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Student Muster

**Time Series Analysis  
for Irregularly Sampled Data**

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Co-Advisor    Your co-supervisor  
Advisor:     Prof. Dr. Your supervisor



To some special person



# Preface

First words and acknowledgements.



# Abstract

Short summary of my thesis.

## Contents

Notation	xiii
<b>1 Introduction</b>	<b>1</b>
1.1 Thesis Objective . . . . .	1
1.2 Thesis Outline . . . . .	2
<b>2 Characteristics of Time Series</b>	<b>3</b>
2.1 Time Series Definition . . . . .	3
2.2 Moments of a Time Series . . . . .	3
2.3 Stationarity . . . . .	3
2.4 Special cases of Time Series Processes . . . . .	4
2.5 Characteristics of the Blood Pressure Time Series . . . . .	4
<b>3 Time Series Decomposition and Regression</b>	<b>5</b>
3.1 Linear Regression . . . . .	5
3.2 Regression with Correlated Errors . . . . .	6
3.2.1 Maximum-Likelihood Estimation . . . . .	6
3.2.2 Sandwich Estimation . . . . .	7
3.2.3 Extension to Irregularly Spaced Time Series . . . . .	7
3.2.4 Confidence Intervals for the Mean Function . . . . .	7
<b>4 Gaussian Process Regression</b>	<b>11</b>
4.1 Gaussian Process Definition . . . . .	11
4.2 Bayesian Linear Regression . . . . .	12
4.3 Bayesian Linear Regression as Gaussian Process Regression . . . . .	15
4.3.1 Time Series Gaussian Process Regression . . . . .	16
4.4 Mean Function . . . . .	17
4.5 Kernel Functions . . . . .	17
4.5.1 Stationary Covariance Function . . . . .	17
4.6 Model Selection - Choosing Hyperparameters . . . . .	19
<b>5 First Chapter</b>	<b>21</b>
5.1 To include a picture . . . . .	21
5.2 To make a proof . . . . .	22
5.3 To include R code . . . . .	22
5.4 Other information . . . . .	22
<b>6 Summary</b>	<b>23</b>
6.1 Future Work . . . . .	23
<b>Bibliography</b>	<b>25</b>
<b>A Complementary information</b>	<b>27</b>
A.1 Including R code with verbatim . . . . .	27
A.2 Including R code with the <i>listings</i> package . . . . .	28
A.3 Using <i>Sweave</i> (or <i>knitr</i> ) to include R code (and more) in your report . . . . .	29



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<b>B</b>	<b>Yet another appendix....</b>	<b>31</b>
B.1	Description . . . . .	31
B.2	Tables . . . . .	31
<b>C</b>	<b>2nd Appendix: More sophisticated R code listing</b>	<b>33</b>
C.1	Chapter 5 . . . . .	33
	<b>Epilogue</b>	<b>35</b>

**List of Figures**

- 5.1 Geyser data: binned histogram, Silverman's and another kernel . . . . . [21](#)
- 5.2 Geyser data: binned histogram, Silverman's and another kernel . . . . . [21](#)

**List of Tables**

B.1 Test results . . . . .	31
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# Notation

BP: blood pressure  
CI: Confidence Intervals  
OLS: Ordinary Least Squares  
Prediction: TODO  
Forecasting: TODO  
Filtering: TODO  
Smoothing: TODO

$\mathcal{N}(\mu, \sigma^2)$  : Normal distribution with mean  $\mu$  and standard deviation  $\sigma$



# Chapter 1

## Introduction

### 1.1 Thesis Objective

The thesis aims at giving an overview of time series analysis methods for irregularly sampled data.

The standard time series analysis methods usually assume discrete equispaced time and introductory textbooks on time series analysis either completely omit the irregularly spaced case or they only dedicate a very small section to continuous time models or to state-space models with missing observations ([Brockwell and Davis](#), [Brockwell and Davis](#), [Cryer and Chan](#), [Chatfield](#)).

