.3939	-1.8608	0.5826	1.9461	4.9661

Coefficients:

	Estimate	Std. Error	t value	Pr(> t )
(Intercept)	-5.20334	11.11810	-0.468	0.644
Wind	-0.42706	0.08645	-4.940	3.58e-05 ***
Temp	0.52035	0.10813	4.812	5.05e-05 ***

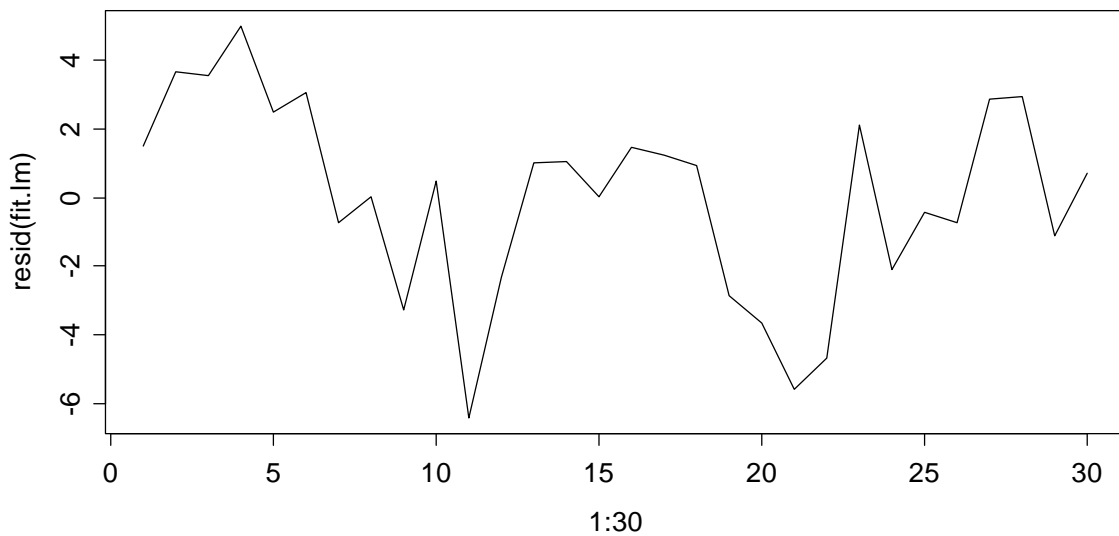
---

Residual standard error: 2.95 on 27 degrees of freedom  
 Multiple R-squared: 0.7773, Adjusted R-squared: 0.7608  
 F-statistic: 47.12 on 2 and 27 DF, p-value: 1.563e-09

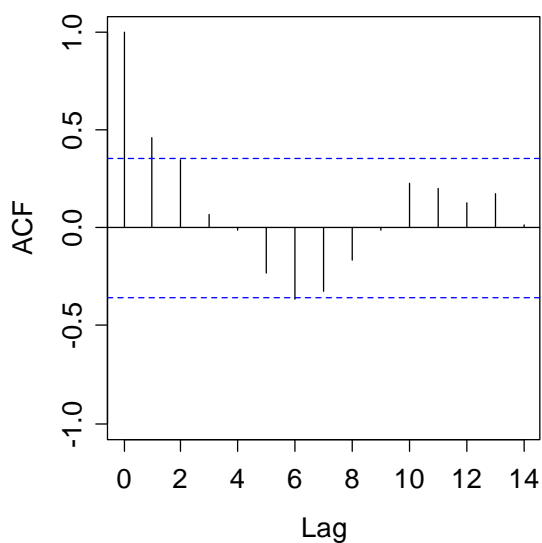
We will do without showing the 4 standard diagnostic plots, and here only report that they do not show any model violations. Because we are performing a time series regression, we also need to check for potential serial correlation of the errors. As before, this is done on the basis of time series plot, ACF and PACF:

```
> plot(1:30, resid(fit.lm), type="l")
> title("Residuals of the lm() Function")
> par(mfrow=c(1,2))
> acf(resid(fit.lm), ylim=c(-1,1), main="ACF of Residuals")
> pacf(resid(fit.lm), ylim=c(-1,1), main="PACF of Residuals")
```

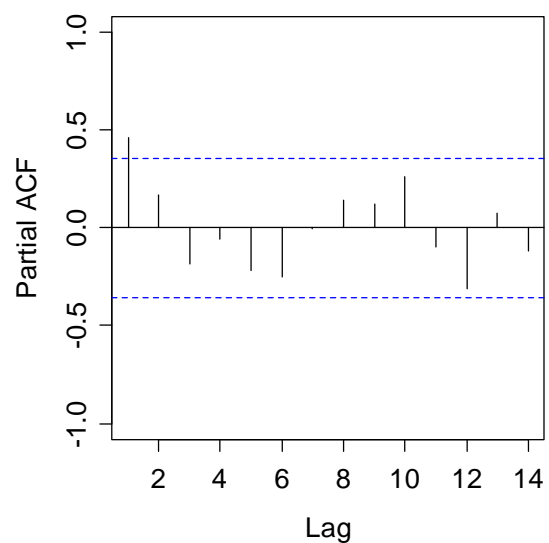
Residuals of the lm() Function



ACF of Residuals



PACF of Residuals



Also in this example, the time series of the residuals exhibits serial dependence. Because the ACF shows an exponential decay and the PACF cuts off at lag 1, we hypothesize that an  $AR(1)$  model is a good description. While the AIC criterion suggests an order of  $p=14$ , the residuals of an  $AR(1)$  show the behavior of White Noise. Additionally, using an  $AR(14)$  would be spending too many degrees of freedom for a series with only 30 observations.

Thus, we can summarize that also in our second example with the air pollution data, we feature a time series regression that has correlated errors. Again, we must not communicate the above regression summary and for sound inference, we require more sophisticated models.

## 7.2.1 Durbin-Watson Test

For the less proficient user, hypothesis tests always seem like an attractive alternative to visual inspection of graphical output. This is certainly also the case when the task is identifying a potential serial correlation in a regression analysis. Indeed, there is a formal test that addresses the issue, called the Durbin-Watson test. While we will here briefly go into it, we do not recommend it for practical application. The Durbin-Watson test tests the null hypothesis  $H_0: \rho(1) = 0$  against the alternative  $H_A: \rho(1) \neq 0$ . The test statistic  $\hat{D}$  is calculated as follows

$$\hat{D} = \frac{\sum_{t=2}^n (r_t - r_{t-1})^2}{\sum_{t=1}^n r_t^2}$$

where  $r_t = y_t - \hat{y}_t$  is the residual from the regression model, observed at time  $t$ . There is an approximate relationship between the test statistic  $\hat{D}$  and the autocorrelation coefficient at lag 1:

$$\hat{D} \approx 2(1 - \hat{\rho}(1))$$

The test statistic takes values between 0 if  $r_t = r_{t-1}$  and 4 if  $r_t = -r_{t-1}$ . These extremes indicate perfect correlation of the residuals. Values around 2, on the other hand, are evidence for uncorrelated errors. The exact distribution of  $\hat{D}$  is rather difficult to derive. However, we do not need to bother with this. The R package `lmtest` holds an implementation of the Durbin-Watson test with function `dwtest()`, where the p-value is either (for large sample size) determined by a normal approximation, or (for short series) by an iterative procedure.

### Example 1: Global Temperature

```
> dwtest(fit.lm)
data: fit.lm
DW = 0.5785, p-value < 2.2e-16
alt. hypothesis: true autocorrelation is greater than 0
```

### Example 2: Air Pollution

```
> dwtest(fit.lm)
data: fit.lm
DW = 1.0619, p-value = 0.001675
alt. hypothesis: true autocorrelation is greater than 0
```

Thus, the null hypothesis is rejected in both examples and we come to the same conclusion (“errors are correlated”) as with our visual inspection. It is very important to note that this is not necessary: In cases where the errors follow an  $AR(p)$  process where  $p > 1$  and  $|\rho(1)|$  is small, the null hypothesis will not be rejected despite the fact that the errors are correlated.

### 7.3 Cochrane-Orcutt Method

The goal of this section is to solve the time series regression problem with errors that have an  $AR(1)$  structure. This simple case is illustrative and helps to build the comprehension for more complicated error dependencies. We consider the Air Pollution example, where we have:

$$Y_t = \beta_0 + \beta_1 x_{t1} + \beta_2 x_{t2} + E_t \text{ with } E_t = \alpha E_{t-1} + U_t, \text{ where } U_t \sim N(0, \sigma_U^2) \text{ iid}.$$

The fundamental trick, on which in fact all time series regression methods are based will be presented here and now. We make the transformation:

$$Y'_t = Y_t - \alpha Y_{t-1}$$

Next, we plug-in the model equation and rearrange the terms. Finally, we build on the fundamental property that  $E_t - \alpha E_{t-1} = U_t$ . The result is:

$$\begin{aligned} Y'_t &= \beta_0 + \beta_1 x_{t1} + \beta_2 x_{t2} + E_t - \alpha(\beta_0 + \beta_1 x_{t-1,1} + \beta_2 x_{t-1,2} + E_{t-1}) \\ &= \beta_0(1-\alpha) + \beta_1(x_{t1} - \alpha x_{t-1,1}) + \beta_2(x_{t2} - \alpha x_{t-1,2}) + E_t - \alpha E_{t-1} \\ &= \beta'_0 + \beta_1 x'_{t1} + \beta_2 x'_{t2} + U_t \end{aligned}$$

Obviously, this is a time series regression problem where the error term  $U_t$  is *iid*. Also note that both the response and the predictors have undergone a transformation. The coefficients however, are identical in both the original and the modified regression equation. For implementing this approach in practice, we require knowledge about the  $AR(1)$  parameter  $\alpha$ . Usually, it is not known previously. A simple idea to overcome this and solve the time series regression problem for the Air Pollution data is as follows:

- 1) Run OLS regression to obtain estimates  $\hat{\beta}_0, \dots, \hat{\beta}_p$
- 2) Estimate an  $AR(1)$  on the OLS residuals to obtain  $\hat{\alpha}$
- 3) Determine the prime variables  $Y'; x'$  and derive  $\hat{\beta}_0^*, \hat{\beta}_1, \dots, \hat{\beta}_p$  by OLS

This procedure is known as the *Cochrane-Orcutt* iterative method. Please note that the estimates  $\hat{\beta}_0, \hat{\beta}_1, \dots, \hat{\beta}_p$  and their standard errors from the OLS regression in step 3) are sound and valid. But while the Cochrane-Orcutt procedure has its historical importance and is very nice for illustration, it lacks of a direct **R** implementation, and, as an iterative procedure, also of mathematical closeness and quality. The obvious improvement is to solve the prime regression problem by simultaneous Maximum-Likelihood estimation of all parameters:

$$\beta_0, \dots, \beta_p; \alpha; \sigma_U^2$$

This is possible and implemented in the **R** function `gls()`. Also, we need to be able to handle more complicated structure for the regression error  $E_t$ . For this, we resort to matrix notation, see the next section.

## 7.4 Generalized Least Squares

The ordinary least squares regression model assumes that  $\text{Var}(E) = \sigma^2 I$ , i.e. the covariance matrix of the errors is diagonal with identical values on the diagonal itself. As we have seen in our examples above, this is not a good model for time series regression. There, we rather have  $\text{Var}(E) = \sigma^2 \Sigma$ , where  $\Sigma$  reports the correlation among the errors. Using a Cholesky decomposition, we can write  $\Sigma = SS^T$ , where  $S$  is a triangular matrix. This allows us to rewrite the regression model in matrix notation as follows:

$$\begin{aligned} y &= X\beta + E \\ S^{-1}y &= S^{-1}X\beta + S^{-1}E \\ y' &= X'\beta + E' \end{aligned}$$

This transformation is successful, because in the prime model, we have uncorrelated errors again:

$$\text{Var}(E) = \text{Var}(S^{-1}E) = S^{-1}\text{Var}(E)S^{-T} = S^{-1}\sigma^2 SS^T S^{-T} = \sigma^2 I$$

With some algebra, it is easy to show that the estimated regression coefficients for the generalized least squares approach turn out to be:

$$\hat{\beta} = (X^T \Sigma^{-1} X)^{-1} X^T \Sigma^{-1} y$$

This is what is known as the *generalized least squares estimator*. Moreover, the covariance matrix of the coefficient vector is:

$$\text{Var}(\hat{\beta}) = (X^T \Sigma^{-1} X)^{-1} \sigma^2$$

This covariance matrix then also contains standard errors in which the correlation of the errors has been accounted for, and with which sound inference is possible. However, while this all neatly lines up, we of course require knowledge about the error covariance matrix  $\Sigma$ , which is generally unknown in practice. What we can do is estimate it from the data, for which two approaches exist.

### Cochrane-Orcutt Method

As we have seen above, this method is iterative: it starts with an ordinary least squares (OLS) regression, from which the residuals are determined. For these residuals, we can then fit an appropriate  $ARMA(p, q)$  model and with its estimated model coefficients  $\alpha_1, \dots, \alpha_p$  and  $\beta_1^{MA(q)}, \dots, \beta_q^{MA(q)}$ . On the basis of the estimated  $AR(MA)$  model coefficients, an estimate of the error covariance matrix  $\Sigma$  can be derived. We denote it by  $\hat{\Sigma}$ , and plug it into the formulae presented above. This yields adjusted regression coefficients and correct standard errors for these regression problems. As mentioned above, the iterative approach is secondary to a simultaneous MLE. Thus, we do without further performing Cochrane-Orcutt on our examples.

## The `gls()` Procedure

A better, yet more sophisticated approach is to estimate the regression coefficients and the *ARMA* parameters simultaneously. This can be done using the Maximum-Likelihood principle. Even under the assumption of Gaussian errors, this is a nonlinear and numerically difficult problem. However, for practical application, we do not need to worry. The **R** package `nlme` features the `gls()` procedure which tackles this problem. Thus, we focus on correct application of the **R** function.

### Example 1: Global Temperature

Every GLS regression analysis starts by fitting an OLS and analyzing the residuals, as we have done above. Remember that the only model violation we found were correlated residuals that were well described with an *AR*(2) model. Please note that for performing GLS, we need to provide a dependency structure for the errors. Here, this is the *AR*(2) model, in general, it is an appropriate *ARMA*( $p, q$ ). The syntax and output is as follows:

```
> library(nlme)
> corStruct <- corARMA(form=~time, p=2)
> fit.gls <- gls(temp~time+season, data=dat, corr=corStruct)
> fit.gls
Generalized least squares fit by REML
  Model: temp ~ time + season
  Data: dat
  Log-restricted-likelihood: 366.3946

Coefficients:
  (Intercept)           time      seasonFeb      seasonMar
-39.896981987    0.020175528    0.008313205   -0.006487876
   seasonApr      seasonMay      seasonJun      seasonJul
-0.009403242   -0.027232895   -0.017405404   -0.015977913
   seasonAug      seasonSep      seasonOct      seasonNov
-0.011664708   -0.024637218   -0.036152584   -0.048582236
   seasonDec
-0.025326174

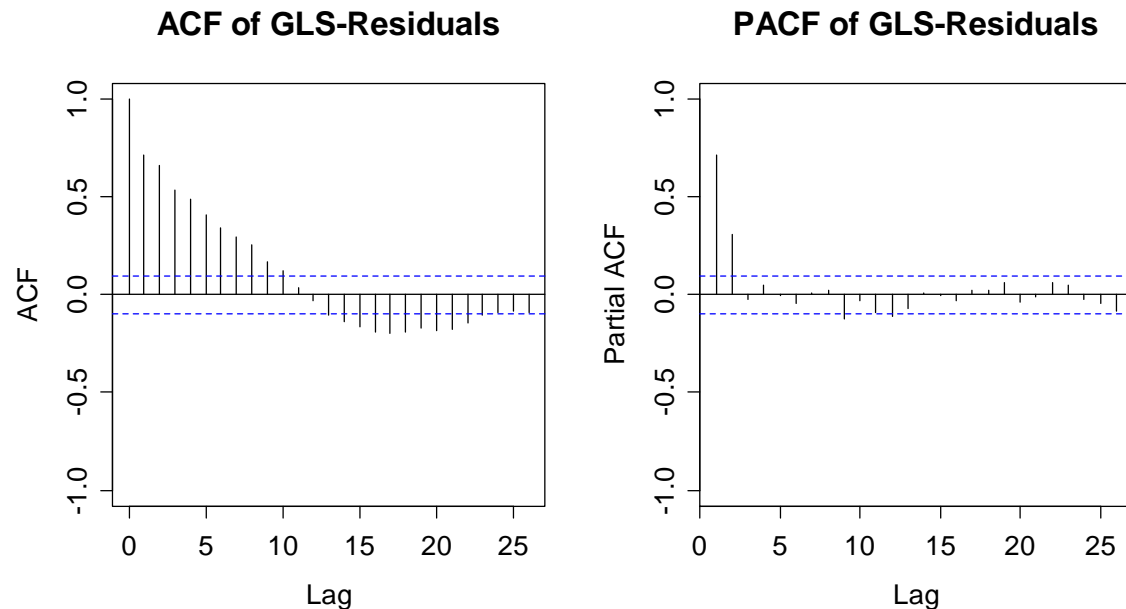
Correlation Structure: ARMA(2,0)
Formula: ~time
Parameter estimate(s):
      Phi1      Phi2
0.5539900 -0.1508046
Degrees of freedom: 420 total; 407 residual
Residual standard error: 0.09257678
```

The result reports the regression and the *AR* coefficients. Using the `summary()` function, even more output with all the standard errors can be generated. We omit this here and instead focus on the necessary residual analysis for the GLS model. We can extract the residuals using the usual `resid()` command. Important: these



residuals must not look like White Noise, but as from an  $ARMA(p, q)$  with orders  $p$  and  $q$  as provided in the `corStruct` object – which in our case, is an  $AR(2)$ .

```
> par(mfrow=c(1,2))
> acf(resid(fit.gls), main="ACF of GLS-Residuals")
> pacf(resid(fit.gls), main="PACF of GLS-Residuals")
```



The plots look similar to the ACF/PACF plots of the OLS residuals. This is often the case in practice, only for more complex situations, there can be a bigger discrepancy. And because we observe an exponential decay in the ACF, and a clear cut-off at lag 2 in the PACF, we conjecture that the GLS residuals meet the properties of the correlation structure we hypothesized, i.e. of an  $AR(2)$  model. Thus, we can now use the GLS fit for drawing inference. We first compare the OLS and GLS point estimate for the trend, along with its confidence interval:

```
> coef(fit.lm)["time"]
      time
0.01822374
> confint(fit.lm, "time")
           2.5 %      97.5 %
time 0.01702668 0.0194208
> coef(fit.gls)["time"]
      time
0.02017553
> confint(fit.gls, "time")
           2.5 %      97.5 %
time 0.01562994 0.02472112
```

We obtain a temperature increase of 0.0182 degrees per year with the OLS, and of 0.0202 with the GLS. While this may seem academic, the difference among the point estimates is around 10%, and theory tells us that the GLS result is more reliable. Moreover, the length of the confidence interval is 0.0024 with the OLS,

and 0.0091 and thus 3.5 times as large with the GLS. Thus, without accounting for the dependency among the errors, the precision of the trend estimate is by far overestimated. Nevertheless, also the confidence interval obtained from GLS regression does not contain the value 0, and thus, the null hypothesis on no global warming trend is rejected (with margin!).

Finally, we investigate the significance of the seasonal effect. Because this is a factor variable, i.e. a set of dummy variables, we cannot just produce a confidence interval. Instead, we have to rely on a significance test, i.e. a partial F-test. Again, we compare what is obtained from OLS and GLS:

```
> drop1(fit.lm, test="F")
Single term deletions

Model:
temp ~ time + season
      Df Sum of Sq    RSS    AIC  F value    Pr(>F)
<none>                 6.4654 -1727.0
time    1    14.2274 20.6928 -1240.4 895.6210 <2e-16 ***
season 11     0.1744  6.6398 -1737.8   0.9982  0.4472

> anova(fit.gls)
Denom. DF: 407
      numDF  F-value p-value
(Intercept)      1 78.40801  <.0001
time              1 76.48005  <.0001
season           11  0.64371  0.7912
```

As for the trend, the result is identical with OLS and GLS. The seasonal effect is non-significant with p-values of 0.45 (OLS) and 0.79 (GLS). Again, the latter is the value we must believe in. We conclude that there is no seasonality in global warming – but there is a trend.

## Example 2: Air Pollution

For finishing the air pollution example, we also perform a GLS fit here. We identified an  $AR(1)$  as the correct dependency structure for the errors. Thus, we define it accordingly:

```
> dat      <- cbind(dat, time=1:30)
> corStruct <- corARMA(form=~time, p=1)
> model     <- formula(Oxidant ~ Wind + Temp)
> fit.gls   <- gls(model, data=dat, correlation=corStruct)
```

The output then is as follows:

```
> fit.gls
Generalized least squares fit by REML
Model: model
Data: dat
Log-restricted-likelihood: -72.00127
```

Coefficients:

(Intercept)	Wind	Temp
-3.7007024	-0.4074519	0.4901431

Correlation Structure: AR(1)

Formula: ~time

Parameter estimate(s):

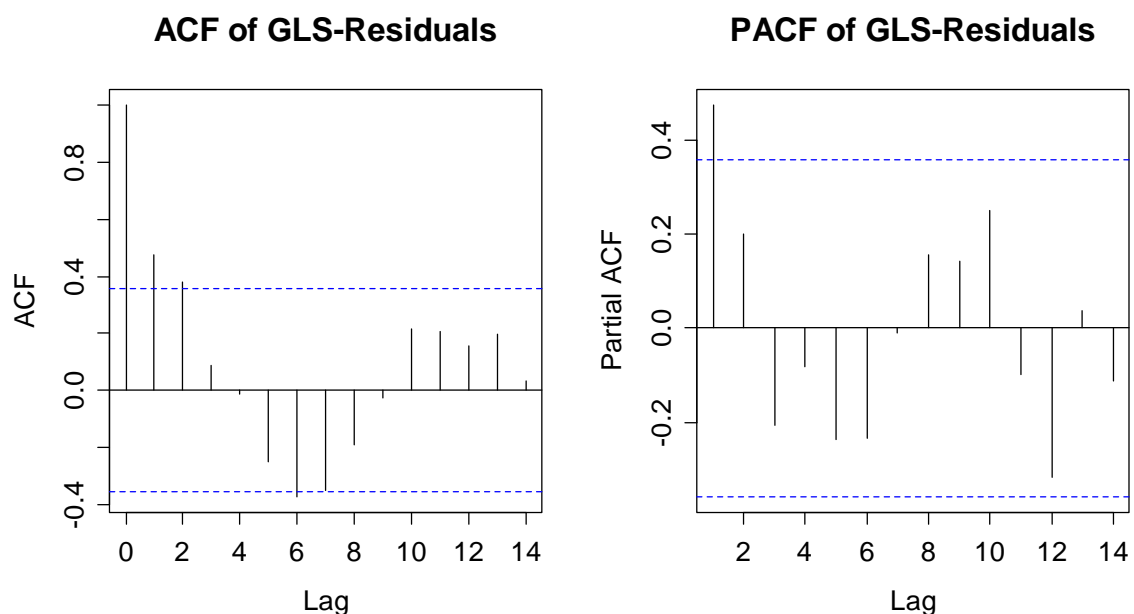
Phi

0.5267549

Degrees of freedom: 30 total; 27 residual

Residual standard error: 3.066183

Again, we have to check if the GLS residuals show the stylized facts of an  $AR(1)$ :



This is the case, and thus we can draw inference from the GLS results. The confidence intervals of the regression coefficients are:

```
> confint(fit.lm, c("Wind", "Temp"))
           2.5 %      97.5 %
Wind -0.6044311 -0.2496841
Temp  0.2984794  0.7422260

> confint(fit.gls, c("Wind", "Temp"))
           2.5 %      97.5 %
Wind -0.5447329 -0.2701709
Temp  0.2420436  0.7382426
```

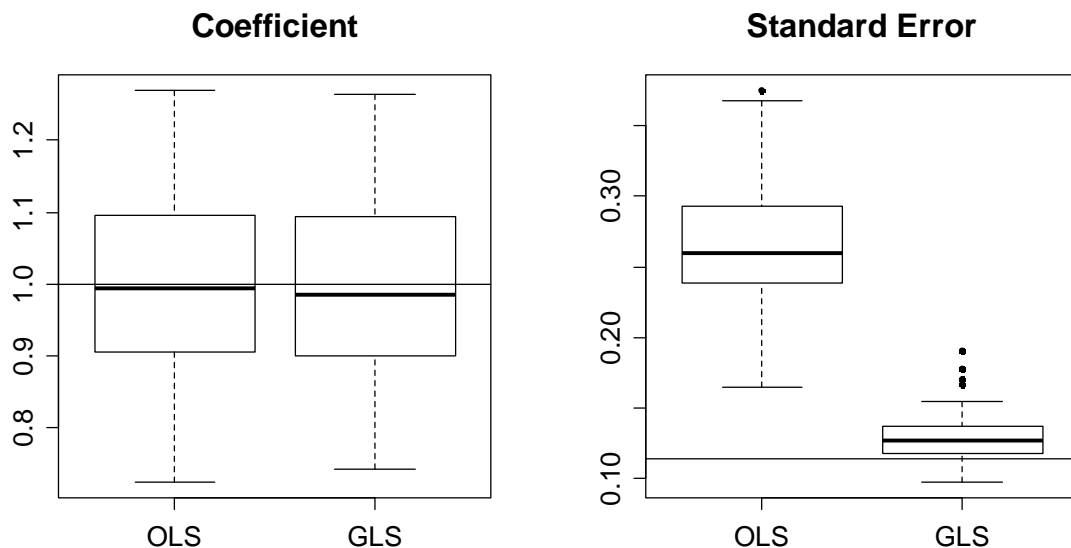
Here the differences among point estimates and confidence intervals are not very pronounced. This has to do with the fact that the correlation among the errors is weaker than in the global temperature example. But we emphasize again that the GLS results are the one to be relied on and the magnitude of the difference between OLS and GLS can be tremendous.

### Simulation Study

We provide further evidence for the importance of the GLS approach by performing a simulation study in which the resulting coefficients and standard errors are compared to the ones obtained from OLS regression. We consider the following, relatively simple model:

$$\begin{aligned}x_t &= t/50 \\ y_t &= x_t + 2(x_t)^2 + E_t\end{aligned}$$

where  $E_t$  is from an  $AR(1)$  process with  $\alpha_1 = -0.65$ . The innovations are Gaussian with  $\sigma = 0.1$ . Regression coefficients and the true standard deviations of the estimators are known in this extraordinary situation. However, we generate 100 realizations with series length  $n = 50$ , on each perform OLS and GLS regression and record both point estimate and standard error.



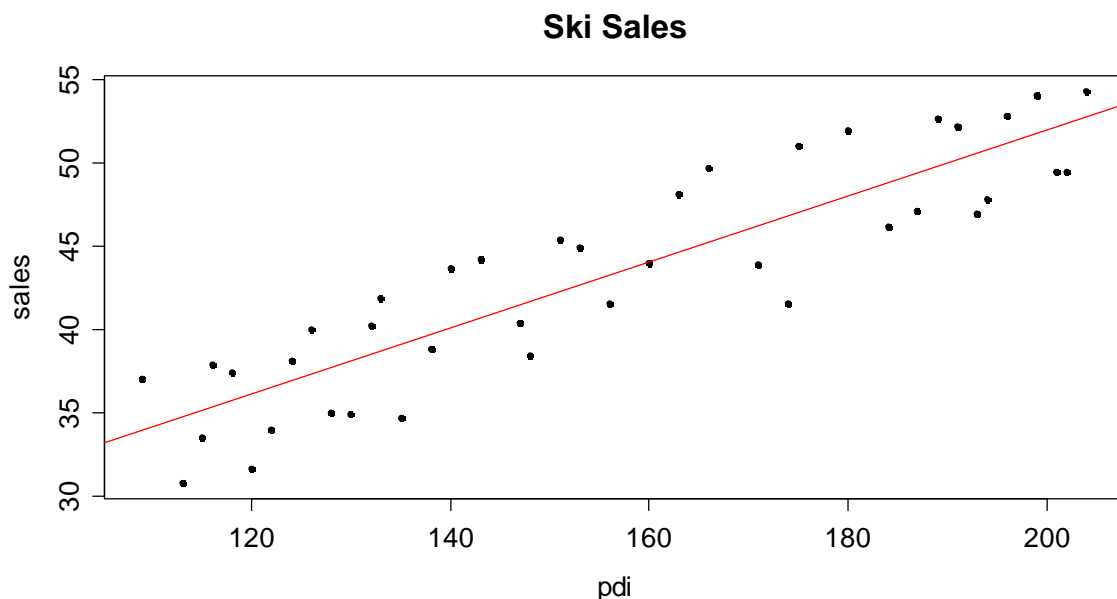
The simulation outcome is displayed by the boxplots in the figure above. While the point estimator for  $\beta_1$  in the left panel is unbiased for both OLS and GLS, we observe that the standard error for  $\hat{\beta}_1$  is very poor when the error correlation is not accounted for. We emphasize again that OLS regression with time series will inevitably lead to spuriously significant predictors and thus, false conclusions. Hence, it is absolutely key to inspect for possible autocorrelation in the regression residuals and apply the `gls()` procedure if necessary.

However, while `gls()` can cure the problem of autocorrelation in the error term, it does not solve the issue from the root. Sometimes, even this is possible. In the next subsection, we conclude the chapter about time series regression by showing how correlated errors can originate, and what practice has to offer for deeper understanding of the problem.

## 7.5 Missing Predictor Variables

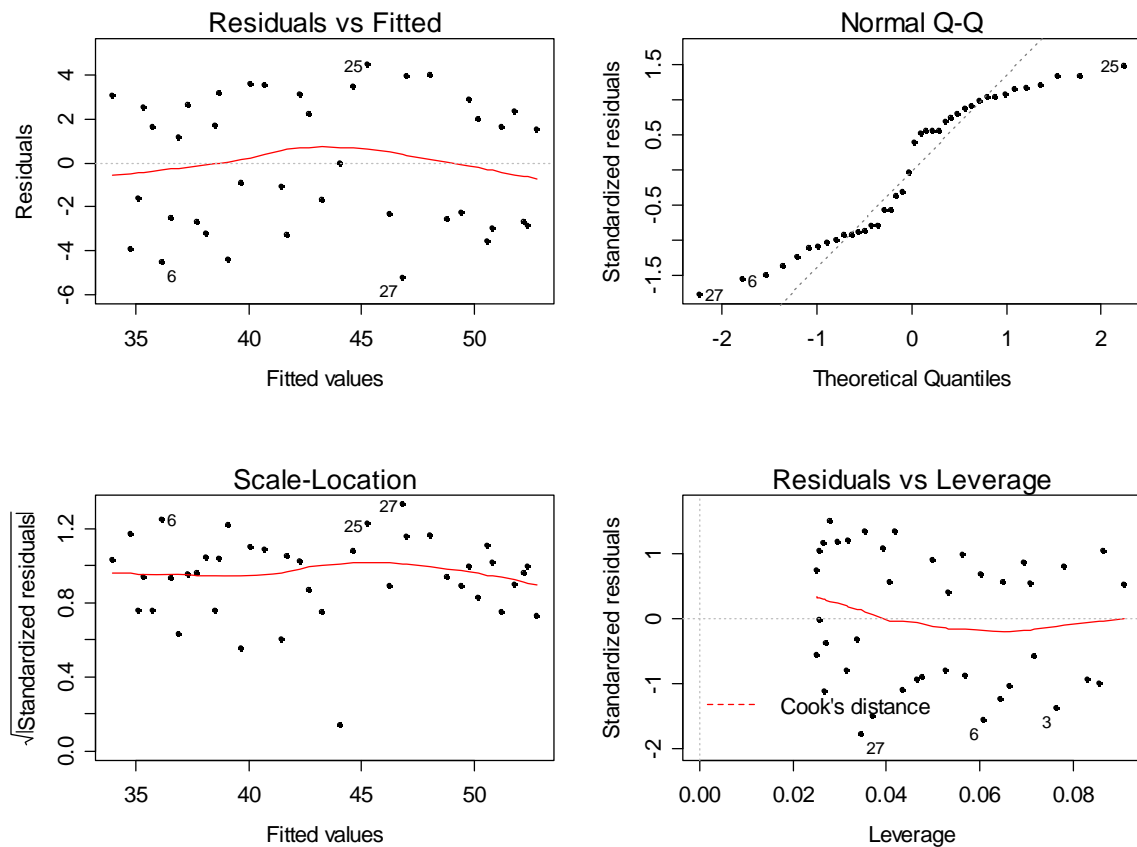
The presence correlated errors is often due to missing predictors. For illustration, we consider a straightforward example of a ski selling company in the US. The quarterly sales  $Y_t$  are regressed on the personal disposable income (PDI) which is the one and only predictor  $x_t$ . We display the two time series in a scatterplot and enhance it with the OLS regression line.

```
> ## Loading the data
> ski      <- read.table("ski.dat",header=TRUE)
> names(ski) <- c("time", "sales", "pdi", "season")
>
> ## Scatterplot
> par(mfrow=c(1,1))
> plot(sales ~ pdi, data=ski, pch=20, main="Ski Sales")
>
> ## LS modeling and plotting the fit
> fit <- lm(sales ~ pdi, data=ski)
> abline(fit, col="red")
```



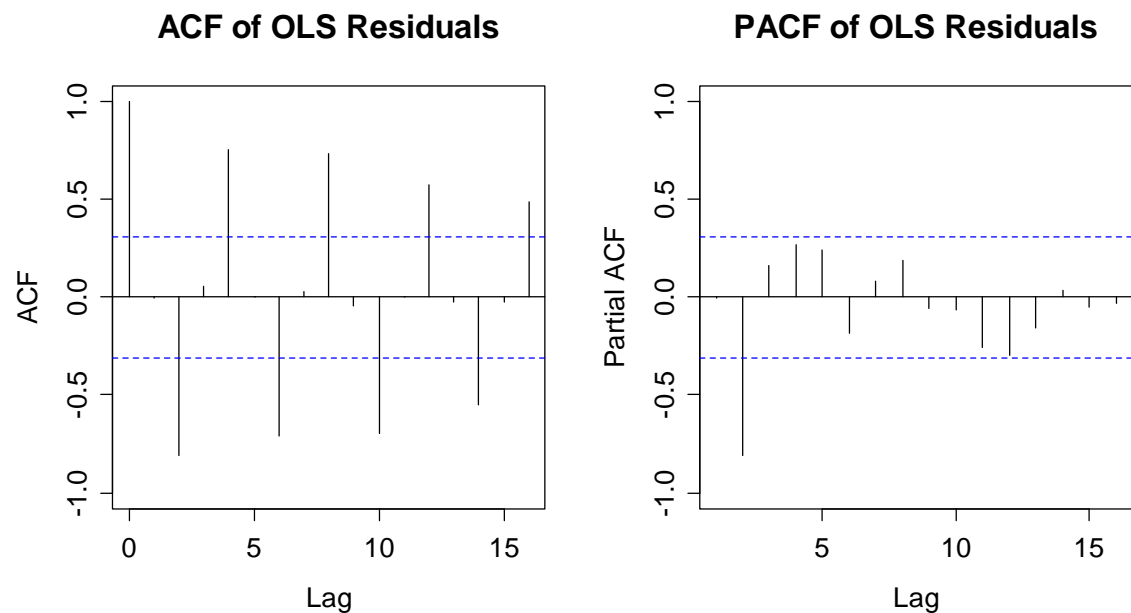
The coefficient of determination is rather large, i.e.  $R^2 = 0.801$  and the linear fit seems adequate, i.e. a straight line seems to correctly describe the systematic relation between sales and PDI. However, the model diagnostic plots (see the next page) show some rather special behavior, i.e. there are hardly any “small” residuals (in absolute value). Or more precisely, the data points almost lie on two lines around the regression line, with almost no points near or on the line itself.

```
> ## Residual diagnostics
> par(mfrow=c(2,2))
> plot(fit, pch=20)
```

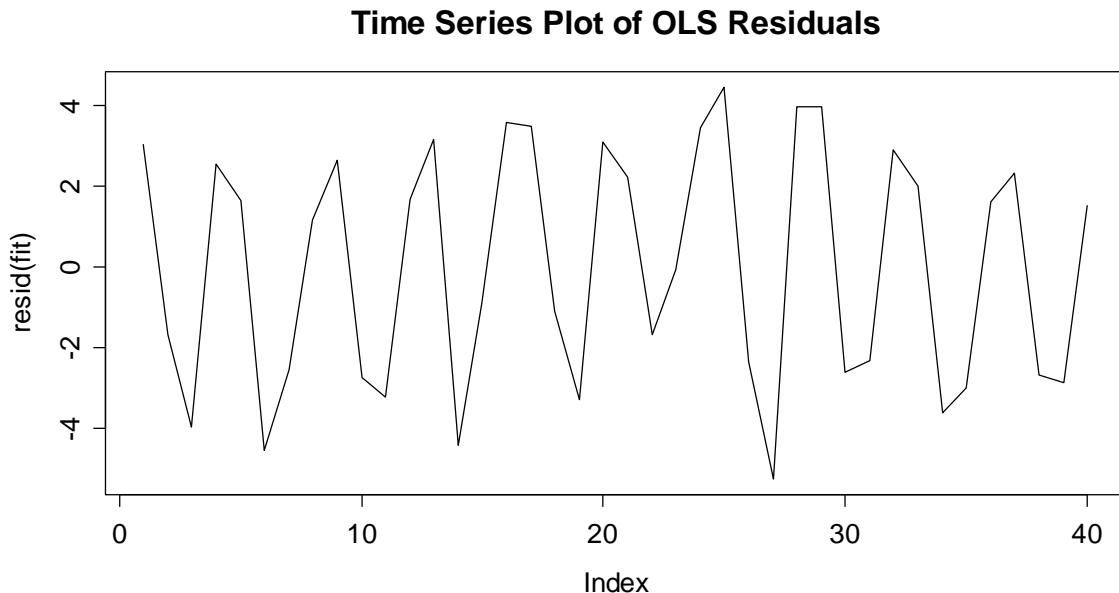


As the next step, we analyze the correlation of the residuals and perform a Durbin-Watson test. The result is as follows:

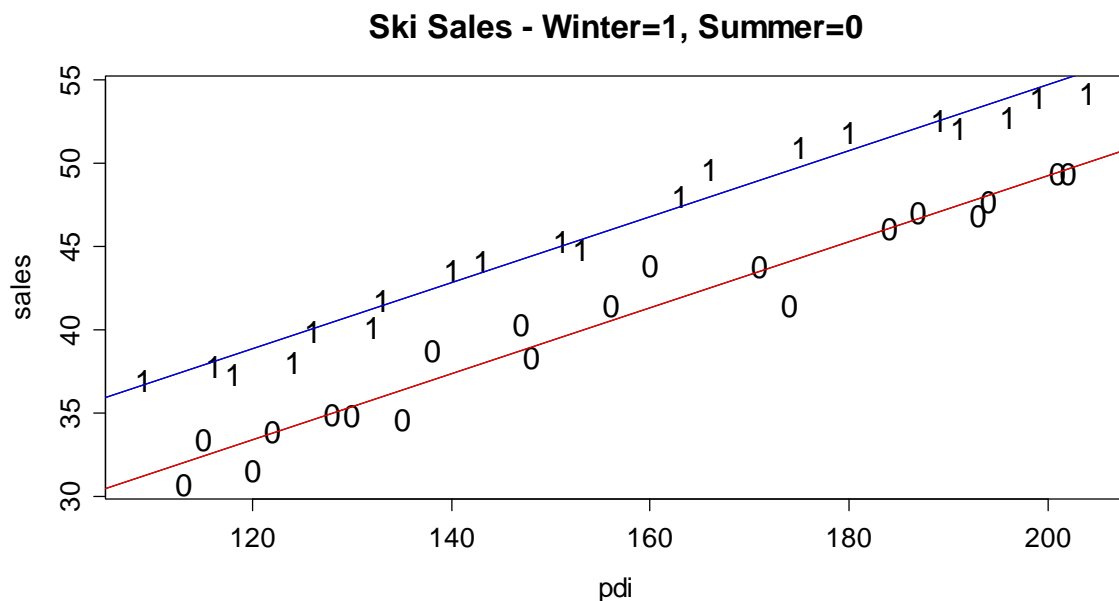
```
> dwtest(fit)
data: fit
DW = 1.9684, p-value = 0.3933
alt. hypothesis: true autocorrelation is greater than 0
```



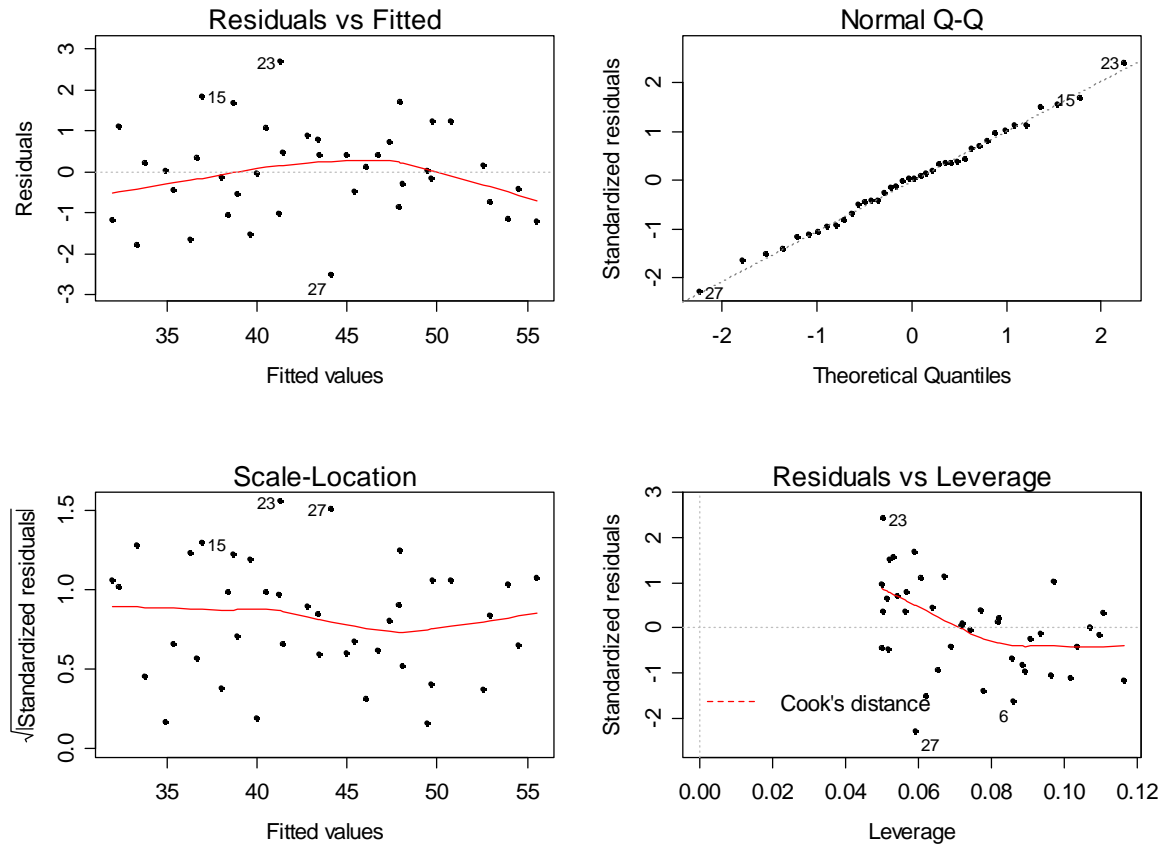
While the Durbin-Watson test does not reject the null hypothesis, the residuals seem very strongly correlated. The ACF exhibits some decay that may still qualify as exponential, and the PACF has a clear cut-off at lag 2. Thus, an  $AR(2)$  model could be appropriate. And because it is an  $AR(2)$  where  $\alpha_1$  and  $\rho(1)$  are very small, the Durbin-Watson test fails to detect the dependence in the residuals. The time series plot is as follows:



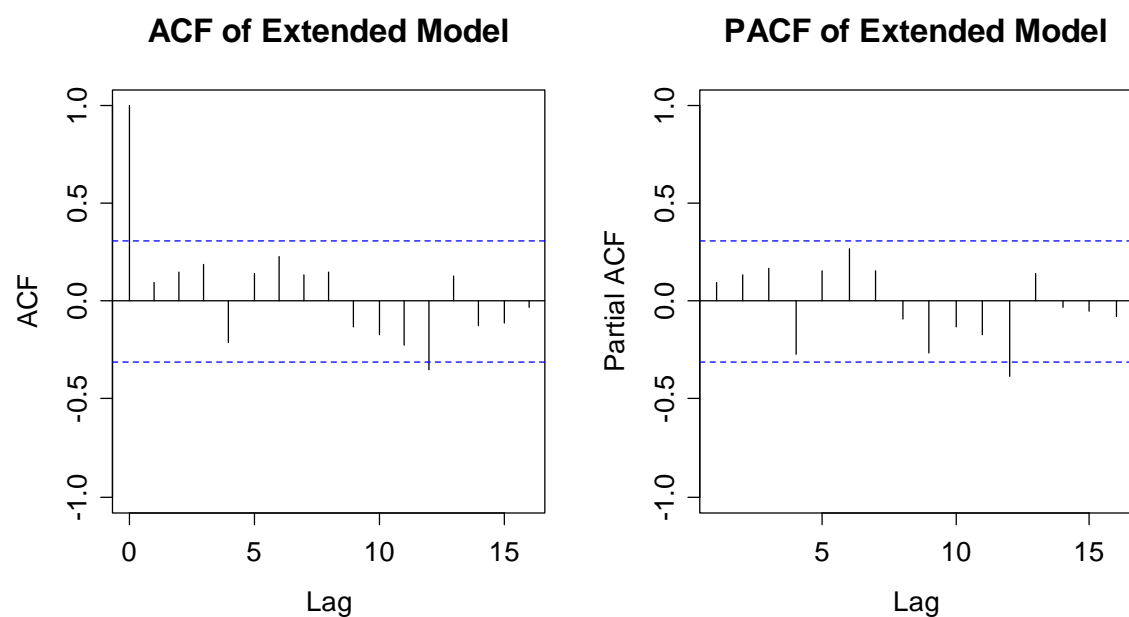
While we could now account for the error correlation with a GLS, it is always better to identify the reason behind the dependence. I admit this is suggestive here, but as mentioned in the introduction of this example, these are quarterly data and we might have forgotten to include the seasonality. It is not surprising that ski sales are much higher in fall and winter and thus, we introduce a factor variable which takes the value 0 in spring and summer, and 1 else.



Introducing the seasonal factor variable accounts to fitting two parallel regression lines for the winter and summer term. Eyeballing already lets us assume that the fit is good. This is confirmed when we visualize the diagnostic plots:



The unwanted structure is now gone, as is the correlation among the errors:





Apparently, the addition of the season as an additional predictor has removed the dependence in the errors. Rather than using GLS, a sophisticated estimation procedure, we have found a simple model extension that describes the data well and is certainly easier to interpret (especially when it comes to prediction) than a model that is built on correlated errors.

We conclude by saying that using GLS for modeling dependent errors should only take place if care has been taken that no important and/or obvious predictors are missing in the model.



## 8 Forecasting

One of the principal goals with time series analysis is to produce predictions which show the future evolution of the data. This is what it is: an extrapolation in the time domain. And as we all know, extrapolation is always (at least slightly) problematic and can lead to false conclusions. Of course, this is no different with time series forecasting.