I will thereafter present the most important concepts and what I have identified to be the basic methods for the analysis of irregularly spaced time series.

The topic is motivated by a "real world" problem from medicine. The problem at hand is the one of extracting time series characteristics from a dataset featuring blood pressure (BP) measurements sampled at irregularly spaced time points. High BP is known to be a risk factor for cardiovascular disease. A person's BP level is generally summarized using the average BP value over available measurements within a given time range. A novel monitoring device already allows to collect BP estimates round the clock. The device is collecting photoplethysmography (PPG) signals and converting them into BP measurements. Typically, the system will yield approximately 1.5 BP measurements per hour, but depending on the quality of the PPG signal and some additional external factors, this sampling frequency can widely vary and the expected range lies roughly between 0 and 5 measurements per hour. Having good estimates of the true BP values at any, potentially not observed, time would allow for a better estimation of the person's cardiovascular risk, and enable the development of novel valuable metrics. The thesis will focus on a set of time series characteristics, which have been considered most relevant for estimating the person's cardiovascular risk. The characteristics of interest are:

- the mean function of the BP time series
- the one-week mean BP value
- any "long-term" trends
- characteristics of the circadian cycle, such as the mean day and night BP

Besides the point estimates also their CIs are of interest. Importantly, the CI should be able to capture the uncertainty due to the lack of data in the proximity of the point of prediction. This implies, that the width of the CI intervals around the mean function will not be constant over time but depend, among other factors, on how much data is available in the proximity of a given time point. The described endpoints are all based on prediction at the not observed passed time points however not on forecasting at new time points in the future. Hence, the thesis will only focus on the task of reconstructing BP values between the first and last time point in the dataset.

This "real world" problem will serve as a running example throughout the Thesis. Although the topic is motivated by a real dataset we will restrict ourselves to simulated data, which will mimic the most important characteristics of BP time series data.

## 1.2 Thesis Outline

TODO



## Chapter 2

# Characteristics of Time Series

### 2.1 Time Series Definition

A potentially unevenly spaced **time series** is a sequence of observation time and value pair  $(t_i, x_i)$  with strictly increasing observation times. Let  $\mathbb{T}$  be a set of observation time points, then the sequence of random variables  $(X_t : t \in \mathbb{T})$  or simply  $(X_t)$  is a **time series process** with observation times  $t \in \mathbb{T}$ . More specifically:

- $(X_t : t \in \{1, 2, \dots, n\})$  refers to a discrete and equispaced time series of length  $n$
- $(X_{t_i} : i \in \{1, 2, \dots, n\})$  refers to an irregularly spaced time series of length  $n$  with observations at time points  $t_1 < t_2 < \dots < t_n$
- $(X_t : t \in (0, T])$  refers to a continuous time series

When  $\mathbb{T}$  has finite length, we will often use a random column vector  $\mathbf{X}$  to refer to the time series process  $(X_t)$ . Sometimes a time series model will be expressed as a random function  $f : \mathbb{T} \rightarrow \mathbb{R}$  instead of a collection of random variables. Throughout the thesis, the term time series is used both to refer to the data  $(x_t)$  and the process  $(X_t)$  from which it is generated.

### 2.2 Moments of a Time Series

A time series process  $(X_t)$  is usually characterized by its first and second moment.

**Definition 2.2.0.1.** (*Brockwell and Davis*) The **mean function** of a time series  $(X_t)$  is:

$$\mu_X(t) = E(X_t)$$

The **covariance function** of a time series  $(X_t)$  is:

$$\gamma_X(r, s) = \text{Cov}(X_r, X_s) = E[(X_r - \mu_X(r))(X_s - \mu_X(s))]$$

### 2.3 Stationarity

Given that one has only one observation  $x_t$  per time point  $t$ , a necessary condition to statistically learn from a time series is stationarity.