The saying is that the task we are faced with can be compared to driving a car by looking through the rear window mirror. While this may work well on a wide motorway that runs mostly straight and has a few gentle bends only, things get more complicated as soon as there are some sharp and unexpected bends in the road. Then, we would need to drive very slowly to stay on track. This all translates directly to time series analysis. For series where the signal is much stronger than the noise, accurate forecasting is possible. However, for noisy series, there is a great deal of uncertainty in the predictions, and they are at best reliable for a very short horizon.

From the above, one might conclude that the principal source of uncertainty is inherent in the process, i.e. comes from the innovations. However, in practice, this is usually different, and several other factors can threaten the reliability of any forecasting procedure. In particular:

- We need to be certain that the data generating process does not change over time, i.e. continues in the future as it was observed in the past.
- When we choose/fit a model based on a realization of data, we have no guarantee that it is the correct, i.e. data-generating one.
- Even if we are so lucky to find the correct data-generating process (or in cases we know it), there is additional uncertainty arising from the estimation of the parameters.

Keeping these general warnings in mind, we will now present several approaches to time series forecasting. First, we deal with stationary processes and present, how AR, MA and ARMA processes can be predicted. These principles can be extended to the case of ARIMA and SARIMA models, such that forecasting series with either trend and/or seasonality is also possible.

As we had seen in section 4.3, the decomposition approach for non-stationary time series helps a great deal for visualization and modeling. Thus, we will present some heuristics about how to produce forecasts with series that were decomposed into trend, seasonal pattern and a stationary remainder. Last but not least, we present the method of exponential smoothing. This was constructed as a model-free, intuitive weighting scheme that allows forecasting of time series. Due to its simplicity and the convenient implementation in the `HoltWinters()` procedure in `R`, it is very popular and often used in applied sciences.

## 8.1 Forecasting ARMA

We suppose that we are given a time series, for which an appropriate AR, MA or ARMA model was identified, the parameters were successfully estimated and where the residuals exhibited the required properties, i.e. looked like White Noise. Under these circumstances, forecasts may be readily computed. Given data up to time  $n$ , the forecasts will involve either involve the past observations, and/or the residuals.

In mathematical statistics, many forecasting methods have been studied on a theoretical basis with the result that the minimum mean squared error forecast  $\hat{X}_{n+k,1n}$  for  $k$  steps ahead is given by the conditional expectation, i.e.:

$$\hat{X}_{n+k,1n} = E[X_{n+k} | X_1, \dots, X_n]$$

In evaluating this term, we use the fact that the best forecast of all future innovation terms  $E_t, t > n$  is simply zero. We will be more specific in the following subsections.

### 8.1.1 Forecasting AR(1)

For simplicity, we first consider a mean-zero, stationary  $AR(1)$  process with model equation:

$$X_t = \alpha_1 X_{t-1} + E_t,$$

where  $E_t$  is the innovation, for which we do not need to assume a particular distribution. As we will see below, it is convenient to assume Gaussian  $E_t$ , because this allows for an easy derivation of a prediction interval. The conditional expectation at time  $n+1$  is given by:

$$E[X_{n+1} | X_1, \dots, X_n] = \alpha_1 x_n.$$

Thus, we can forecast the next instance of a time series with the observed value of the previous one, in particular:

$$\hat{X}_{n+1,1n} = \alpha_1 x_n.$$

For the  $k$ -step forecast with  $k > 1$ , we just need to repeatedly plug-in the model equation, and as use the fact that the conditional expectation of the innovations is zero:

$$\begin{aligned} \hat{X}_{n+k,1n} &= E[X_{n+k} | X_1, \dots, X_n] \\ &= E[\alpha_1 X_{n+k-1} + E_{n+k} | X_1, \dots, X_n] \\ &= \alpha_1 E[X_{n+k-1} | X_1, \dots, X_n] \\ &= \dots \\ &= \alpha_1^k x_n \end{aligned}$$

For any stationary  $AR(1)$  process, the  $k$ -step forecast beyond the end of a series depends on the last observation  $x_n$  only and goes to zero exponentially quickly. For practical implementation with real data, we would just plug-in the estimated model parameter  $\hat{\alpha}_1$  and can so produce a forecast for any desired horizon.

As always, a prediction is much more useful in practice if one knows how precise it is. Under the assumption of Gaussian innovations, a 95% prediction interval can be derived from the conditional variance  $Var(X_{n+k} | X_1, \dots, X_n)$ . For the special case of  $k = 1$  we obtain:

$$\alpha_1 x_n \pm 1.96 \cdot \sigma_E.$$

Again, for practical implementation, we need to plug-in  $\hat{\alpha}_1$  and  $\hat{\sigma}_E$ . For a  $k$ -step prediction, the 95% prognosis interval is:

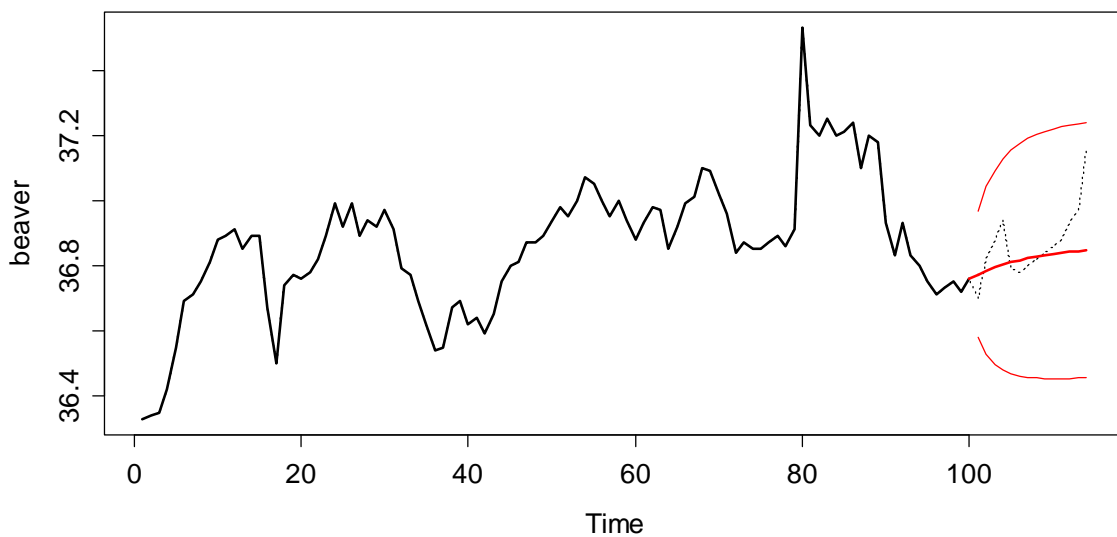
$$\alpha_1 x_n \pm 1.96 \cdot \left(1 + \sum_{j=1}^{k-1} \alpha_1^{2j}\right) \cdot \sigma_E.$$

For increasing prediction horizon  $k$ , the conditional variance goes to  $\sigma_E^2 / (1 - \alpha_1^2)$ , which is the process variance  $\sigma_X^2$ . Thus, for the 1-step forecast, the uncertainty in the prediction is given by the innovation variance  $\sigma_E$  alone, while for increasing horizon  $k$  the prognosis interval gets wider and is finally determined by the process variance.

### Practical Example

We now turn our attention to a practical example, where we apply the  $\mathfrak{R}$  functions which implement the above theory. This is the Beaver data we had already discussed in section 4.4.3. An  $AR(1)$  model is appropriate, and for estimating the coefficients, we omit the last 14 observations from the data. These will be predicted, and the true values are needed for verifying the prediction.

**Beaver Data: 14-Step Prediction Based on  $AR(1)$**



The **R** commands for fitting the model on the training data and producing the 14-step prediction are as follows:

```
> btrain <- window(beaver, 1, 100)
> fit <- ar.burg(btrain, order=1)
> forecast <- predict(fit, n.ahead=14)
```

The `forecast` object is a list that has two components, `pred` and `se`, which contain the point predictions and the standard error, respectively. We now turn our attention to how the forecast is visualized:

```
> plot(beaver, lty=3)
> lines(btrain, lwd=2)
> lines(pred$pred, lwd=2, col="red")
> lines(pred$pred+pred$se*1.96, col="red")
> lines(pred$pred-pred$se*1.96, col="red")
```

One more issue requires some attention here: for the Beaver data, a pure  $AR(1)$  process is not appropriate, because the global series mean is clearly different from zero. The way out is to de-mean the series, then fit the model and produce forecasts, and finally re-adding the global mean. **R** does all this automatically.

We conclude by summarizing what we observe in the example: the forecast is based on the last observed value  $x_{100}=36.76$ , and from there approaches the global series mean  $\hat{\mu}=36.86$  exponentially quick. Because the estimated coefficient is  $\hat{\alpha}_1=0.87$ , and thus relatively close to one, the approach still takes some time.

## 8.1.2 Forecasting $AR(p)$

Forecasting from  $AR(p)$  processes works based on the same principles as explained above for the  $AR(1)$ , i.e. we use the conditional expected value. The algebra for writing the forecasting formulae is somewhat more laborious, but not more difficult. Thus, we do without displaying it here, and directly present the 1-step-forecast:

$$\hat{X}_{n+1,1:n} = \alpha_1 x_n + \alpha_2 x_{n-1} + \dots + \alpha_p x_{n-p}$$

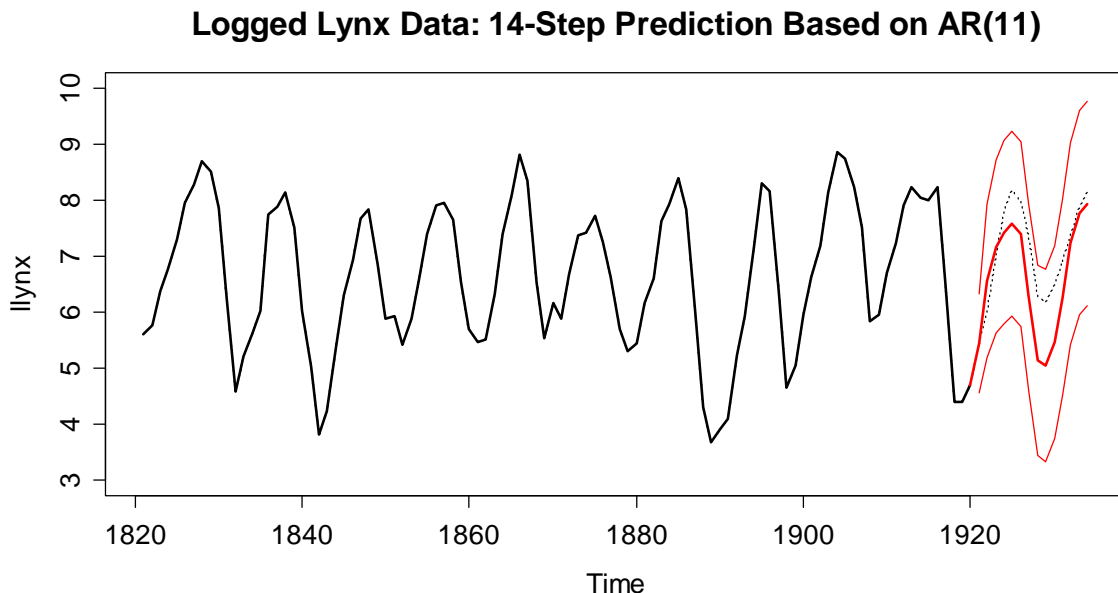
The question is, what do we do for longer forecasting horizons? There, the forecast is again based on the linear combination of the  $p$  past instances. For the ones with an index between 1 and  $n$ , the observed value  $x_t$  is used. Else, if the index exceeds  $n$ , we just plug-in the forecasted values  $\hat{x}_{t,1:n}$ . Thus, the general formula is:

$$\hat{X}_{n+k,1:n} = \alpha_1 \hat{X}_{n+k-1,1:n} + \dots + \alpha_p \hat{X}_{n+k-p,1:n},$$

where  $\hat{X}_{t,1:n} = x_t$  in all cases where  $t \leq n$ , i.e. an observed value is available.

### Practical Example

We consider the lynx data for which we had identified an  $AR(11)$  as a suitable model. Again, we use the first 100 observations for fitting the model and lay aside the last 14, which are in turn used for verifying the result. Also, we do without showing the R code, because it is identical to the one from the previous example.



We observe that the forecast tracks the general behavior of the series well, though the level of the series is underestimated somewhat. This is, however, not due to an “error” of ours, it is just that the values were higher than the past observations suggested. We finish this section with some remarks:

- Forecasting from an  $AR(p)$  only requires knowledge about the last  $p$  instances of the series, plus the model parameters  $\alpha_1, \dots, \alpha_p$  and the global series mean  $\mu$ . Earlier values of the series are not required, the model thus has a Markov property of order  $p$ .
- The prediction intervals only account for the uncertainty caused by the innovation variance, but not for the one caused by model misconception, and the plug-in of estimated parameters. Thus in practice, a true 95% interval would most likely be wider than shown above.

### 8.1.3 Forecasting $MA(1)$

We here consider an invertible  $MA(1)$  process, where the model equation is as follows:

$$X_t = E_t + \beta_1 E_{t-1},$$

where  $E_t$  is an innovation with expectation zero and constant variance.

As above, the forecast  $\hat{X}_{n+k,ln}$  will again be based on the conditional expectation  $E[X_{n+k} | X_1, \dots, X_n]$ . We get to a solution if we plug-in the model equation. First, we assume that  $k \geq 2$ , i.e. predict at least 2 time steps ahead.

$$\begin{aligned}\hat{X}_{n+k,ln} &= E[X_{n+k} | X_1, \dots, X_n] \\ &= E[E_{n+k} + \beta_1 E_{n+k-1} | X_1, \dots, X_n] \\ &= E[E_{n+k} | X_1, \dots, X_n] + \beta_1 E[E_{n+k-1} | X_1, \dots, X_n] \\ &= 0\end{aligned}$$

The best forecast  $MA(1)$  forecast for horizons 2 and up is thus zero. Remember that we require  $E_t$  being an innovation, and thus independent from previous instances  $X_s, s < t$  of the time series process. Next, we address the 1-step forecast. This is more problematic, because the above derivation leads to:

$$\begin{aligned}\hat{X}_{n+1,ln} &= \dots \\ &= \beta_1 E[E_n | X_1, \dots, X_n] \\ &\neq 0 \text{ (generally)}\end{aligned}$$

The 1-step forecast thus generally is different from zero. Moreover, the term  $E[E_n | X_1, \dots, X_n]$  is difficult to determine. Using some mathematical trickery, we can at least propose an approximate value. This trick is to move the point of reference into the infinite past, i.e. conditioning on all previous instances of the  $MA(1)$  process. We denote

$$e_n := E[E_n | X_{-\infty}^n].$$

By successive substitution, we then write the  $MA(1)$  as an  $AR(\infty)$ . This yields

$$E_n = \sum_{j=0}^{\infty} (-\beta_1)^j X_{n-j}.$$

If we condition the expectation of  $E_n$  on the infinite past of the series  $X_t$ , we can plug-in the realizations  $x_t$  and obtain:

$$E[E_n | X_{-\infty}^n] = e_n = \sum_{j=0}^{\infty} (-\beta_1)^j x_{n-j}.$$

This is of course somewhat problematic for practical implementation, because we only have realizations for  $x_1, \dots, x_n$ . However, because for invertible  $MA(1)$  processes,  $|\beta_1| < 1$ , the impact of early observations dies out exponentially quickly. Thus, we let  $x_t = 0$  for  $t < 1$ , and thus also have that  $e_t = 0$  for  $t < 1$ . Also, we plug-in the estimated model parameter  $\hat{\beta}_1$ , and thus, the 1-step forecast for an  $MA(1)$  is:

$$\hat{X}_{n+1,ln} = \sum_{j=0}^{n-1} \hat{\beta}_1 (-\hat{\beta}_1)^j x_{n-j}$$



This is a sum of all observed values, with exponentially decaying weights.

### 8.1.4 Forecasting MA(q)

When forecasting from  $MA(q)$  processes, we encounter the same difficulties as above. The prediction for horizons exceeding  $q$  are all zero, but anything below contains terms for which the considerations in section 8.1.3 are again necessary. We do without displaying this, and proceed to giving the formulae for  $ARMA(p, q)$  forecasting, from which the ones for  $MA(q)$  can be learned.

### 8.1.5 Forecasting ARMA(p,q)

We are considering stationary and invertible  $ARMA(p, q)$  processes. The model equation for  $X_{n+1}$  then is:

$$X_{n+1} = \alpha_1 X_n + \dots + \alpha_p X_{n+1-p} + E_{n+1} + \beta_1 E_n + \dots + \beta_q E_{n+1-q}$$

As this model equation contains past innovations, we face the same problems as in section 8.1.3 when trying to derive the forecast for horizons  $\leq q$ . These can be mitigated, if we again condition on the infinite past of the process.

$$\begin{aligned} \hat{X}_{n+1,1n} &= E[X_{n+1} | X_{-\infty}^n] \\ &= \sum_{i=1}^p \alpha_i E[X_{n+1-i} | X_{-\infty}^n] + E[E_{n+1} | X_{-\infty}^n] + \sum_{j=1}^q \beta_j E[E_{n+1-j} | X_{-\infty}^n] \\ &= \sum_{i=1}^p \alpha_i x_{n+1-i} + \sum_{j=1}^q \beta_j E[E_{n+1-j} | X_{-\infty}^n] \end{aligned}$$

If we are aiming for  $k$ -step forecasting, we can use a recursive prediction scheme:

$$\hat{X}_{n+k,1n} = \sum_{i=1}^p \alpha_i E[X_{n+k-i} | X_{-\infty}^n] + \sum_{j=1}^q \beta_j E[E_{n+k-j} | X_{-\infty}^n],$$

where for the  $AR$ - and  $MA$ -part the conditional expectations are:

$$\begin{aligned} E[X_t | X_{-\infty}^n] &= \begin{cases} x_t, & \text{if } t \leq n \\ \hat{X}_{t,1n}, & \text{if } t > n \end{cases} \\ E[E_t | X_{-\infty}^n] &= \begin{cases} e_t, & \text{if } t \leq n \\ 0, & \text{if } t > n \end{cases} \end{aligned}$$

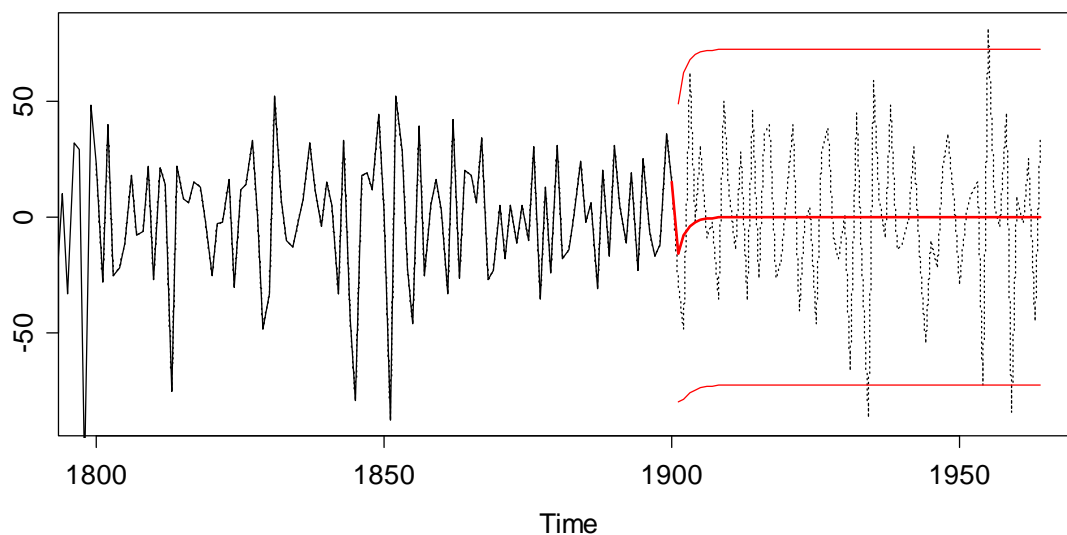
The terms  $e_t$  are then determined as outlined above in section 8.1.3, and for the model parameters, we are plugging-in the estimates. This allows us to generate any forecast from an  $ARMA(p, q)$  model that we wish. The procedure is also known as Box-Jenkins procedure, after the two researchers who first introduced it.

Next, we illustrate this with a practical example, though in  $\mathbb{R}$ , things are quite unspectacular. It is again the `predict()` procedure that is applied to a fit from `arima()`, the Box-Jenkins scheme that is employed runs in the background.

### Practical Example

We here consider the Douglas Fir data which show the width of the year rings over a period from 1107 to 1964. Because the data are non-stationary, we take differences and model these. An  $ARMA(1,1)$  seems appropriate. We put the last 64 observations aside so that we can verify our predictions. Then, the model is fitted and the Box-Jenkins predictions are obtained. The result, including a 95% prognosis interval, is shown below.

**Differenced Douglas Fir Data: 64-Step Prediction Based on  $ARMA(1,1)$**



We observe that the forecast goes to zero exponentially quickly. However, it is in fact different from zero for all times. Moreover, all observations down to the very first one are used for obtaining the predictions. Again, the  $ARMA$  model combines the properties from pure  $AR$  and  $MA$  processes.

## 8.2 Exponential Smoothing

### 8.2.1 Simple Exponential Smoothing

The objective in this section is to predict some future values  $X_{n+k}$  given an observed series  $\{X_1, \dots, X_n\}$ , and thus no different than before. We first assume that the data do not exhibit any deterministic trend or seasonality, or that these have been identified and removed. The (conditional) expected value of the process can change from one time step to the next, but we do not have any information about the direction of this change. A typical application is forecasting sales of a well-established product in a stable market. The model is:

$$X_t = \mu_t + E_t,$$

where  $\mu_t$  is the non-stationary mean of the process at time  $t$ , and  $E_t$  are independent random innovations with expectation zero and constant variance  $\sigma_E^2$ . We will here use the same notation as  $\mathfrak{R}$  does, and let  $a_t$ , called *level* of the series, be our estimate of  $\mu_t$ . By assuming that there is no deterministic trend, an intuitive estimate for the level at time  $t$  is to take a weighted average of the current time series observation and the previous level:

$$a_t = \alpha x_t + (1 - \alpha)a_{t-1}, \text{ with } 0 < \alpha < 1.$$

Apparently, the value of  $\alpha$  determines the amount of smoothing: if it is near 1, there is little smoothing and the level  $a_t$  closely tracks the series  $x_t$ . This would be appropriate if the changes in the mean of the series are large compared to the innovation variance  $\sigma_E^2$ . At the other extreme, an  $\alpha$ -value near 0 gives highly smoothed estimates of the current mean which take little account of the most recent observation. This would be the way to go for series with a large amount of noise compared to the signal size. A typical default value is  $\alpha = 0.2$ , chosen in the light that for most series, the change in the mean between  $t$  and  $t-1$  is smaller than  $\sigma_E^2$ . Alternatively, it is (with  $\mathfrak{R}$ ) also possible to estimate  $\alpha$ , see below.

Because we assume absence of deterministic trend and seasonality, the best forecast at time  $n$  for the future level of the series, no matter what horizon we are aiming for, is given by the level estimate at time  $n$ , i.e.

$$\hat{X}_{n+k,1n} = a_n, \text{ for all } k = 1, 2, \dots$$

We can rewrite the weighted average equation in two further ways, which yields insight into how exponential smoothing works. Firstly, we can write the level at time  $t$  as the sum of  $a_{t-1}$  and the 1-step forecasting error and obtain the *update formula*:

$$a_t = \alpha(x_t - a_{t-1}) + a_{t-1}$$

Now, if we repeatedly apply back substitution, we obtain:

$$a_t = \alpha x_t + \alpha(1 - \alpha)x_{t-1} + \alpha(1 - \alpha)^2 x_{t-2} + \dots$$

When written in this form, we see that the level  $a_t$  is a linear combination of the current and all past observations with more weight given to recent observations. The restriction  $0 < \alpha < 1$  ensures that the weights  $\alpha(1 - \alpha)^i$  become smaller as  $i$  increases. In fact, they are exponentially decaying and form a geometric series. When the sum over these terms is taken to infinity, the result is 1. In practice, the infinite sum is not feasible, but can be avoided by specifying  $a_1 = x_1$ .

For any given smoothing parameter  $\alpha$ , the update formula plus the choice of  $a_1 = x_1$  as a starting value can be used to determine the level  $a_t$  for all times  $t = 2, 3, \dots$ . The 1-step prediction errors  $e_t$  are given by:

$$e_t = x_t - \hat{x}_{t|t(t-1)} = x_t - a_{t-1}.$$

By default, R obtains a value for the smoothing parameter  $\alpha$  by minimizing the sum of squared 1-step prediction errors, called *SS1PE* :

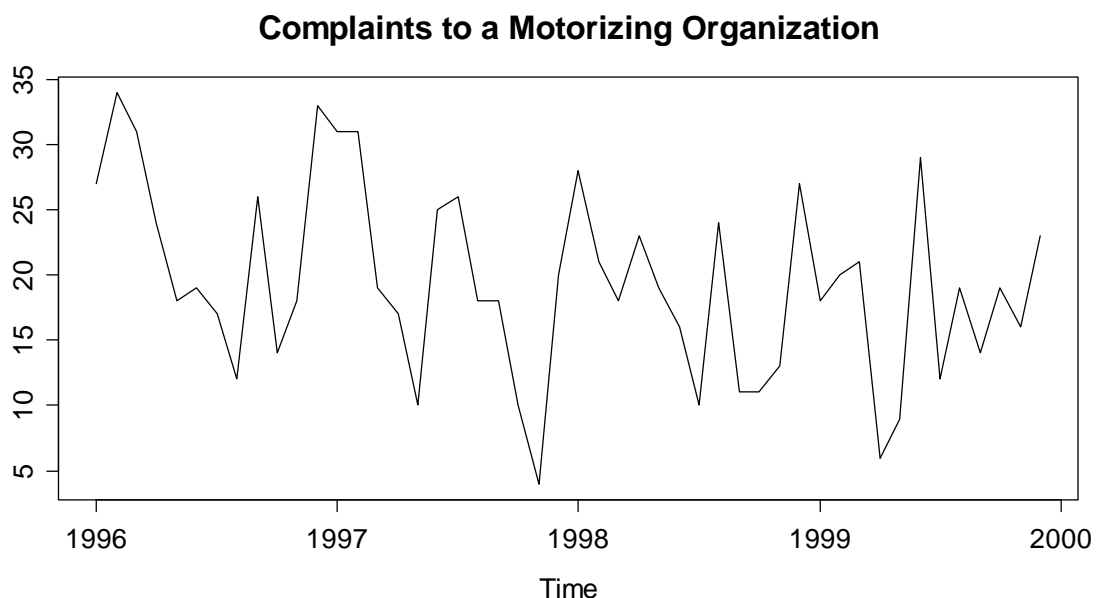
$$SS1PE = \sum_{t=2}^n e_t^2.$$

There is some mathematical theory that examines the quality of the *SS1PE* - minimizing  $\alpha$ . Not surprisingly, this depends very much on the true, underlying process. However in practice, this value is reasonable and allows for good predictions.

### Practical Example

We here consider a time series that shows the number of complaint letters that were submitted to a motoring organization over the four years 1996-1999. At the beginning of year 2000, the organization wishes to estimate the current level of complaints and investigate whether there was any trend in the past. We import the data and do a time series plot:

```
> www <- "http://staff.elela.aut.ac.nz/Paul-Cowpertwait/ts/"
> dat <- read.table(paste(www,"motororg.dat",sep=" ", head=T)
> cml <- ts(dat$complaints, start=c(1996,1), freq=12)
> plot(cml, ylab="", main="Complaints ...")
```



The series is rather short, and there is no clear evidence for a deterministic trend and/or seasonality. Thus, it seems sensible to use exponential smoothing here. The algorithm that was described above is implemented in R's `HoltWinters()` procedure. Please note that `HoltWinters()` can do more than plain exponential smoothing, and thus we have to set arguments `beta=FALSE` and `gamma=FALSE`.

If we do not specify a value for the smoothing parameter  $\alpha$  with argument `alpha`, it will be estimated using the *SS1PE* criterion.

```
> fit <- HoltWinters(cmpl, beta=FALSE, gamma=FALSE); fit
```

Holt-Winters exponential smoothing without trend and without seasonal component.

Call:

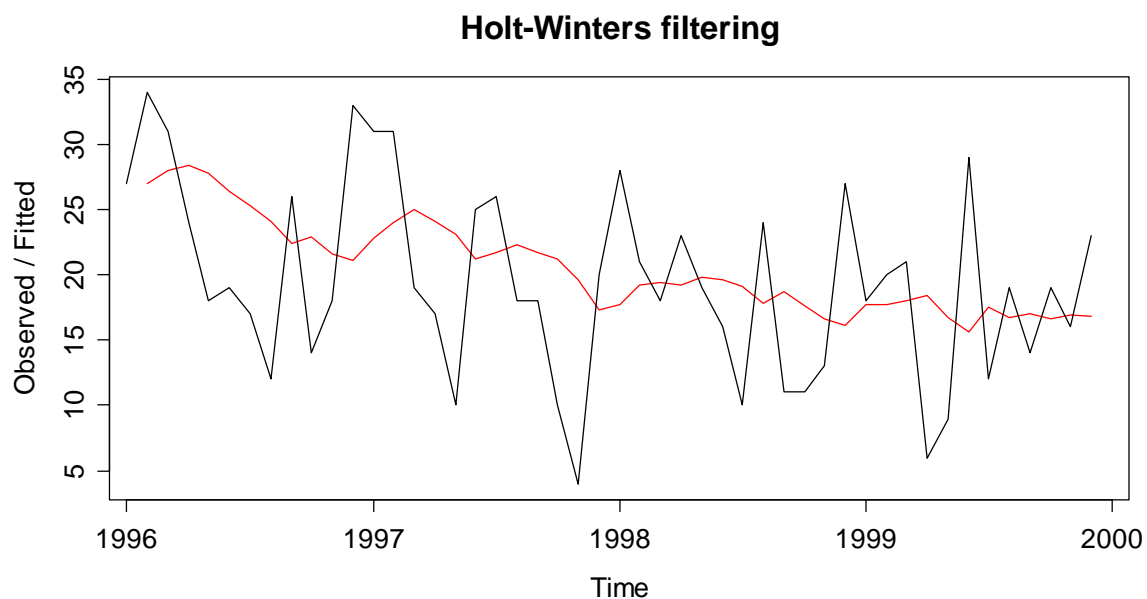
```
HoltWinters(x = cmpl, beta = FALSE, gamma = FALSE)
```

Smoothing parameters:

```
alpha: 0.1429622
beta : FALSE
gamma: FALSE
```

Coefficients:

```
      [,1]
a 17.70343
> plot(fit)
```



The output shows that the level in December 1999, this is  $a_{48}$ , is estimated as 17.70. The optimal value for  $\alpha$  according to the *SS1PE* criterion is 0.143, and the sum of squared prediction errors was 2502. Any other value for  $\alpha$  will yield a worse result, thus we proceed and display the result visually.

## 8.2.2 The Holt-Winters Method

The simple exponential smoothing approach from above can be generalized for series which exhibit deterministic trend and/or seasonality. As we have seen in many examples, such series are the norm rather than the exception and thus, such a method comes in handy. It is based on these formulae:

$$\begin{aligned}
 a_t &= \alpha(x_t - s_{t-p}) + (1-\alpha)(a_{t-1} + b_{t-1}) \\
 b_t &= \beta(a_t - a_{t-1}) + (1-\beta)b_{t-1} \\
 s_t &= \gamma(x_t - a_t) + (1-\gamma)s_{t-p}
 \end{aligned}$$

In the above equations,  $a_t$  is again the level at time  $t$ ,  $b_t$  is called the slope and  $s_t$  is the seasonal effect. There are now three smoothing parameters  $\alpha, \beta, \gamma$  which are aimed at level, slope and season. The explanation of these equations is as follows:

- The first updating equation for the level takes a weighted average of the most recent observation with the existing estimate of the previous' period seasonal effect term subtracted, and the 1-step level forecast at  $t-1$ , which is given by level plus slope.
- The second updating equation takes a weighted average of the difference between the current and the previous level with the estimated slope at time  $t-1$ . Note that this can only be computed if  $a_t$  is available.
- Finally, we obtain another estimate for the respective seasonal term by taking a weighted average of the difference between observation and level with the previous estimate of the seasonal term for the same unit, which was made at time  $t-p$ .

If nothing else is known, the typical choice for the smoothing parameters is  $\alpha = \beta = \gamma = 0.2$ . Moreover, starting values for the updating equations are required. Mostly, one chooses  $a_1 = x_1$ , the slope  $b_1 = 0$  and the seasonal effects  $s_1, \dots, s_p$  are either also set to zero or to the mean over the observations of a particular season. When applying the R function `HoltWinters()`, the starting values are obtained from the `decompose()` procedure, and it is possible to estimate the smoothing parameters through *SS1PE* minimization. The most interesting aspect are the predictions, though: the  $k$ -step forecasting equation for  $X_{n+k}$  at time  $n$  is:

$$\hat{X}_{n+k,1:n} = a_n + kb_n + s_{n+k-p},$$

i.e. the current level with linear trend extrapolation plus the appropriate seasonal effect term. The following practical example nicely illustrates the method.

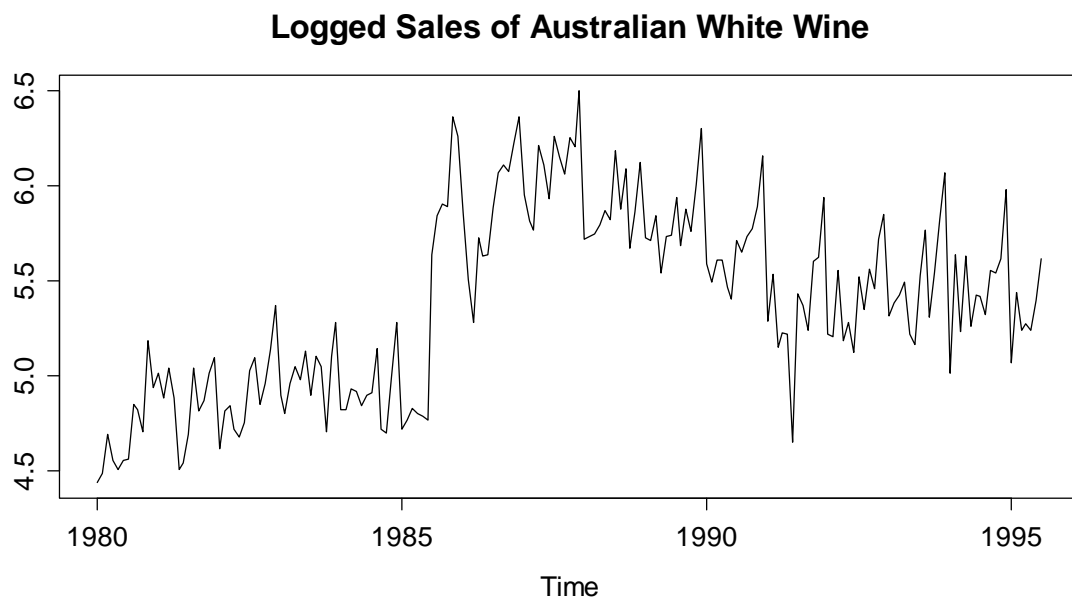
### Practical Example

We here discuss the series of monthly sales (in thousands of litres) of Australian white wine from January 1980 to July 1995. This series features a deterministic trend, the most striking feature is the sharp increase in the mid-80ies, followed by a reduction to a distinctly lower level again. The magnitude of both the seasonal effect and the errors seem to be increasing with the level of the series, and are thus multiplicative rather than additive. We will cure this by a log-transformation of the series, even though there exists a multiplicative formulation of the Holt-Winters algorithm, too.

```
> www <- "http://staff.elena.aut.ac.nz/Paul-Cowpertwait/ts/"
> dat <- read.table(paste(www,"wine.dat",sep="", header=T)
> aww <- ts(dat$sweetw, start=c(1980,1), freq=12)
> plot(aww, ylab="", main="Sales of Australian White Wine")
```



```
> plot(log(aww), ylab="", main="Logged Sales ...")
```



The transformation seems successful, thus we proceed to the Holt-Winters modeling. When we apply parameter estimation by *SS1PE*, this is straightforward. The fit contains the current estimates for level, trend and seasonality. Note that these are only valid for time  $n$ , and not for the entire series. Anyhow, it is much better to visualize the sequence of  $a_t, b_t$  and  $\gamma_t$  graphically. Moreover, plotting the fitted values along with the time series is informative, too.

```
> fit
Holt-Winters exponential smoothing with trend and additive
seasonal component.
```

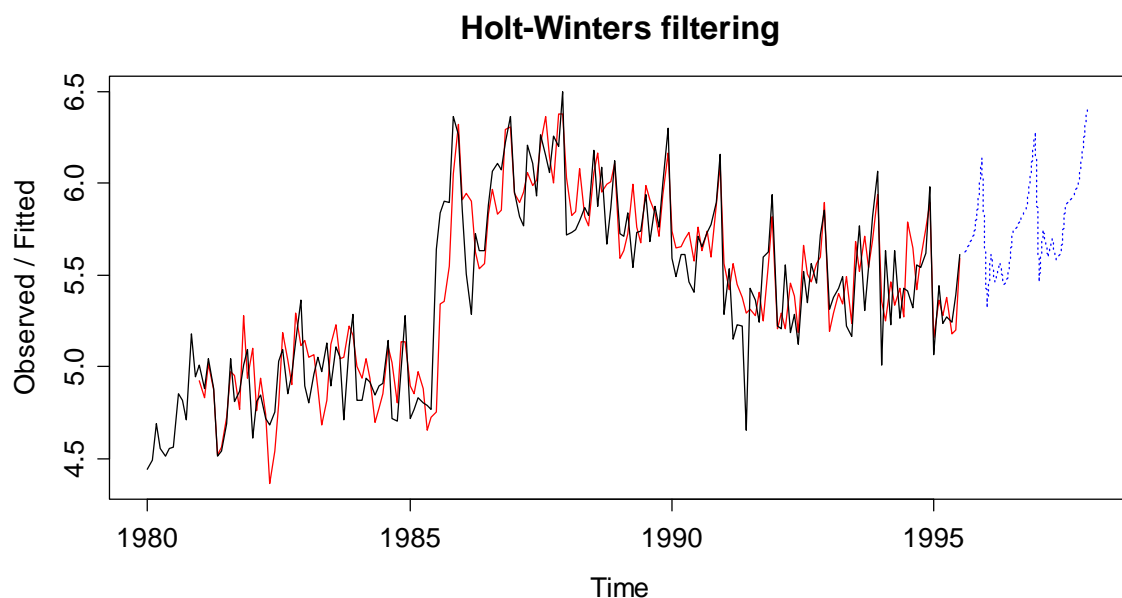
```
Call:
HoltWinters(x = log(aww))
```

```
Smoothing parameters:
  alpha: 0.4148028
  beta : 0
  gamma: 0.4741967
```

```
Coefficients:
a      5.62591329
b      0.01148402
s1     -0.01230437
s2      0.01344762
s3      0.06000025
s4      0.20894897
s5      0.45515787
s6     -0.37315236
s7     -0.09709593
s8     -0.25718994
s9     -0.17107682
s10    -0.29304652
s11    -0.26986816
s12    -0.01984965
```

The coefficient values (at time  $n$ ) are also the ones which are used for forecasting from that series with the formula given above. We produce a prediction up until the end of 1998, which is a 29-step forecast. The R commands are:

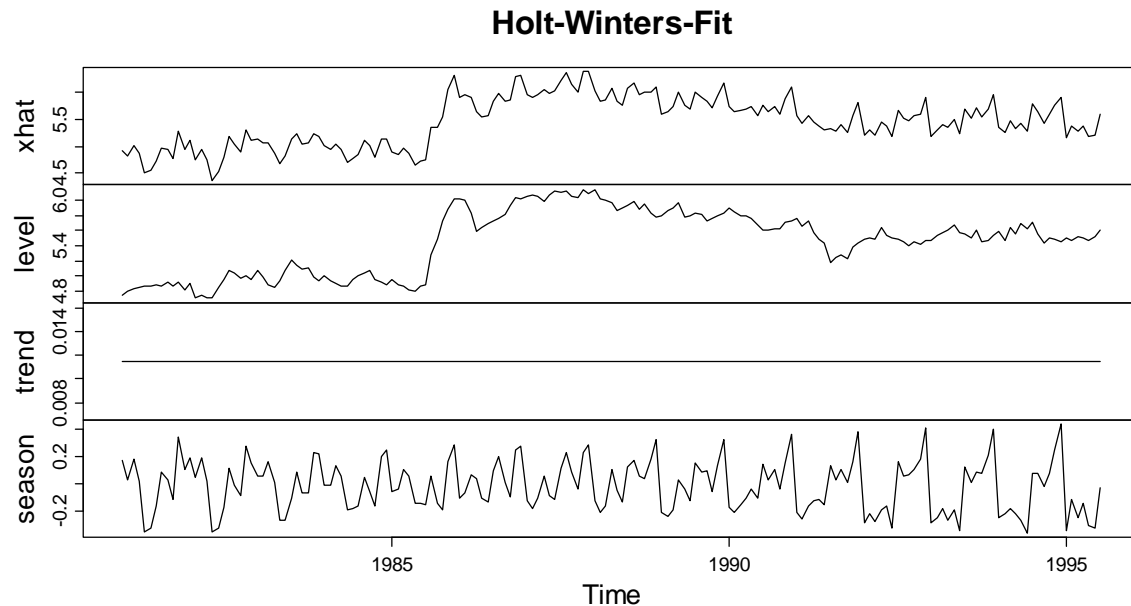
```
> plot(fit, xlim=c(1980, 1998))
> lines(predict(fit, n.ahead=29), col="blue", lty=3)
```





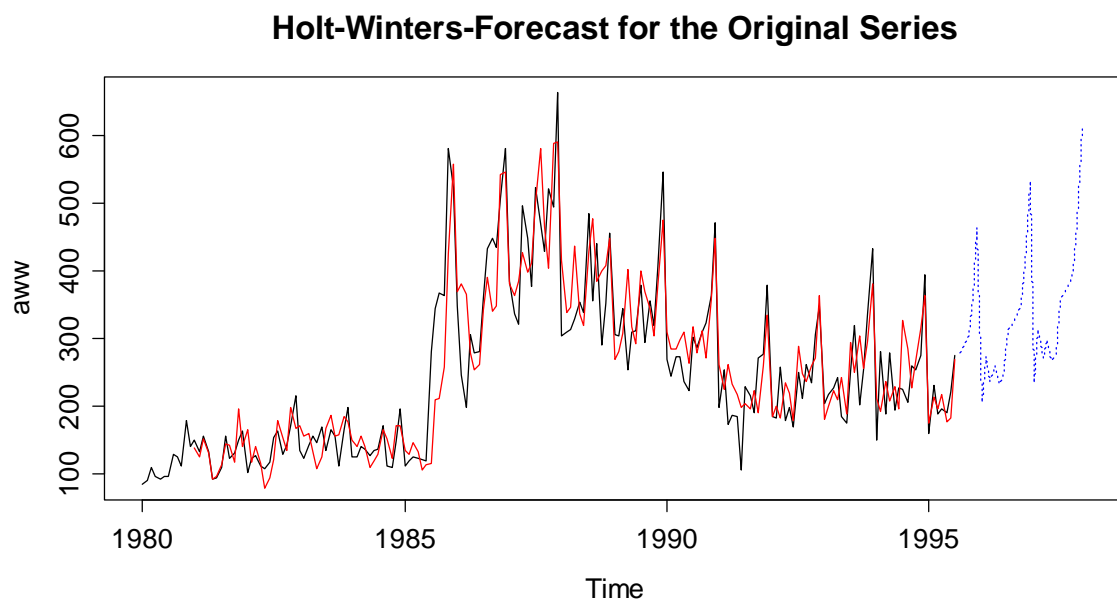
It is also very instructive to plot how level, trend and seasonality evolved over time. This can be done very simply in **R**:

```
> plot(fit$fitted, main="Holt-Winters-Fit")
```



Since we are usually more interested in the prediction on the original scale, i.e. in liters rather than log-liters of wine, we just re-exponentiate the values. Please note that the result is an estimate of the median rather than the mean of the series. There are methods for correction, but the difference is usually only small.

```
> plot(aww, xlim=c(1980, 1998))
> lines(exp(fit$fitted[,1]), col="red")
> lines(exp(predict(fit, n.ahead=29)), col="blue", lty=3)
```



Also, we note that the (insample) 1-step prediction error is equal to 50.04, which is quite a reduction when compared to the series' standard deviation which is 121.4. Thus, the Holt-Winters fit has substantial explanatory power. Of course, it would now be interesting to test the accuracy of the predictions. We recommend that you, as an exercise, put aside the last 24 observations of the Australian white wine data, and run a forecasting evaluation where all the methods (SARIMA, decomposition approaches, Holt-Winters) compete against each other.

## 9 Multivariate Time Series Analysis

While the header of this section says *multivariate* time series analysis, we will here restrict to two series series  $X_1 = (X_{1,t})$  and  $X_2 = (X_{2,t})$ , and thus *bivariate* time series analysis, because an extension to more than two series is essentially analogous. Please note that a prerequisite for all the theory in this section is that the series  $X_1$  and  $X_2$  are stationary.

Generally speaking, the goal of this section is to describe and understand the (inter)dependency between two series. We introduce the basic concepts of cross correlation and transfer function models, warn of arising difficulties in interpretation and show how these can be mitigated.

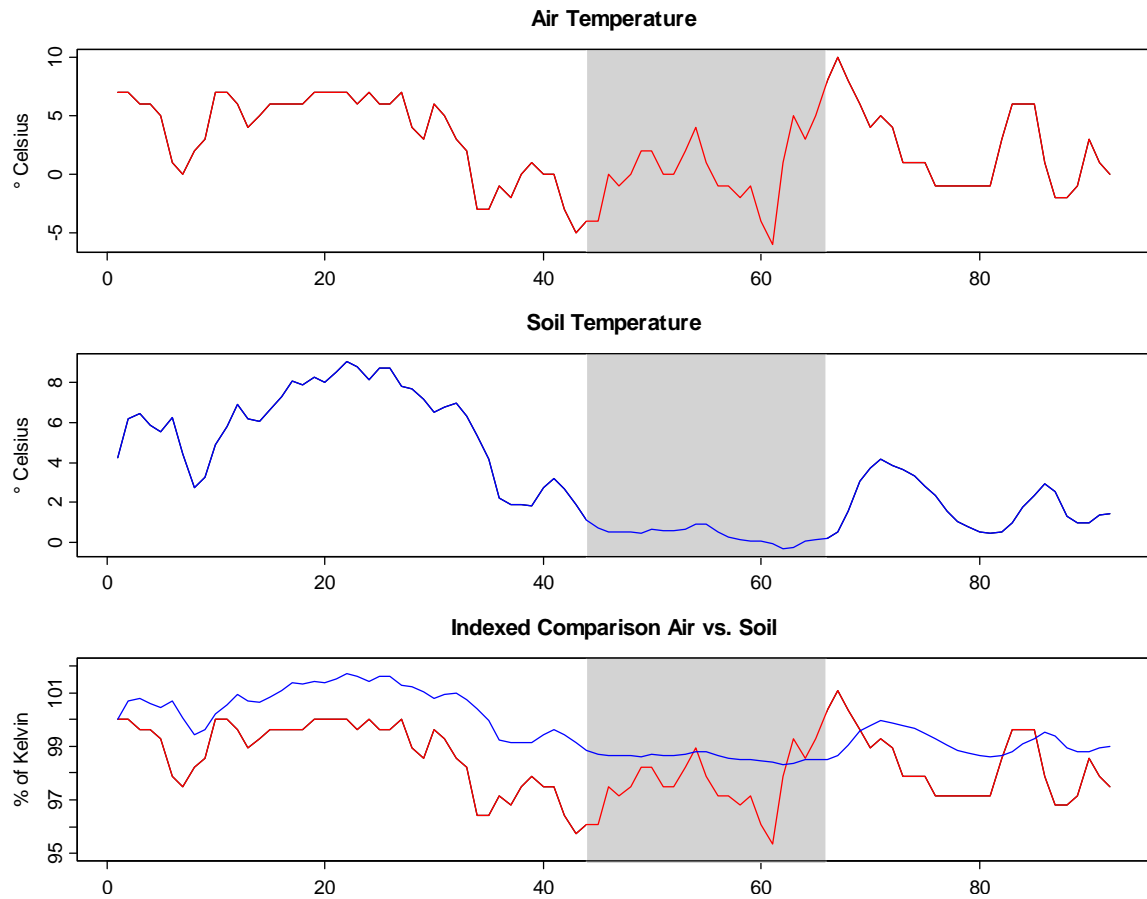
### 9.1 Practical Example

We will illustrate the theory on multivariate time series analysis with a practical example. The data were obtained in the context of the diploma thesis of Evelyn Zenklusen Mutter, a former WBL student who works for the Swiss Institute for Snow and Avalanche Research SLF. The topic is how the ground temperature in permafrost terrain depends on the ambient air temperature. The following section gives a few more details.