**Definition 2.3.0.1.** (*Brockwell and Davis*) A time series  $(X_t)$  is strictly stationary iff the distribution of  $(X_{t_1}, \dots, X_{t_n})$  is identical to the distribution of  $(X_{t_1+h}, \dots, X_{t_n+h})$  for all  $n \in \mathbb{N}^+$  and shifts  $h \in \mathbb{Z}$ :

**Definition 2.3.0.2.** (*Brockwell and Davis*) A time series  $(X_t)$  is weakly stationary if

$$\mu_X(t) \text{ is independent of } t,$$

and

$$\gamma_X(t+h, t) \text{ is independent of } t \text{ for each } h$$

Whenever the term stationary is used, it is referring to weak stationarity.

## 2.4 Special cases of Time Series Processes

**Example 2.4.0.1.** If  $(X_t)$  is a **white noise** process, then  $X_t \sim WN(0, \sigma^2)$ , that is  $X_t \sim F$  iid for some distribution  $F$  with mean 0 and variance  $\sigma^2$ . A special case is Gaussian White noise where  $W_t \sim \mathcal{N}(0, \sigma^2)$  and  $F = \Phi$

**Example 2.4.0.2.** An equispaced time series process  $(X_t : t \in \{1, 2, \dots\})$  is called **autoregressive process** of order  $p$  or  $AR(p)$  if:

$$X_t = \phi_1 X_{t-1} + \dots + \phi_p X_{t-p} + W_t$$

where  $\phi_p \neq 0$  and  $(W_t)$  is a white noise process. The variable  $W_t$  is called the innovation at time  $t$  and is independent of all  $X_k, k < t$ .

**Example 2.4.0.3.** An equispaced time series process  $(X_t : t \in \{1, 2, \dots\})$  is called **moving average process** of order  $q$  or  $MA(q)$  if:

$$X_t = W_t + \theta_1 W_{t-1} + \dots + \theta_q W_{t-q}$$

where  $\theta_q \neq 0$  and  $(W_t)$  is a white noise process. The variable  $W_t$  is called the innovation at time  $t$  and is independent of all  $X_k, k < t$ .

**Example 2.4.0.4.** An equispaced time series process  $(X_t : t \in \{1, 2, \dots\})$  is called **autoregressive moving average process** of autoregressive order  $p$  and moving average order  $q$  or  $ARMA(p, q)$  if:

$$X_t = \phi_1 X_{t-1} + \dots + \phi_p X_{t-p} + \theta_1 W_{t-1} + \dots + \theta_q W_{t-q} + W_t$$

where  $\phi_p \neq 0, \theta_q \neq 0$  and  $(W_t)$  is a white noise process. The variable  $W_t$  is called the innovation at time  $t$  and is independent of all  $X_k, k < t$

## 2.5 Characteristics of the Blood Pressure Time Series

TODO circadian cycle

## Chapter 3

# Time Series Decomposition and Regression

As most time series, the mean function of the BP time series is not constant in time and hence it is not stationary. One can try to decompose the time series  $Y(t)$  into a deterministic component, the mean function  $\mu(t)$  and a zero mean stationary process  $E(t)$ . This can be expressed in the form of a regression problem:

$$Y(t) = \mu(t) + E(t)$$

The decomposition allows to extract a stationary component  $E(t)$ , for which we can find a probabilistic model using the theory of such stationary time series processes. The idea is to then use this model in combination with an estimate of  $\mu(t)$  to obtain a probability distribution of  $Y^*$  at some time  $t^*$ . Hence time series decomposition comes for free in regression analysis and we start with estimation of the deterministic component  $\mu(t)$  which might be an arbitrary function of  $t$ .