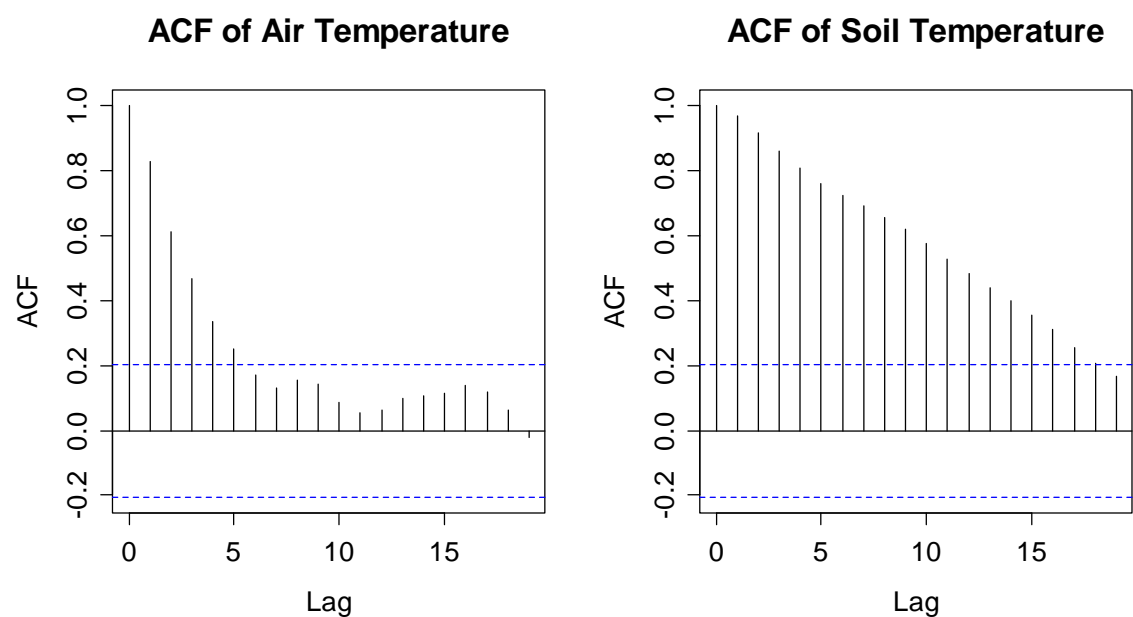
*Ambient air temperatures influence ground temperatures with a certain temporal delay. Borehole temperatures measured at 0.5m depth in alpine permafrost terrain, as well as air temperatures measured at or nearby the boreholes will be used to model this dependency. The reaction of the ground on the air temperature is influenced by various factors such as ground surface cover, snow depth, water or ground ice content. To avoid complications induced by the insulating properties of the snow cover and by phase changes in the ground, only the snow-free summer period when the ground at 0.5m is thawed will be considered.*

We here consider only one single borehole, it is located near the famous *Hörnli hut* at the base of *Matterhorn* near Zermatt/CH on 3295m above sea level. The air temperature was recorded on the nearby *Platthorn* at 3345m of elevation and 9.2km distance from the borehole. Data are available from beginning of July 2006 to the end of September 2006. After the middle of the observation period, there is a period of 23 days during which the ground was covered by snow, highlighted in grey color in the time series plots on the next page.

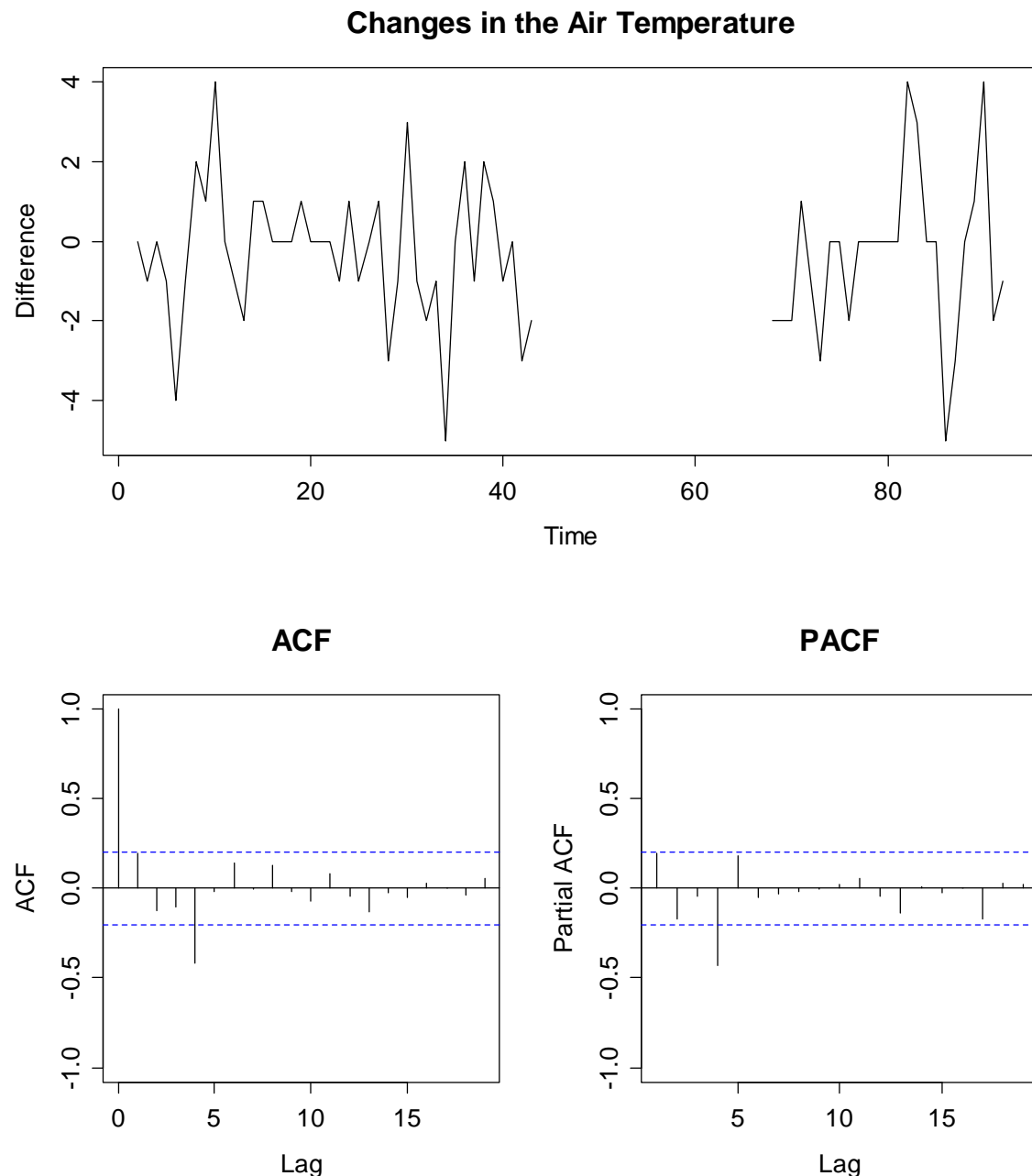
Because the snow insulates the ground, we do not expect the soil to follow the air temperature during that period. Hence, we set all values during that period equal to NA. The time series plots, and especially the indexed plot where both series are shown, clearly indicate that the soil reacts to the air temperature with a delay of a few days. We now aim for analyzing this relationship on a more quantitative basis, for which the methods of multivariate time series analysis will be employed.



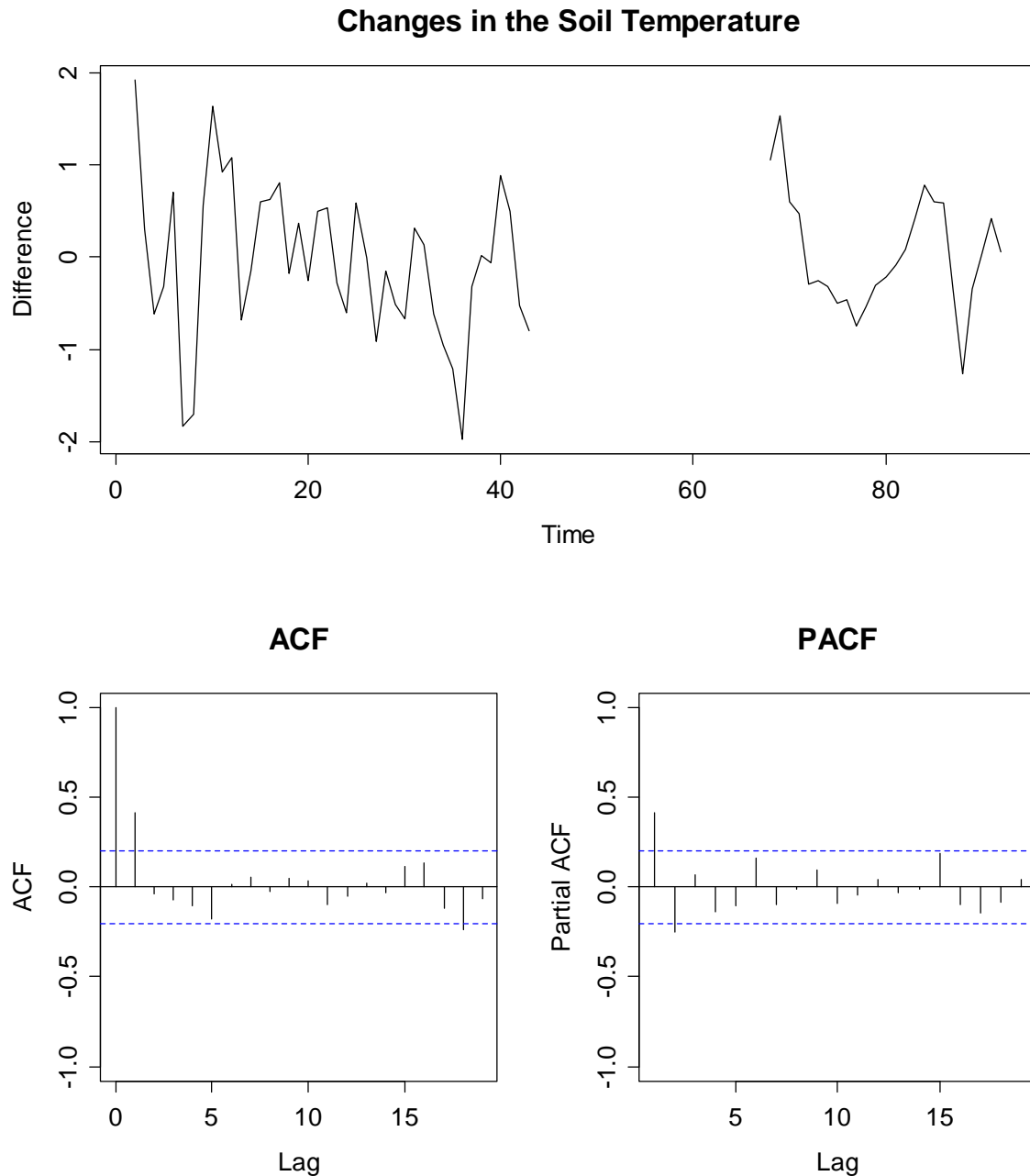
As we had stated above, multivariate time series analysis requires stationarity. Is this met with our series? The time series plot does not give a very clear answer. Science tells us that temperature has a seasonal pattern. Moreover, the correlogram of the two series is enlightening.



The ACF exhibits a slow decay, especially for the soil temperature. Thus, we decide to perform lag 1 differencing before analyzing the series. This has another advantage: we are then exploring how changes in the air temperature are associated with changes in the soil temperature and if so, what the time delay is. These results are easier to interpret than a direct analysis of air and soil temperatures. Next, we display the differenced series with their ACF and PACF. The observations during the snow cover period are now omitted.



The differenced air temperature series seems stationary, but is clearly not iid. There seems to be some strong negative correlation at lag 4. This may indicate the properties of the meteorological weather patterns at that time of year in that part of Switzerland. We now perform the same analysis for the changes in the soil temperature.



In the course of our discussion of multivariate time series analysis, we will require some  $ARMA(p, q)$  models fitted to the changes in air and soil temperature. For the former series, model choice is not simple, as in both ACF and PACF, the coefficient at lag 4 sticks out. A grid search shows that an  $AR(5)$  model yields the best AIC value, and also, the residuals from this model do look as desired, i.e. it seems plausible that they are White Noise.

For the changes in the soil temperature, model identification is easier. ACF and PACF suggest either a  $MA(1)$ , an  $ARMA(2, 1)$  or an  $AR(2)$ . From these three models, the  $MA(1)$  shows both the lowest AIC value as well as the “best looking” residuals. Furthermore, it is the parsimonious choice, and hence we got with it.

## 9.2 Cross Correlation

To begin with, we consider the (theoretical) cross covariance, the measure that describes the amount of linear dependence between the two time series processes. Firstly, we recall the definition of the within-series autocovariances, denoted by  $\gamma_{11}(k)$  and  $\gamma_{22}(k)$ :

$$\gamma_{11}(k) = \text{Cov}(X_{1,t+k}, X_{1,t}), \gamma_{22}(k) = \text{Cov}(X_{2,t+k}, X_{2,t})$$

The cross covariances between the two processes  $X_1$  and  $X_2$  are given by:

$$\gamma_{12}(k) = \text{Cov}(X_{1,t+k}, X_{2,t}), \gamma_{21}(k) = \text{Cov}(X_{2,t+k}, X_{1,t})$$

Note that owing to the stationarity of the two series, the cross covariances  $\gamma_{12}(k)$  and  $\gamma_{21}(k)$  both do not depend on the time  $t$ . Moreover, there is some obvious symmetry in the cross covariance:

$$\gamma_{12}(-k) = \text{Cov}(X_{1,t-k}, X_{2,t}) = \text{Cov}(X_{1,t}, X_{2,t+k}) = \gamma_{21}(k)$$

Thus, for practical purposes, it suffices to consider  $\gamma_{12}(k)$  for positive and negative values of  $k$ . Note that we will preferably work with correlations rather than covariances, because they are scale-free and thus easier to interpret. We can obtain the cross correlations by standardizing the cross covariances:

$$\rho_{12}(k) = \frac{\gamma_{12}(k)}{\sqrt{\gamma_{11}(0)\gamma_{22}(0)}}, \rho_{21}(k) = \frac{\gamma_{21}(k)}{\sqrt{\gamma_{11}(0)\gamma_{22}(0)}}.$$

Not surprisingly, we also have symmetry here, i.e.  $\rho_{12}(-k) = \rho_{21}(k)$ . Additionally, the cross correlations are limited to the interval between -1 and +1, i.e.  $|\rho_{12}(k)| \leq 1$ . As for the interpretation,  $\rho_{12}(k)$  measures the linear association between two values of  $X_1$  and  $X_2$ , if the value of the first time series is  $k$  steps ahead. Concerning estimation of cross covariances and cross correlations, we apply the usual sample estimators:

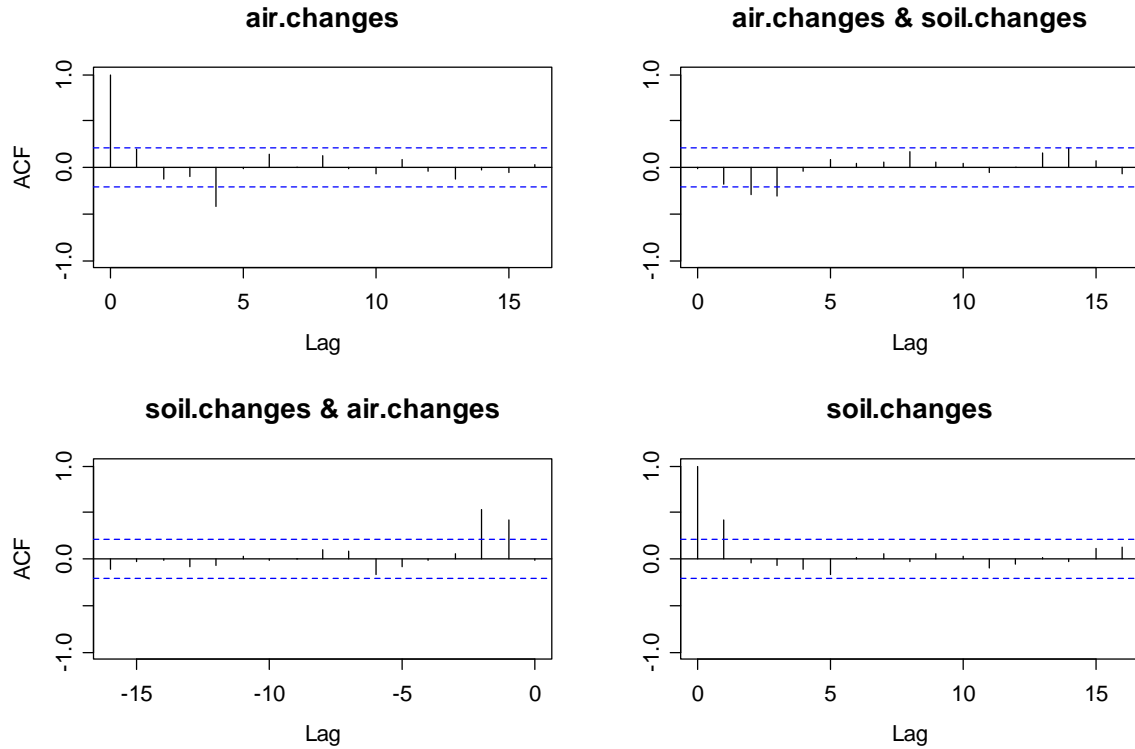
$$\hat{\gamma}_{12}(k) = \frac{1}{n} \sum_t (x_{1,t+k} - \bar{x}_1)(x_{2,t} - \bar{x}_2) \text{ and } \hat{\gamma}_{21}(k) = \frac{1}{n} \sum_t (x_{2,t+k} - \bar{x}_2)(x_{1,t} - \bar{x}_1),$$

where the summation index  $t$  for  $k \geq 0$  goes from 1 to  $n-k$  and for  $k < 0$  goes from  $1-k$  to  $n$ . With  $\bar{x}_1$  and  $\bar{x}_2$  we denote the mean values of  $x_{1,t}$  and  $x_{2,t}$ , respectively. We define the estimation of the cross-correlations as

$$\hat{\rho}_{12}(k) = \frac{\hat{\gamma}_{12}(k)}{\sqrt{\hat{\gamma}_{11}(0)\hat{\gamma}_{22}(0)}}, \hat{\rho}_{21}(k) = \frac{\hat{\gamma}_{21}(k)}{\sqrt{\hat{\gamma}_{11}(0)\hat{\gamma}_{22}(0)}}.$$

The plot of  $\hat{\rho}_{12}(k)$  against  $k$  is called the cross-correlogram. Note that this must be viewed for both positive and negative  $k$ . In  $\mathbf{R}$ , we the job is done by the `acf()` function, applied to a multiple time series object.

```
> both <- ts.union(diff(air.na), diff(soil.na))
> acf(both, na.action=na.pass, ylim=c(-1,1))
```



The top left panel shows the ACF of the differenced air temperature, the bottom right one holds the pure autocorrelations of the differenced soil temperature. The two off-diagonal plots contains estimates of the cross correlations: The top right panel has  $\hat{\rho}_{12}(k)$  for positive values of  $k$ , and thus shows how changes in the air temperature depend on changes in the soil temperature.

Note that we do not expect any significant correlation coefficients here, because the ground temperature has hardly any influence on the future air temperature at all. Conversely, the bottom left panel shows  $\hat{\rho}_{12}(k)$  for negative values of  $k$ , and thus how the changes in the soil temperature depend on changes in the air temperature. Here, we expect to see significant correlation.

## 9.2.1 Interpreting the Cross Correlogram

Interpreting the cross correlogram is tricky, because the within-series dependency results in a mixing of the correlations. It is very important to note that the confidence bounds shown in the above plots are usually wrong and can thus be strongly misleading. If not the additional steps to be discussed below are taken, interpreting the raw cross correlograms will lead to false conclusions.

The reason for these problems is that the variances and covariances of the  $\hat{\rho}_{12}(k)$  are very complicated functions of  $\rho_{11}(j), \rho_{22}(j)$  and  $\rho_{12}(j), j \in \mathbb{Z}$ . For illustrative purposes, we will treat some special cases explicitly.



### Case 1: No correlation between the two series for large lags

In the case where the cross correlation  $\rho_{12}(j) = 0$  for  $|j| \geq m$ , we have for  $|k| \geq m$ :

$$\text{Var}(\hat{\rho}_{12}(k)) \approx \frac{1}{n} \sum_{j=-\infty}^{\infty} \{\rho_{11}(j)\rho_{22}(j) + \rho_{12}(j+k)\rho_{12}(j-k)\}.$$

Thus, the variance of the estimated cross correlation coefficients goes to zero for  $n \rightarrow \infty$ , but for a deeper understanding with finite sample size, we must know *all* true auto and cross-correlations, which is of course impossible in practice.

### Case 2: No correlation between the series for all lags

If the two processes  $X_1$  and  $X_2$  are independent, i.e.  $\rho_{12}(j) \equiv 0$  for all  $j$ , then the variance of the cross correlation estimator simplifies to:

$$\text{Var}(\hat{\rho}_{12}(k)) \approx \frac{1}{n} \sum_{j=-\infty}^{\infty} \rho_{11}(j)\rho_{22}(j).$$

If, for example,  $X_1$  and  $X_2$  are two independent  $AR(1)$  processes with parameters  $\alpha_1$  and  $\alpha_2$ , then  $\rho_{11}(j) = \alpha_1^{|j|}$ ,  $\rho_{22}(j) = \alpha_2^{|j|}$  and  $\rho_{12}(j) \equiv 0$ . For the variance of  $\hat{\rho}_{12}(k)$  we have, because the autocorrelations form a geometric series:

$$\text{Var}(\hat{\rho}_{12}(k)) \approx \frac{1}{n} \sum_{j=-\infty}^{\infty} (\alpha_1 \alpha_2)^{|j|} = \frac{1}{n} \frac{1 + \alpha_1 \alpha_2}{1 - \alpha_1 \alpha_2}.$$

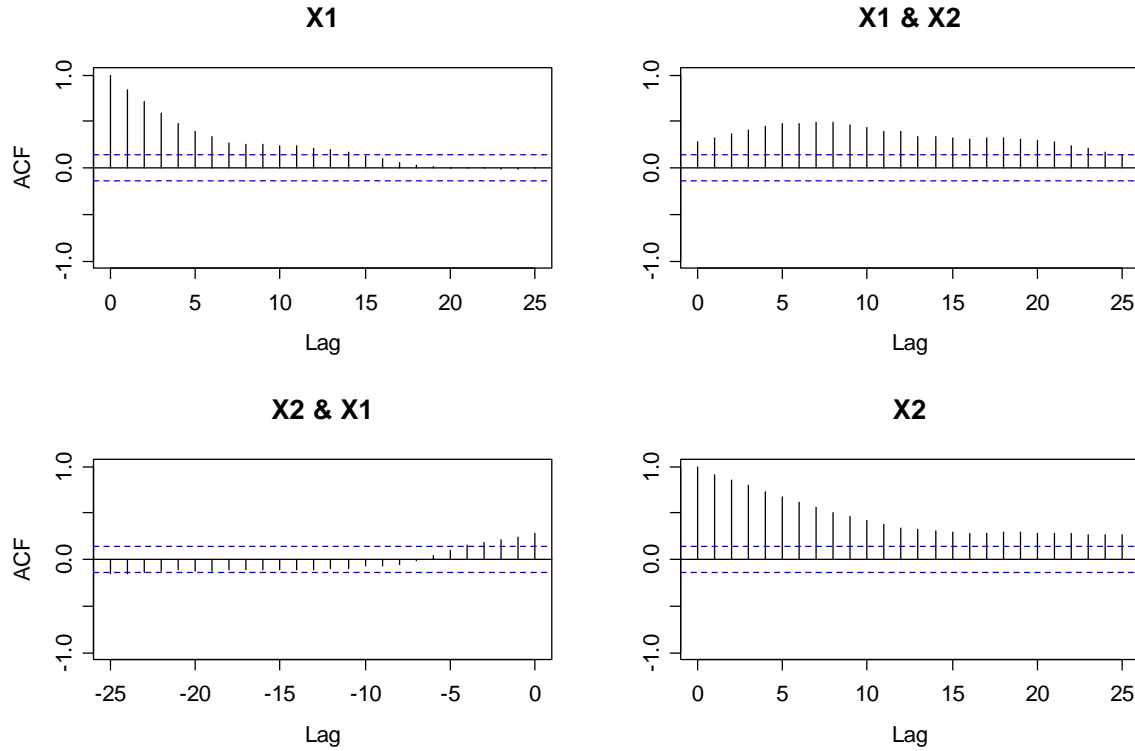
For  $\alpha_1 \rightarrow 1$  and  $\alpha_2 \rightarrow 1$  this expression goes to  $\infty$ , i.e. the estimator  $\hat{\rho}_{12}(k)$  can, for a finite time series, differ greatly from the true value 0. We would like to illustrate this with two simulated  $AR(1)$  processes with  $\alpha_1 = \alpha_2 = 0.9$ . According to theory all cross-correlations are 0. However, as we can see in the figure on the next page, the estimated cross correlations differ greatly from 0, even though the length of the estimated series is 200. In fact,  $2\sqrt{\text{Var}(\hat{\rho}_{12}(k))} \approx 0.44$ , i.e. the 95% confidence interval is  $\pm 0.44$ . Thus even with an estimated cross-correlation of 0.4 the null hypothesis “true cross-correlation is equal to 0” cannot be rejected.

### Case 3: No cross correlations for all lags and one series uncorrelated

Only now, in this special case, the variance of the cross correlation estimator is significantly simplified. In particular, if  $X_1$  is a White Noise process which is independent of  $X_2$ , we have, for large  $n$  and small  $k$ :

$$\text{Var}(\hat{\rho}_{12}(k)) \approx \frac{1}{n}.$$

Thus, in this special case, the rule of thumb  $\pm 2/\sqrt{n}$  yields a valid approximation to a 95% confidence interval for the cross correlations and can help to decide whether they are significantly or just randomly different from zero.



In most practical examples, however, the data will be auto- and also cross correlated. Thus, the question arises whether it is at all possible to do something here. Fortunately, the answer is yes: with the method of *prewhitening*, described in the next chapter, we do obtain a theoretically sound and practically useful cross correlation analysis.

### 9.3 Prewhitening

The idea behind *prewhitening* is to transform one of the two series such that it is uncorrelated, i.e. a White Noise series, which also explains the name of the approach. Formally, we assume that the two stationary processes  $X_1$  and  $X_2$  can be transformed as follows:

$$U_t = \sum_{i=0}^{\infty} a_i X_{1,t-i}$$

$$V_t = \sum_{i=0}^{\infty} b_i X_{2,t-i}$$

Thus, we are after coefficients  $a_i$  and  $b_i$  such that an infinite linear combination of past terms leads to White Noise. We know from previous theory that such a representation exists for all stationary and invertible  $ARMA(p, q)$  processes, it is the  $AR(\infty)$  representation. For the cross-correlations between  $U_t$  and  $V_t$  and between  $X_t$  and  $Y_t$ , the following relation holds:

$$\rho_{UV}(k) = \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} a_i b_j \rho_{X_1 X_2}(k+i-j)$$

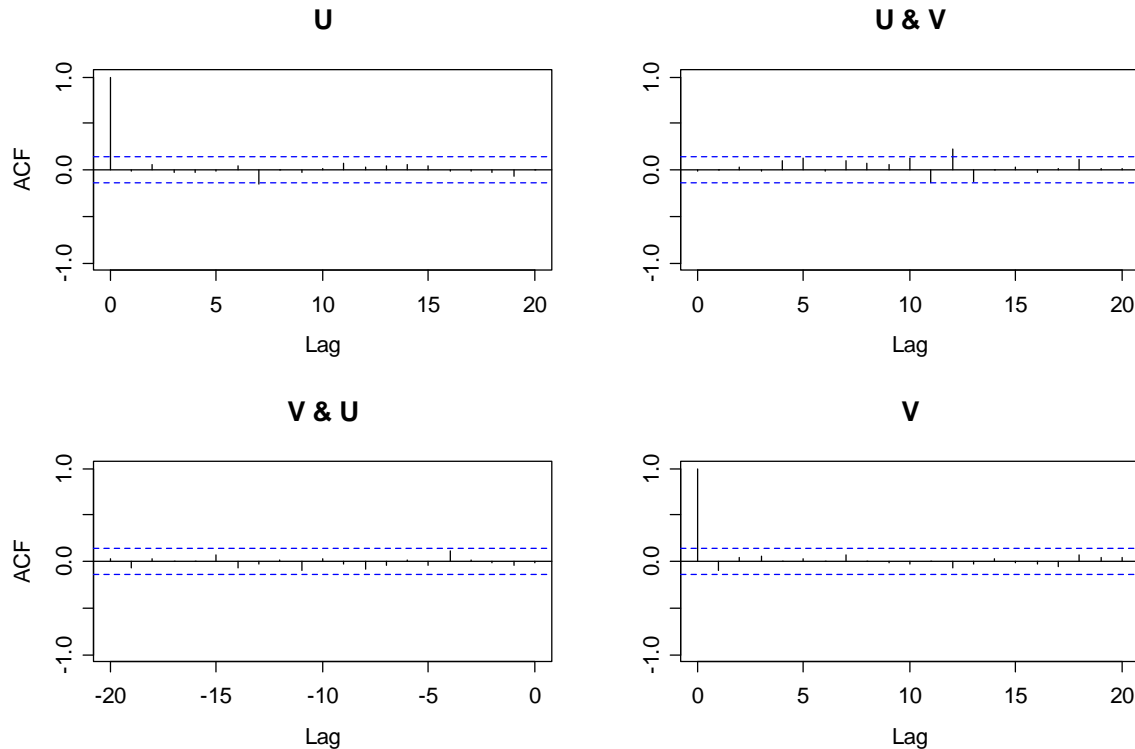
We conjecture that for two independent processes  $X_1$  and  $X_2$ , where all cross correlation coefficients  $\rho_{X_1 X_2}(k) = 0$ , also all  $\rho_{UV}(k) = 0$ . Additionally, the converse is also true, i.e. it follows from “ $U_t$  and  $V_t$  uncorrelated” that the original processes  $X_1$  and  $X_2$  are uncorrelated, too. Since  $U_t$  and  $V_t$  are White Noise processes, we are in the above explained case 3, and thus the confidence bounds in the cross correlograms are valid. Hence, any cross correlation analysis on “real” time series starts with representing them in terms of  $u_t$  and  $v_t$ .

### Example: AR(1) Simulations

For our example with the two simulated AR(1) processes, we can estimate the AR model coefficients with the Burg method and plug them in for prewhitening the series. Note that this amounts considering the residuals from the two fitted models!

$$u_t = x_{1,t} - \hat{\alpha}_1 x_{1,t-1}, \text{ where } \hat{\alpha}_1 = 0.889, \text{ and}$$

$$v_t = x_{2,t} - \hat{\alpha}_2 x_{2,t-1}, \text{ where } \hat{\alpha}_2 = 0.917.$$



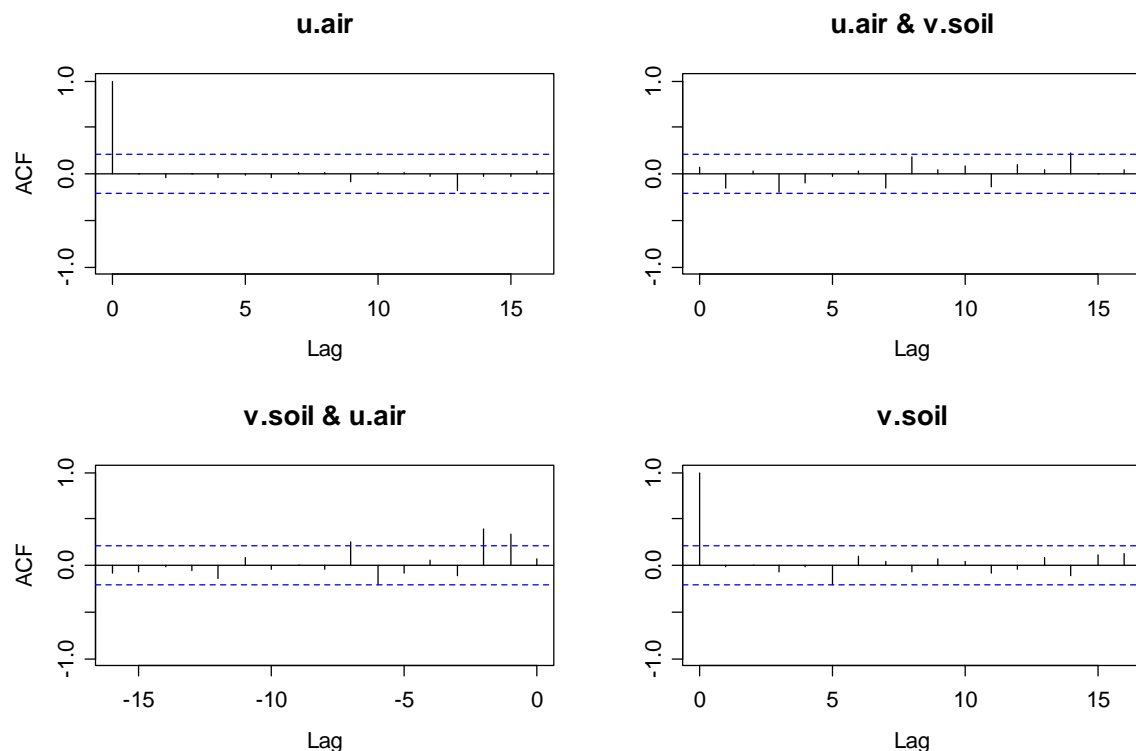
The figure on the previous page shows both the auto and cross correlations of the prewhitened series. We emphasize again that we here consider the residuals from the AR(1) models that were fitted to series  $X_1$  and  $X_2$ . We observe that, as we expect, there are no significant autocorrelations, and there is just one cross correlation coefficient that exceeds the 95% confidence bounds. We can attribute this to random variation.

The theory suggests, because  $U_t$  and  $V_t$  are uncorrelated, that also  $X_1$  and  $X_2$  do not show any linear dependence. Well, owing to how we set up the simulation, we know this for a fact, and take the result as evidence that the prewhitening approach works in practice.

### Example: Air and Soil Temperatures

For verifying whether there is any cross correlation between the changes in air and soil temperatures, we have to perform prewhitening also for the two differenced series. Previously, we had identified an  $AR(5)$  and a  $MA(1)$  model as. We can now just take their residuals and perform a cross correlation analysis:

```
> fit.air <- arima(diff(air.na), order=c(5,0,0))
> fit.soil <- arima(diff(soil.na), order=c(0,0,1))
> u.air <- resid(fit.air); v.soil <- resid(fit.soil)
> acf(ts.union(u.air, v.soil), na.action=na.pass)
```



The bottom left panel shows some significant cross correlations. A change in the air temperature seems to induce a change in the ground with a lag of 1 or 2 days.

## 9.4 Transfer Function Models

In the previous section we had observed significant cross correlations between the prewhitened air and soil temperature changes. This means that the cross correlations between the original air and soil temperature changes will also be different from zero. However, due to the prewhitening, inferring the magnitude of the linear association is different. The aim of this section is to clarify this issue.

The transfer function models are a possible way to capture the dependency between two time series. We must assume that the first series influences the second, but the second does not influence the first. Furthermore, the influence occurs only at simultaneously or in the future, but not on past values. Both assumptions are met in our example. The transfer function model is:

$$X_{2,t} - \mu_2 = \sum_{j=0}^{\infty} \nu_j (X_{1,t-j} - \mu_1) + E_t$$

We call  $X_1$  the *input* and correspondingly,  $X_2$  is named the *output*. For the error term  $E_t$  we require zero expectation and that they are independent from the input series, in particular:

$$E[E_t] = 0 \text{ and } Cov(E_t, X_{1,s}) = 0 \text{ for all } t \text{ and } s.$$

However, the errors  $E_t$  are usually autocorrelated. Note that this model is very similar to the time series regression model. However, here we have infinitely many unknown coefficients  $\nu_j$ , i.e. we do not know (a priori) on which lags to regress the input for obtaining the output. For the following theory, we assume (w.l.o.g.) that  $\mu_1 = \mu_2 = 0$ , i.e. the two series were adjusted for their means. In this case the cross covariances  $\gamma_{21}(k)$  are given by:

$$\gamma_{21}(k) = Cov(X_{2,t+k}, X_{1,t}) = Cov\left(\sum_{j=0}^{\infty} \nu_j X_{1,t+k-j}, X_{1,t}\right) = \sum_{j=0}^{\infty} \nu_j \gamma_{11}(k-j).$$

In cases where the transfer function model has a finite number of coefficients  $\nu_j$  only, i.e.  $\nu_j = 0$  for  $j > K$ , then the above formula turns into a linear system of  $K+1$  equations that we could theoretically solve for the unknowns  $\nu_j, j = 0, \dots, K$ .

If we replaced the theoretical  $\gamma_{11}$  and  $\gamma_{21}$  by the empirical covariances  $\hat{\gamma}_{11}$  and  $\hat{\gamma}_{21}$ , this would yield, estimates  $\hat{\nu}_j$ . However, this method is statistically inefficient and the choice of  $K$  proves to be difficult in practice. We again resort to some special case, for which the relation between cross covariance and transfer function model coefficients simplifies drastically.

### Special Case: Uncorrelated input series $X_1$

In this case,  $\gamma_{11}(k) = 0$  for  $k \neq 0$  and we have  $\gamma_{21}(k) = \nu_k \gamma_{11}(0)$ . For the coefficients  $\nu_k$  this results in the simplified transfer function model:

$$\nu_k = \frac{\gamma_{21}(k)}{\gamma_{11}(0)} = \rho_{21} \sqrt{\frac{\gamma_{22}(0)}{\gamma_{11}(0)}}, \text{ for } k \geq 0.$$

However,  $X_1$  generally is not a White Noise process. We can resort to prewhitening the input series. As we will show below, we can obtain an equivalent transfer function model with identical coefficients if a smart transformation is

applied to the output series. Namely, we have to filter the output with the model coefficients from the input series.

$$X_{1,t} = 0.296 \cdot X_{1,t-1} - 0.242 \cdot X_{1,t-2} - 0.119 \cdot X_{1,t-3} - 0.497 \cdot X_{1,t-4} + 0.216 \cdot X_{1,t-5} + D_t,$$

where  $D_t$  is the innovation, i.e. a White Noise process, for which we estimate the variance to be  $\hat{\sigma}_D^2 = 2.392$ . We now solve this equation for  $D_t$  and get:

$$\begin{aligned} D_t &= X_{1,t} - 0.296 \cdot X_{1,t-1} + 0.242 \cdot X_{1,t-2} + 0.119 \cdot X_{1,t-3} + 0.497 \cdot X_{1,t-4} - 0.216 \cdot X_{1,t-5} \\ &= (1 - 0.296B + 0.242B^2 + 0.119B^3 + 0.497B^4 - 0.216B^5)X_{1,t} \end{aligned}$$

We now apply this same transformation, i.e. the characteristic polynomial of the AR(5) also on the output series  $X_2$  and the transfer function model errors  $E_t$ :

$$Z_t = (1 - 0.296B + 0.242B^2 + 0.119B^3 + 0.497B^4 - 0.216B^5)X_{2,t}$$

$$U_t = (1 - 0.296B + 0.242B^2 + 0.119B^3 + 0.497B^4 - 0.216B^5)E_t.$$

We can now equivalently write the transfer function model with the new processes  $D_t$ ,  $Z_t$  and  $U_t$ . It takes the form:

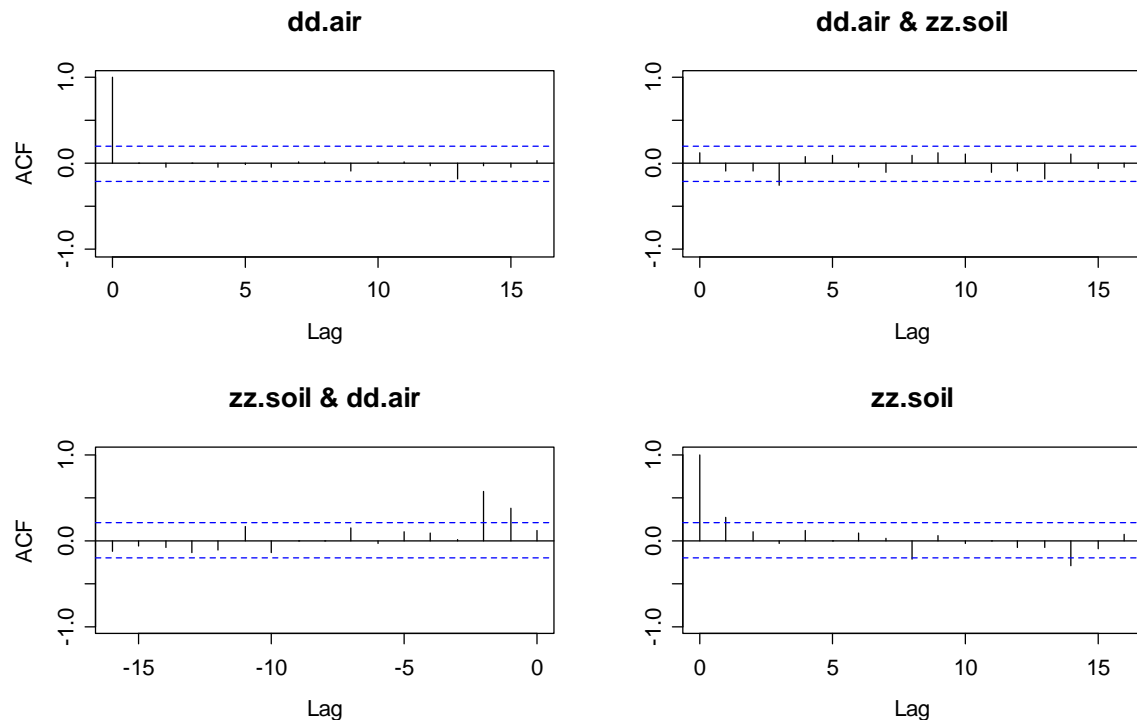
$$Z_t = \sum_{j=0}^{\infty} \nu_j D_{t-j} + U_t,$$

where the coefficients  $\nu_j$  are identical than for the previous formulation of the model. The advantage of this latest formulation, however, is that the input series  $D_t$  is now White Noise, such that the above special case applies, and the transfer function model coefficients can be obtained by a straightforward computation from the cross correlations:

$$\hat{\nu}_k = \frac{\hat{\gamma}_{21}(k)}{\hat{\sigma}_D^2} = \frac{\hat{\sigma}_Z}{\hat{\sigma}_D} \hat{\rho}_{21}(k), \text{ where } k \geq 0.$$

where  $\hat{\gamma}_{21}$  and  $\hat{\rho}_{21}$  denote the empirical cross covariances and cross correlations of  $D_t$  and  $Z_t$ . However, keep in mind that  $Z_t$  and  $U_t$  are generally correlated. Thus, the outlined method is not a statistically efficient estimator either. While efficient approaches exist, we will not discuss them in this course and scriptum. Furthermore, for practical application the outlined procedure usually yields reliable results. We conclude this section by showing the results for the permafrost example: the transfer function model coefficients in the example are based on the cross correlation between the AR(5) residuals of the air changes and the ground changes that had been filtered with these AR(5) coefficients.

```
> dd.air <- resid(fit.air)
> coefs <- coef(fit.air)[1:5]
> zz.soil <- filter(diff(soil.na), c(1, -coefs, sides=1))
> as.int <- ts.intersect(dd.air, zz.soil)
> acf.val <- acf(as.int, na.action=na.pass)
```



Again, in all except for the bottom left panel, the correlation coefficients are mostly zero, respectively only insignificantly or by chance different from that value. This is different in the bottom left panel. Here, we have substantial cross correlation at lags 1 and 2. Also, these values are proportional to the transfer function model coefficients. We can extract these as follows:

```
> multip <- sd(zz.soil, na.rm=TRUE)/sd(dd.air, na.rm=TRUE)
> multip*acf.val$acf[,2,1]
[1] 0.054305137 0.165729551 0.250648114 0.008416697
[5] 0.036091971 0.042582917 -0.014780751 0.065008411
[9] -0.002900099 -0.001487220 -0.062670672 0.073479065
[13] -0.049352348 -0.060899602 -0.032943583 -0.025975790
```

Thus, the soil temperature in the permafrost boreholes reacts to air temperature changes with a delay of 1-2 days. An analysis of further boreholes has suggested that the delay depends on the type of terrain in which the measurements were made. Fastest response times are found for a very coarse-blocky rock glacier site, whereas slower response times are revealed for blocky scree slopes with smaller grain sizes.





# 10 Spectral Analysis

During this course, we have encountered several time series which show periodic behavior. Prominent examples include the number of shot lynx in the Mackenzie River district in Canada, as well as the wave tank data from section 4.4. In these series, the periodicity is not deterministic, but stochastic. An important goal is to understand the cycles at which highs and lows in the data appear.

In this chapter, we will introduce *spectral analysis* as a descriptive means for showing the character of, and the dependency structure within a time series. This will be based on interpreting the series as a superposition of cyclic components, namely as a *linear combination of harmonic oscillations*. We will introduce the *periodogram*, where the aim is to show which frequencies contribute most importantly to the variation in the series.

In spirit, such an analysis is related to the correlogram. In fact, one can show that the information in the correlogram and the periodogram are mathematically equivalent. However, the two approaches still provide different, complementary views on a series and it is thus often worthwhile to pursue both approaches. Finally, we here also mention that in some areas time series are preferably analyzed in the time domain, whereas in other applied fields, e.g. electrical engineering, geophysics and econometrics, the frequency approach predominates.

## 10.1 Decomposing in the Frequency Domain

We will here first introduce some background and theory on how to decompose time series into cyclic components and then lay the focus on the efficient estimation of these.

### 10.1.1 Harmonic Oscillations

The simplest and best known periodic functions are sine and cosine. It is thus appealing to use these as a basis for decomposing time series. A harmonic oscillation is of the form

$$y(t) = a \cdot \cos(2\pi\nu t - \phi) .$$

Here, we call  $a$  the amplitude,  $\nu$  is the frequency and  $\phi$  is the phase. Apparently, the function  $y(t)$  is periodic, and the period is  $T = 1/\nu$ . It is common to write the above harmonic oscillation in a different form, i.e.:

$$y(t) = \alpha \cdot \cos(2\pi\nu t) + \beta \cdot \sin(2\pi\nu t) ,$$

where in fact  $\alpha = a \cos(\phi)$  and  $\beta = a \sin(\phi)$ . The advantage of this latter form is that if we want to fit a harmonic oscillation with fixed frequency to data, which means estimating amplitude and phase, we face a linear problem instead of a non-linear one, as it was the case in the previous formulation. The time can be either continuous or discrete. In the context of our analysis of discrete time series, only the latter will be relevant.

Now, if fitting a harmonic oscillation to discrete data, we face an identification problem: If frequency  $\nu$  fits, then all higher frequencies such as  $\nu+1, \nu+2, \dots$  will fit as well. This phenomenon is known as aliasing. The plot below shows harmonics where  $a=1$  and  $\phi=0$ . As frequencies, we choose both  $\nu=1/6$  and  $\nu=1+1/6$ . We observe that we cannot decide upon which of the two frequencies generated our discrete time observations. Naturally, the time resolution of our series determines which frequencies we can identify. Or more clearly: we take the point that our data do not allow to identify periodicities with frequency  $\nu > 1/2$ , i.e. that harmonics which oscillate more than once between two observations.

### 10.1.2 Superposition of Harmonics

In a real-world stationary time series, it is rare to nonexistent that only one single periodicity that can be attributed to a single frequency makes up for all the variation that is observed. Thus, for a decomposition of the series into a number of periodicities with different frequency, we choose the regression approach:

$$X_t = \alpha_0 + \sum_{k=1}^m (\alpha_k \cos(2\pi\nu_k t) + \beta_k \sin(2\pi\nu_k t)) + E_t,$$

where  $\alpha_k, \beta_k$  are interpreted as the unknown parameters,  $E_t$  is an *iid* error term with expectation zero and  $\nu_1, \dots, \nu_m$  is a set of pre-defined frequencies. Under these assumptions, we can obtain estimates  $\hat{\alpha}_k, \hat{\beta}_k$  with the ordinary least squares algorithm. As for the frequencies, we choose multiples of  $1/n$ , i.e.

$$\nu_k = k/n, \text{ for } k = 1, \dots, m \text{ with } m = \lfloor n/2 \rfloor.$$

These are called the *Fourier frequencies*. Using some mathematics, one can prove that the above regression problem has an orthogonal design. Thus, the estimated coefficients  $\hat{\alpha}_k, \hat{\beta}_k$  are uncorrelated and (for  $k > 0$ ) have variance  $2\sigma_E^2/n$ . Because we are also spending  $n$  parameters for the  $n$  observations, the frequency decomposition model fits perfectly, i.e. all residuals are zero. Another very important result is that the

$$\text{sum of squared residuals } \sum_{i=1}^n r_i^2 \text{ increases by } \frac{n}{2}(\hat{\alpha}_k^2 + \hat{\beta}_k^2)$$

if the frequency  $\nu_k$  is omitted from the model. We can use this property to gauge the prominence of a particular frequency in the decomposition model, and exactly that is the aim with the periodogram which will be discussed below.

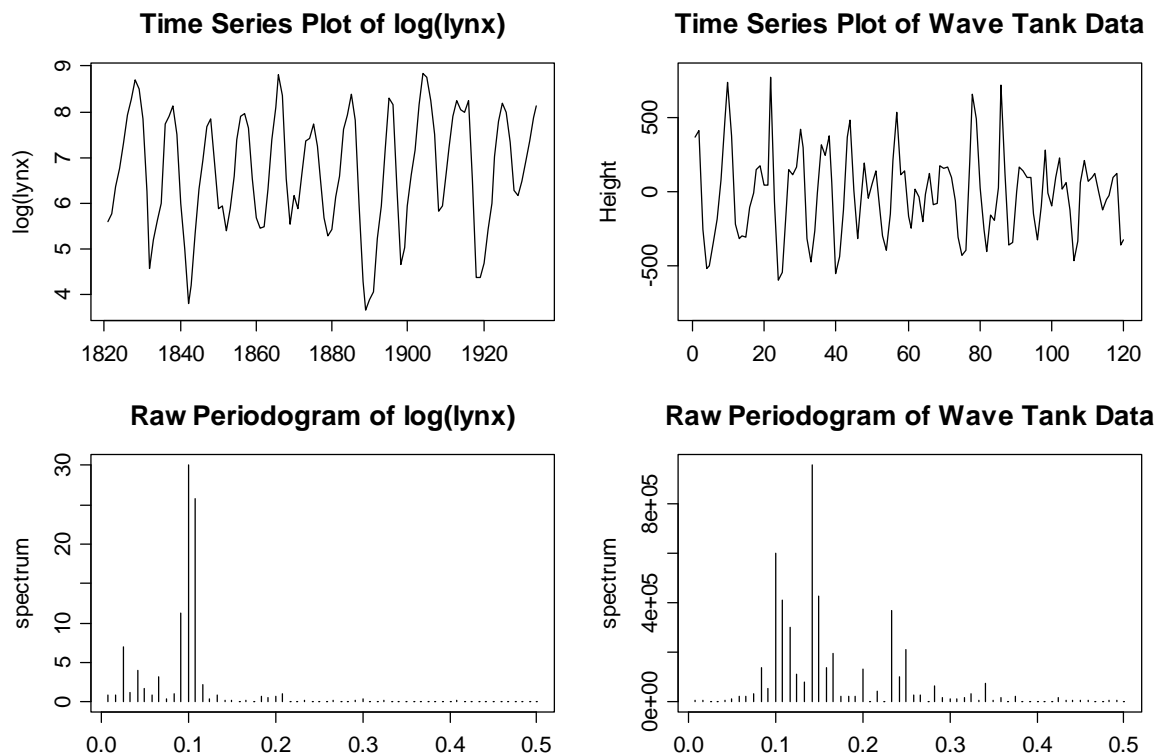
### 10.1.3 The Periodogram

The periodogram quantifies the presence of periodicities in a time series. It is based on half of the increase in sum of squared residuals in the decomposition model if a particular frequency is omitted. We can rewrite that directly as a function of the observations:

$$\begin{aligned} I_n(\nu_k) &= \frac{n}{4}(\hat{\alpha}_k^2 + \hat{\beta}_k^2) \\ &= \frac{1}{n} \left( \sum_{t=1}^n x_t \cos(2\pi\nu_k t) \right)^2 + \frac{1}{n} \left( \sum_{t=1}^n x_t \sin(2\pi\nu_k t) \right)^2 \end{aligned}$$

The result is then plotted versus the frequency  $\nu_k$ , and this is known as the raw periodogram. In R, we can use the convenient function `spec.pgram()`. We illustrate its use with the lynx and the wave tank data:

```
> spec.pgram(log(lynx), log="no", type="h")
> spec.pgram(wave, log="no", type="h")
```



The periodogram of the logged lynx data is easy to read: the most prominent frequencies in this series with 114 observations are the ones near 0.1, more exactly, these are  $\nu_{11} = 11/114 = 0.096$  and  $\nu_{12} = 12/114 = 0.105$ . The period of these frequencies is  $1/\nu_k$  and thus,  $114/11 = 10.36$  and  $114/12 = 9.50$ . This suggests that the series shows a peak at around every 10<sup>th</sup> observation which is clearly the case in practice. We can also say that the highs/lows appear between 11 and 12 times in the series. Also this can easily be verified in the time series plot.

Then, there is a secondary peak at  $\nu_3 = 3/114$ . This must be a cyclic component that appears three times in our data, and the period is  $114/3 = 38$ . Thus, these are the 40-year-superhigh and -lows that we had identified already earlier.

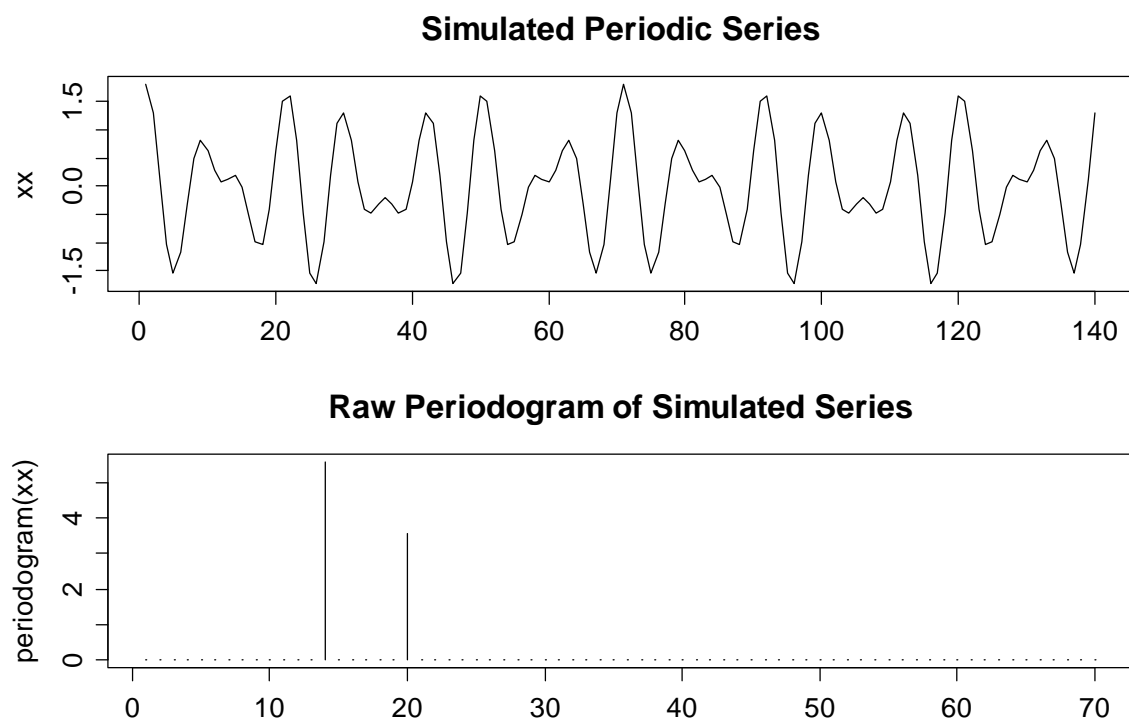
For the wave tank data, we here consider the first 120 observations only. The periodogram is not as clean as for the logged lynx data, but we will try with an interpretation, too. The most prominent peaks are at  $k = 12, 17$  and  $30$ . Thus we have a superposition of cycles which last 4, 7 and 10 observations. The verification is left to you.

### 10.1.4 Leakage

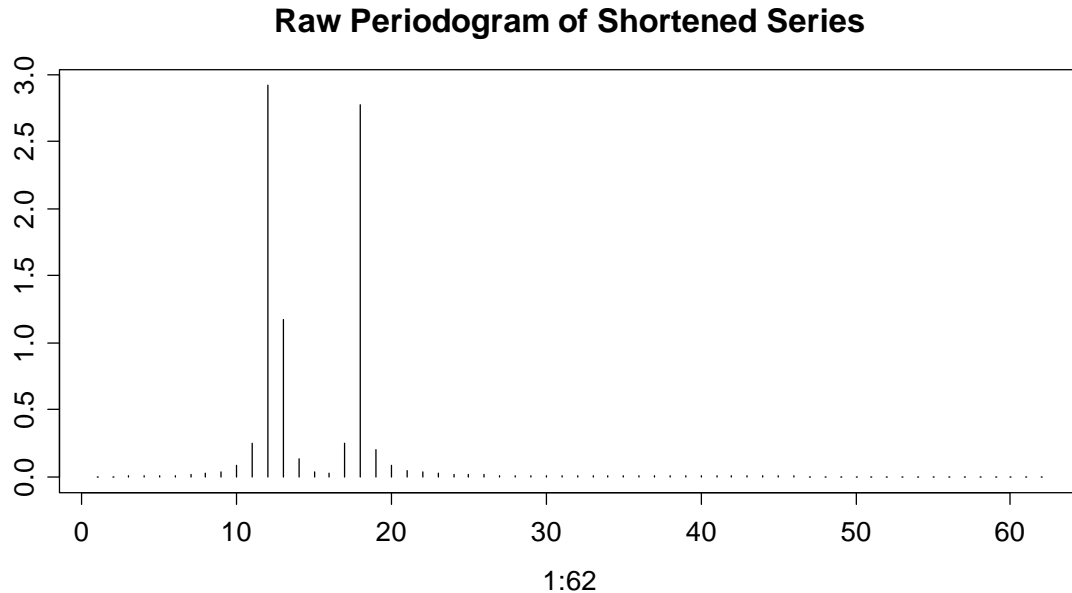
While some basic inspections of the periodogram can and sometimes do already provide valuable insight, there are a few issues which need to be taken care of. The first one which is discussed here is the phenomenon called *leakage*. It appears if there is no Fourier frequency that corresponds to the true periodicity in the data. Usually, the periodogram then shows higher values in the vicinity of the true frequency. The following simulation example is enlightening:

$$X_t = \cos\left(\frac{2\pi \cdot 13 \cdot t}{140}\right) + 0.8 \cdot \cos\left(\frac{2\pi \cdot 20 \cdot t}{140}\right), \text{ for } t = 0, \dots, 139$$

We have a series of 140 observations which is made up as the superposition of two harmonic oscillations with frequencies  $13/140$  and  $20/140$ . These correspond to periods of 7.00 and 10.77, and both are Fourier frequencies. We display the time series plot, as well as the periodogram:



Now if we shorten this very same series by 16 data points so that 124 observations remain, the true frequencies  $20/140$  and  $13/140$  do no longer appear in the decomposition model, i.e. are not Fourier frequencies anymore. The periodogram now shows leakage:



If not all of the true frequencies in the data generating model are Fourier frequencies, then,  $\hat{\alpha}_k, \hat{\beta}_k$  from the decomposition model are only approximations to the true contribution of a particular frequency for the variation in the series.



# 11 State Space Models

State space modeling is a very flexible tool that from which one can benefit in almost all applied fields. It would certainly merit an own full course, exclusively focusing on its applied aspects. Due to restrictions in time, we here provide only a small overview on the potential and a few examples. While one can write most time series models in state space formulation, it is usually simpler to do without, and use their own genuine notation. The real benefits of state space models only come into play when one has to deal with observations that are blurred with additional measurement noise, or in situations, where some parameters are required to adapt over time.

We will here first introduce the general formulation of state space models, and then illustrate with a number of examples. The first two concern AR processes with additional observation noise, then there are two regressions with time-varying coefficients, and finally we consider a linear growth model. The conditional means and variances of the state vectors are usually estimated with the Kalman Filter. Because this is mathematically rather complex topic, and not in the primary focus of the applied user, this scriptum only provides the coarse rationale for it.

## 11.1 State Space Formulation

State space models are built on two equations. One is the state equation, and the other is the observation equation. We here introduce the general notation; their meaning will become clearer with the examples discussed below.

### State Equation

The state of the system at time  $t$  is represented by a column vector  $X_t$ , and it is a linear transformation of the state at time  $t-1$ , plus some random vector  $W_t$  (system noise) from a multivariate normal distribution. The linear transformation of the state at time  $t-1$  is defined with a matrix  $G_t$ , and the covariance matrix of the multivariate normal is denoted with  $w_t$ .

$$X_t = G_t X_{t-1} + W_t, \text{ where } W_t \sim N(0, w_t)$$

### Observation Equation

The observation at time  $t$  is denoted by a column vector  $Y_t$  that is a linear combination of the states, determined by a matrix  $F_t$ , and random variation (measurement noise) from a normal distribution with covariance matrix  $v_t$ .

$$Y_t = F_t X_t + V_t, \text{ where } V_t \sim N(0, v_t)$$

Note that in this general formulation, all matrices can be time varying, but in most of our examples, they will be constant. Also, the nomenclature is different depending on the source, but we here adopt the notation of  $\mathbf{R}$ .

## 11.2 AR Processes with Measurement Noise

We are interested in a stochastic process  $X_t$  (which may be an AR process). Then, one usually makes measurements to obtain observations, i.e. acquires a realization of the process. So far, we operated under the assumption that the measurements were error-free, i.e. that there was no measurement noise and our data were exact. In many cases where the data are measured using physical devices, this is hardly realistic, and we may rather have realizations of some random variable

$$Y_t = X_t + V_t, \text{ where } V_t \sim N(0, \sigma_V^2).$$

Thus, the realizations of the process of interest,  $X_t$  are latent, i.e. hidden under some random noise. We will now discuss how this issue can be solved in practice.

**Example:**  $AR(1)$

As the simplest example of a state space model, we consider an  $AR(1)$  process which is superposed with some additional measurement noise. The *state equation* is as follows:

$$X_t = \alpha_1 X_{t-1} + W_t.$$

We assume that  $W_t$  is an iid innovation with Gaussian distribution, i.e.  $W_t \sim N(0, \sigma_W^2)$ . Also note that matrix  $G_t$  has dimension  $1 \times 1$ , is time-constant and equal to  $\alpha_1$ . If there is additional measurement noise, our observations can be perceived as realizations of the random variable  $Y_t$ :

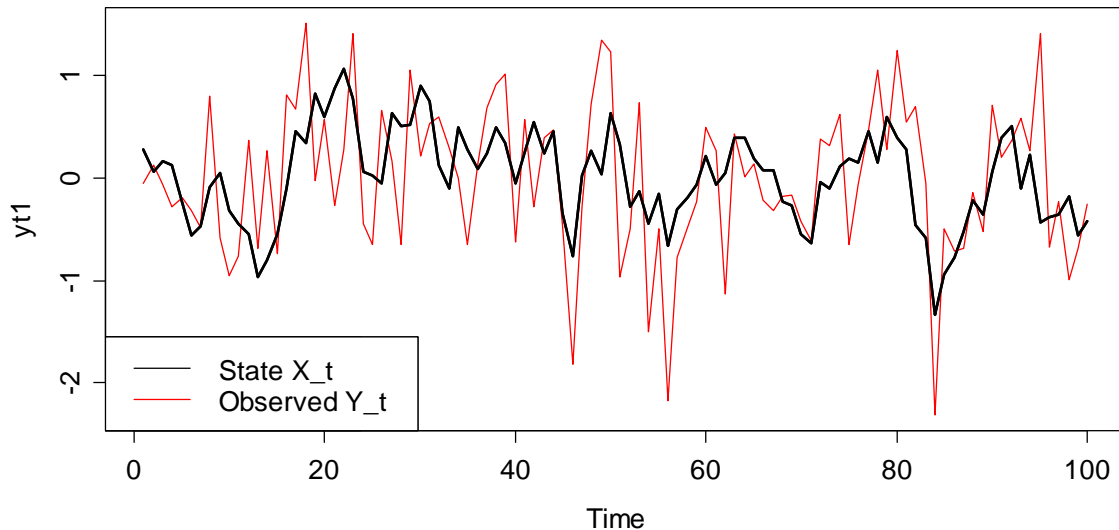
$$Y_t = X_t + V_t, \text{ where } V_t \sim N(0, \sigma_V^2).$$

This is the *observation equation*, note that  $F_t$  is also time-constant and equal to the  $1 \times 1$  identity matrix. We here assume that the errors  $V_t$  are iid, and also independent of  $X_s$  and  $W_s$  for all  $t$  and  $s$ . It is important to note that  $W_t$  is the process innovation that impacts future instances  $X_{t+k}$ . In contrast,  $V_t$  is pure measurement noise with no influence on the future of process  $X_t$ . For illustration, we consider a simulation example. We use  $\alpha_1 = 0.7$ , the innovation variance  $\sigma_W^2$  is 0.1 and the measurement error variance  $\sigma_V^2$  is 0.5. The length of the simulated series is 100 observations. On the next page, we show a number of plots. They include a time series plot with both series  $X_t$  and  $Y_t$ , and the individual plots of  $X_t$  with its ACF/PACF, and of  $Y_t$  with ACF/PACF. We clearly observe that the appearance of the two processes is very different. While  $X_t$  looks like an autoregressive process, and has ACF and PACF showing the stylized facts very prominently,  $Y_t$  almost appears to be White Noise. We here know that this is not

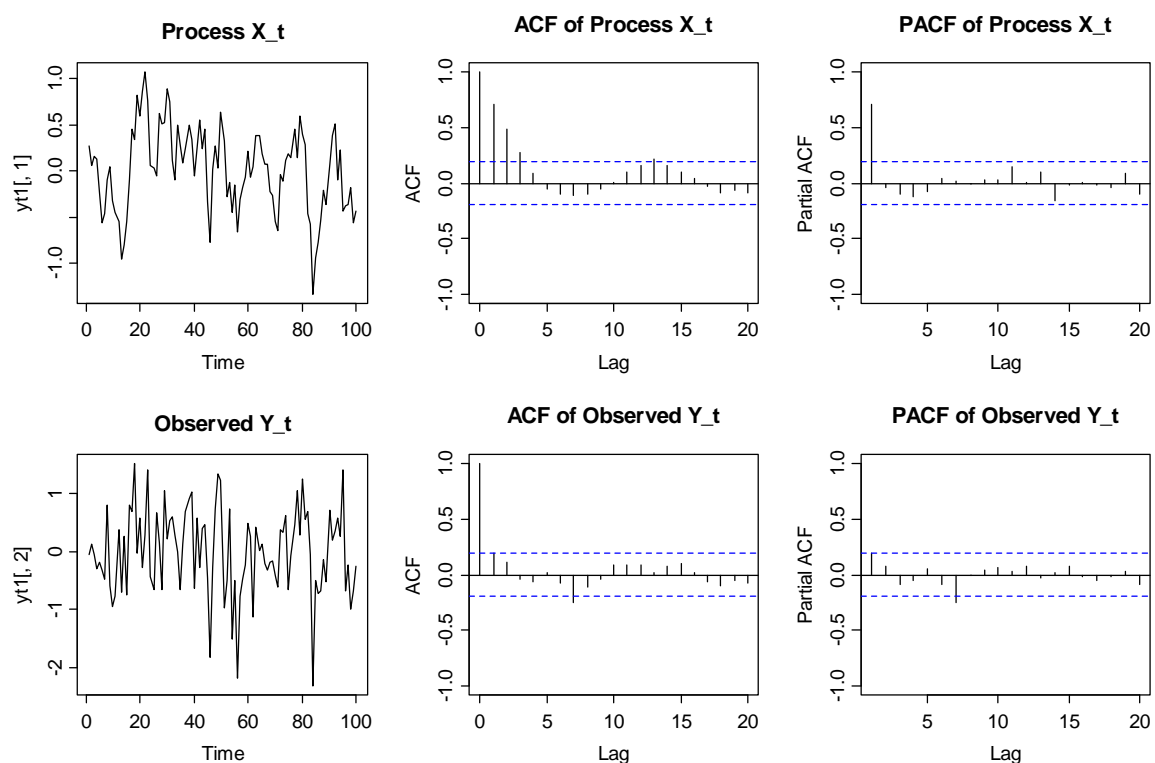


true. There is some dependency also in  $Y_t$ , but it is blurred by strong noise component, and it seems like a difficult task to recover the weak underlying signal.

### AR(1) Simulation Example



We here emphasize that the state space formulation allowed to write a model comprised of a true signal plus additional noise. However, if we face an observed series of this type, we are not any further yet. We need some means to separate the two components. *Kalman filtering*, which is implemented in **R** package *sspir*, allows doing so: it recovers the (expected value of) the states  $X_t$  by some recursive algorithm. For details see below.



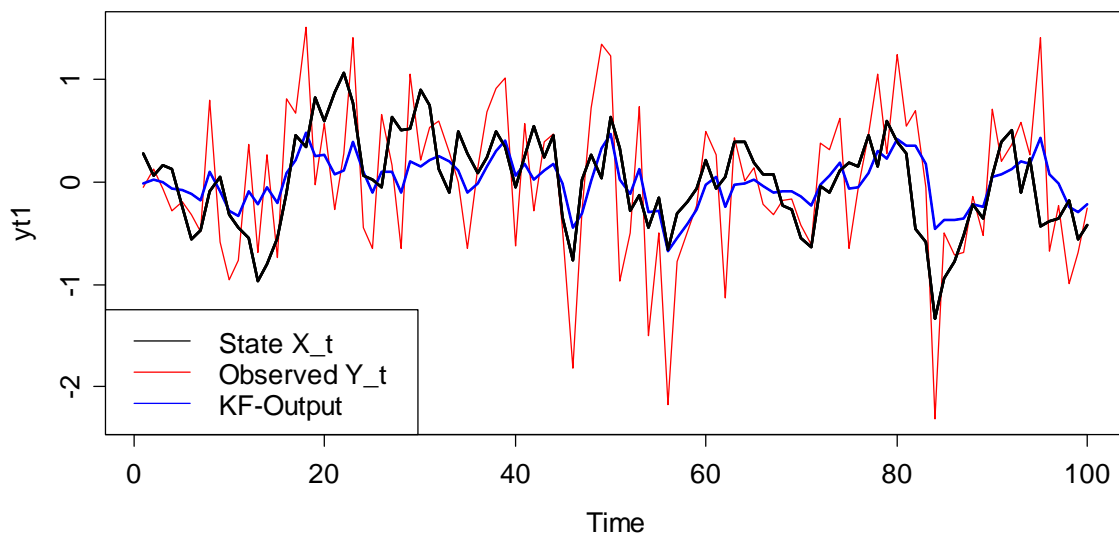
```

> ## Load the package for Kalman filtering
> library(sspir)
>
> ## State Space Formulation
> ssf <- SS(y = as.matrix(obs),
>           Fmat = function(tt,x,phi) {return(matrix(1))},
>           Gmat = function(tt,x,phi) {return(matrix(0.7))},
>           Vmat = function(tt,x,phi) {return(matrix(0.5))},
>           Wmat = function(tt,x,phi) {return(matrix(0.1))},
>           m0 = matrix(0),
>           C0 = matrix(0.1))
>
> ## Kalman Filtering
> fit <- kfilter(ssf)
> plot(fit$m, col="blue", lwd=2, ...)

```

Kalman filtering in **R** requires to specify the state space model first. We need to supply argument  $y$  which stands for the observed time series data. They have to come in form of a matrix. Moreover, we have to specify the matrices  $F_t, G_t$ , as well as the covariance structures  $v_t, w_t$ . In our case, these are all simple  $1 \times 1$  matrices. Finally, we have to provide  $m_0$ , the starting value of the initial state, and  $C_0$ , the variance of the initial state.

### AR(1) Simulation Example with Kalman Filter Output



We can then employ the Kalman filter to recover the original signal  $X_t$ . It was added as the blue line in the above plot. While it is not 100% accurate, it still does a very good job of filtering the noise out. However, note that with this simulation example, we have some advantage over the real-life situation. Here, we could specify the correct state space formulation. In practice, we might have problems to identify appropriate values for  $G_t$  (the true  $AR(1)$  parameter) and the variances in  $v_t, w_t$ . On the other hand, in reality the precision of many measurement devices is more or less known, and thus some educated guess is possible.

**Example:**  $AR(2)$ 

Here, we demonstrate the formulation of a state space model for an  $AR(2)$  process that is superimposed with some measurement error. This example is important, because now, we need to use matrices in the state equation. It is as follows:

$$\begin{pmatrix} X_t \\ X_{t-1} \end{pmatrix} = \begin{pmatrix} \alpha_1 & \alpha_2 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} X_{t-1} \\ X_{t-2} \end{pmatrix} + \begin{pmatrix} W_t \\ 0 \end{pmatrix}$$

Apparently, this is a two-dimensional model. The observation equation is:

$$Y_t = (1 \ 0) \cdot \begin{pmatrix} X_t \\ X_{t-1} \end{pmatrix} + V_t$$

Once the equations are set up, it is straightforward to derive the matrices:

$$G_t = G = \begin{pmatrix} \alpha_1 & \alpha_2 \\ 1 & 0 \end{pmatrix}, \quad H_t = H = (1 \ 0), \quad w_t = \begin{pmatrix} \sigma_w^2 & 0 \\ 0 & 0 \end{pmatrix}, \quad v_t = \sigma_v^2$$

Similar to the example above, we could now simulate from an  $AR(2)$  process, add some artificial measurement noise and then try to uncover the signal using the Kalman filter. This is left as an exercise.

## 11.3 Dynamic Linear Models

A specific, but very useful application of state space models is to generalize linear regression such that the coefficients can vary over time. We consider a very simple example where the sales manager in a house building company uses the following model: the company's house sales at time  $t$ , denoted as  $S_t$ , depends on the general levels of sales in that area  $L_t$  and the company's pricing policy  $P_t$ .

$$S_t = L_t + \beta_t P_t + V_t$$

This is a linear regression model with price as the predictor, and the general level as the intercept. The assumption is that their influence varies over time, but generally only in small increments. We can use the following notation:

$$L_t = L_{t-1} + \Delta L_t$$

$$\beta_t = \beta_{t-1} + \Delta \beta_t$$

In this model, we assume that  $v_t$ ,  $\Delta L_t$  and  $\Delta \beta_t$  are random deviations with mean zero that are independent over time. While we assume independence of  $\Delta L_t$  and  $\Delta \beta_t$ , we could also allow for correlation among the two. The relative magnitudes of these perturbations are accounted for with the variances in the matrices  $V_t$  and  $W_t$  of the state space formulation. Note that if we set  $W_t = 0$ , then we are in the case

of plain OLS regression with constant parameters. Hence, we can also formulate any regression models in state space form. Here, we have:

$$Y_t = S_t, \quad X_t = \begin{pmatrix} L_t \\ \beta_t \end{pmatrix}, \quad W_t = \begin{pmatrix} \Delta L_t \\ \Delta \beta_t \end{pmatrix}, \quad F_t = \begin{pmatrix} 1 \\ P_t \end{pmatrix}, \quad G = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

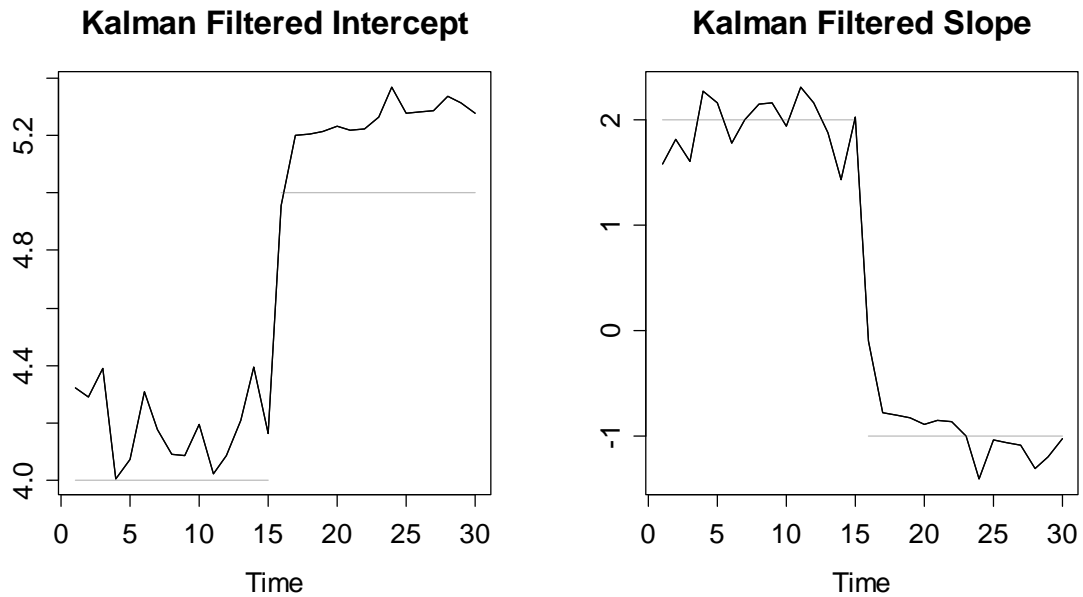
Because we do not have any data for this sales example, we again rely on a simulation. Evidently, this has the advantage that we can evaluate the Kalman filter output versus the truth. Thus, we let

$$y_t = a + bx_t + z_t$$

$$x_t = 2 + t/10$$

We simulate 30 data points from  $t = 1, \dots, 30$  and assume errors which are standard normally distributed, i.e.  $z_t \sim N(0,1)$ . The regression coefficients are  $a = 4$  and  $b = 2$  for  $t = 1, \dots, 15$  and  $a = 5$  and  $b = -1$  for  $t = 16, \dots, 30$ . We will fit a straight line with time-varying coefficients, as this is the model that matches what we had found for the sales example above.

```
> ## Simulation
> set.seed(1)
> x1      <- 1:30
> x1      <- x1/10+2
> aa      <- c(rep(4,15), rep( 5,15))
> bb      <- c(rep(2,15), rep(-1,15))
> nn      <- length(x1)
> y1      <- aa+bb*x1+rnorm(nn)
> x0      <- rep(1,nn)
> xx      <- cbind(x0,x1)
> x.mat   <- matrix(xx, nrow=nn, ncol=2)
> y.mat   <- matrix(y1, nrow=nn, ncol=1)
>
> ## State Space Formulation
> ssf <- SS(y=y.mat, x=x.mat,
>          Fmat=function(tt,x,phi)
>              return(matrix(c(x[tt,1],x[tt,2]),2,1)),
>          Gmat=function(tt,x,phi) return(diag(2)),
>          Wmat=function(tt,x,phi) return(0.1*diag(2)),
>          Vmat=function(tt,x,phi) return(matrix(1)),
>          m0=matrix(c(5,3),1,2),
>          C0=10*diag(2))
>
> ## Kalman-Filtering
> fit <- kfilter(ssf)
> par(mfrow=c(1,2))
> plot(fit$m[,1], type="l", xlab="Time", ylab="")
> title("Kalman Filtered Intercept")
> plot(fit$m[,2], type="l", xlab="Time", ylab="")
> title("Kalman Filtered Slope")
```



The plots show the Kalman filter output for intercept and slope. The estimates pick up the true values very quickly, even after the change in the regime. It is worth noting that in this example, we had a very clear signal with relatively little noise, and we favored recovering the truth by specifying the state space formulation with the true error variances that are generally unknown in practice.

### Example: Batmobile

We here consider another regression problem where time-varying coefficients may be necessary. The description of the practical situation is as follows: *In April 1979 the Albuquerque Police Department began a special enforcement program aimed at countering driving while intoxicated accidents. The program was composed of a squad of police officers, breath alcohol testing (BAT) devices, and a van named batmobile, which housed a BAT device and was used as a mobile station. The data were collected by the Division of Governmental Research of the University of New Mexico under a contract with the National Highway Traffic Safety Administration of the Department of Transportation to evaluate the batmobile program.* Source: <http://lib.stat.cmu.edu/DASL/Datafiles/batdat.html>

The data comprise of quarterly figures of traffic accidents and the fuel consumption in the Albuquerque area as a proxy of the driven mileage. The first 29 quarters are the control period, and observations 30 to 52 were recorded during the experimental (batmobile) period. We would naturally assume a time series regression model for the number of accidents:

$$ACC_t = \beta_0 + \beta_1 \cdot FUEL_t + \beta_2 \cdot 1_{Q_2(t)} + \beta_3 \cdot 1_{Q_3(t)} + \beta_4 \cdot 1_{Q_4(t)} + E_t$$

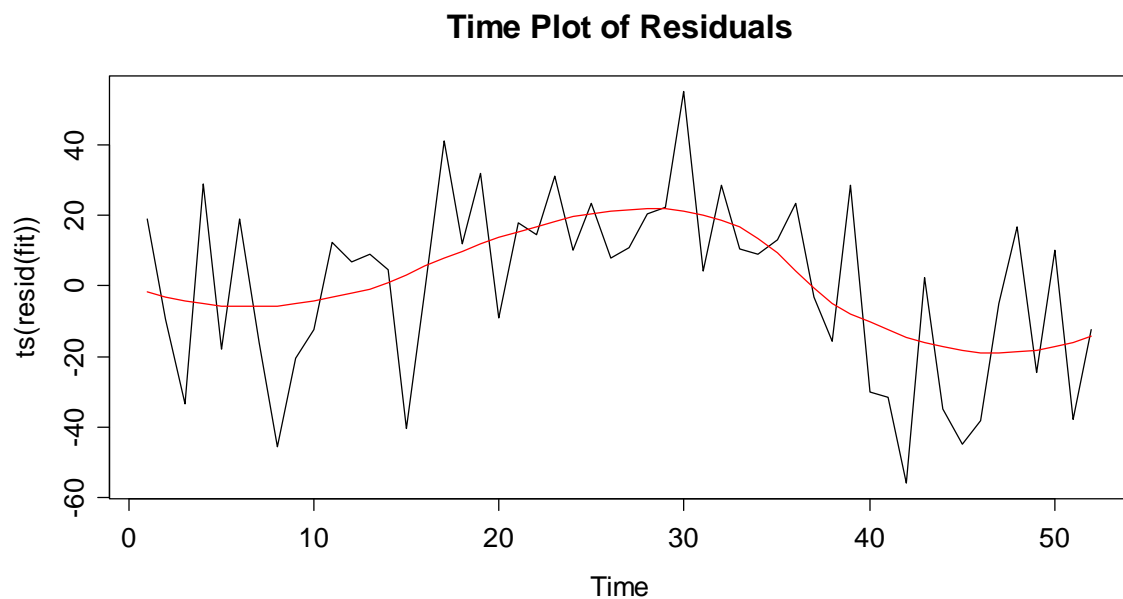
The accidents depend on the mileage driven and there is a seasonal effect. In the above model the intercept  $\beta_0$  is assumed to be constant. In the light of the BAT program, we might well replace it by  $\beta_0 = L_t$ , i.e. some general level of accidents that is time-dependent. Let us first perform regression and check residuals.

```

> ## Regression and Time Plot of Residuals
> fit <- lm(ACC ~ FUEL + season, data=regdat)
> plot(ts(resid(fit)), main="Time Plot of Residuals")
>
> ## Fitting a Loess Smoother to the Residuals
> times <- 1:52
> fit.loess <- loess(resid(fit) ~ times, span=0.65, degree=2)
> lines(times, fitted(fit.loess), col="red")

```

The time series plot of the residuals shows very clear evidence that there is timely dependence. In contrast to what the regression model with constant coefficients suggests, the level of accidents seems to rise in the control period, then drops markedly after the BAT program was introduced. The conclusion is that our above regression model is not adequate and needs to be enhanced. However, just adding an indicator variable that codes for the times before and after the introduction of the BAT program will not solve the issue. It is evident that the level of the residuals is not constant before the program started, and it does not suddenly drop to a constant lower level thereafter.



The alternative is to formulate a state space model and estimate it with the Kalman filter. We (conceptually) assume that all regression parameters are time dependent, and rewrite the model as:

$$ACC_t = L_t + \beta_{1t} \cdot FUEL_t + \beta_{2t} \cdot 1_{Q_2(t)} + \beta_{3t} \cdot 1_{Q_3(t)} + \beta_{4t} \cdot 1_{Q_4(t)} + E_t$$

Our main interest lies in the estimation of the modified intercept term  $L_t$ , which we now call the level. We expect it to drop after the introduction of the BAT program, but let's see if this materializes. The state vector  $X_t$  we are using contains the regression coefficients, and the state equation which describes their evolution over time is as follows:

$$X_t = GX_{t-1} + W_t, \text{ where } X_t = \begin{pmatrix} L_t \\ \beta_{1t} \\ \beta_{2t} \\ \beta_{3t} \\ \beta_{4t} \end{pmatrix}, G = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}, w_t = \begin{pmatrix} 10 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

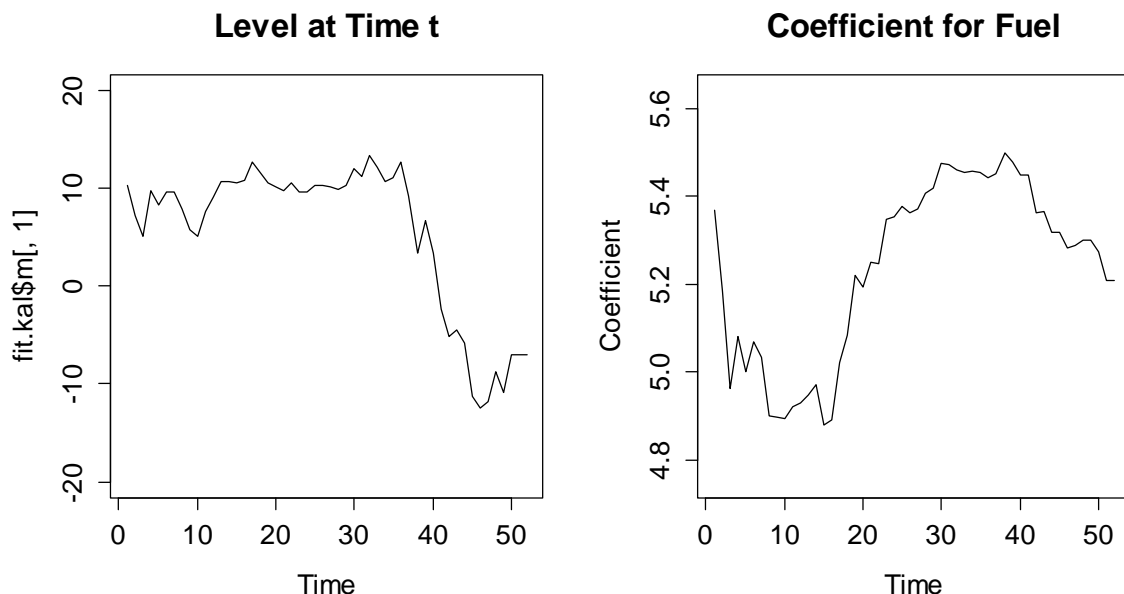
As we can see, we only allow for some small, random permutations in the level  $L_t$ , but not in the other regression coefficients. The observation equation then describes the regression problem, i.e.

$$Y_t = F_t X_t + V_t, \text{ where } Y_t = ACC_t, F_t = (1, Fuel_t, 1_{Q_2(t)}, 1_{Q_3(t)}, 1_{Q_4(t)}), V_t \sim N(0, \sigma_V^2)$$

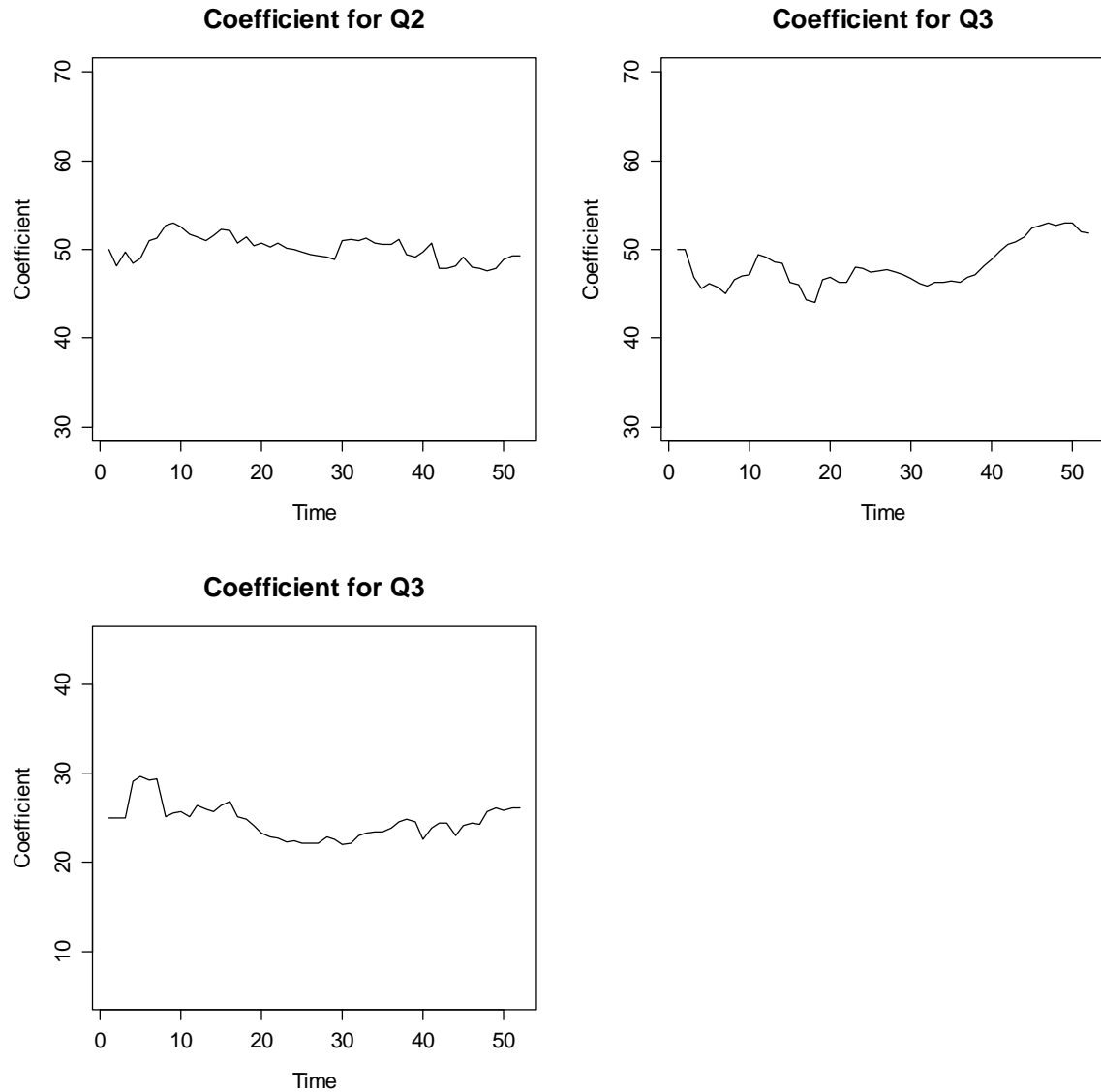
The variance of the noise term  $\sigma_V^2$  is set to 600, which is the error variance in the canonical regression fit. Also the starting values for Kalman filtering, as well as the variances of these initial states are taken from there. Hence, the code for the state space formulation, as well as for Kalman filtering is as follows:

```
> y.mat <- as.matrix(regdat$ACC)
> x.mat <- model.matrix(fit)
> ssf <- SS(y=y.mat, x=x.mat,
+   Fmat=function(tt,x,phi) return(t(x[tt,,drop=FALSE])),
+   Gmat=function(tt,x,phi) return(diag(5)),
+   Wmat=function(tt,x,phi) return(diag(c(10,0,0,0,0))),
+   Vmat=function(tt,x,phi) return(matrix(600)),
+   m0=matrix(c(0,5,50,50,25),1,5),
+   C0=diag(c(900,1,100,100,100)))
> fit.kal <- kfilter(ssf)
```

The filtered output is in object `m` in the output list. We can extract the estimates for the mean of the state vector at time  $t$ , which we display versus time.



Indeed, the level  $L_t$  shows a pronounced drop from  $t = 35$  to  $t = 45$ . Hence, the BAT program shows an effect, but there is some delay after the intervention and it takes some time until it has full effect. Finally, we track the estimates for the seasonal coefficients.



The estimates for these coefficients slightly wiggle around over time. However, they do not seem to change systematically, as we had previously guessed.