### 3.1 Linear Regression

Based on the knowledge we have about the system we might restrict ourselves to a family of functions for  $\mu(t)$ . An obvious choice for the BP time series is the family of functions featuring a linear trend with an additive seasonal component. If the seasonal component is represented by a cosine of the form  $\alpha \cos(2\pi ft - \phi)$  with phase shift  $\phi$  and known frequency  $f$ , we get the following model for the BP time series  $Y(t)$ :

$$Y(t) = \beta_0 + \beta_1 t + \beta_2 \cos(2\pi ft) + \beta_3 \sin(2\pi ft) + E(t),$$

where based on the trigonometric angle sum identities we know that  $\beta_2 = \alpha \cos(\phi)$  and  $\beta_3 = \alpha \sin(\phi)$ .

If we assume BP observations at potentially unequally spaced time points  $t_1, t_2 \dots t_n$  and  $t_1 < t_2 < \dots t_n$ , we can write in matrix notation:

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

Where  $\mathbf{Y} = [Y_{t_1}, \dots, Y_{t_n}]^\top$  is the observed time series,  $X = [x_{t_1}, \dots, x_{t_n}]^\top \in \mathbb{R}^{n \times 4}$  is the design matrix with  $i$ -th row, written as a column vector  $x_{t_i} = [1, t_i, \cos(2\pi f t_i), \sin(2\pi f t_i)]^\top$  and  $\mathbf{E} = [E_{t_1}, \dots, E_{t_n}]^\top$  the zero-mean stationary time series, which we will call errors.

We can use ordinary least squares to find unbiased and asymptotically normal estimates  $\hat{\beta}_{OLS} = (X^\top X)^{-1} X^\top Y$  for the regression coefficients  $\beta$ , without the requirement of regularly spaced data points or uncorrelated errors  $E_{t_1}, \dots, E_{t_n}$  (White). In the case of uncorrelated errors with constant variance  $\sigma^2$  we have  $\text{Var}(\mathbf{E}) = \sigma^2 I_n$  and an unbiased and consistent estimator for  $\Psi = \text{Var}(\hat{\beta}_{OLS})$  is given by:

$$\hat{\Psi} = \hat{\sigma}^2 (X^\top X)^{-1}$$

where  $\hat{\sigma}^2 = \frac{1}{n-p} \sum_{i=1}^n (y_{t_i} - x_{t_i}^\top \hat{\beta}_{OLS})^2$  and  $p = 4$  in our example

Since  $\mathbf{E}$  is a time series, the assumption of uncorrelated errors is usually violated and the covariance matrix  $\hat{\Psi}$  is thus no longer unbiased (Brockwell and Davis).

## 3.2 Regression with Correlated Errors

The argument presented in this section is based on the textbook of Brockwell and Davis.

If the covariance matrix of the errors  $\text{Var}(\mathbf{E}) = \Sigma$  is known, we can use generalized least squares to obtain a unbiased, consistent and efficient coefficient estimate:

$$\hat{\beta}_{GLS} = (X^\top \Sigma^{-1} X)^{-1} X^\top \Sigma^{-1} Y$$

with unbiased and consistent covariance matrix estimate:

$$\text{Var}(\hat{\beta}_{GLS}) = (X^\top \Sigma^{-1} X)^{-1}$$

If  $\Sigma$  is unknown one can exploit the knowledge we have about the stationary time series process  $\mathbf{E}$  to estimate it. The following subsections will present two approaches to estimate  $\Sigma$ ,  $\beta$  and its covariance matrix. Both methods assume an ARMA(p,q) process for  $\mathbf{E}$  and equispaced time points, hence  $\mathbf{E} = (E_t : t \in \{1, 2, \dots, n\})$  and:

$$\Phi(B)E_t = \Theta(B)W_t, \text{ where } W_t \sim WN(0, \sigma_w^2)$$

### 3.2.1 Maximum-Likelihood Estimation

If we additionally assume  $W_t \sim N(0, \sigma_w^2)$ , we can simultaneously estimate the regression coefficients and  $\Sigma$  by maximizing the Gaussian likelihood:

$$L(\beta, \phi, \theta, \sigma_w^2) = (2\pi)^{-\frac{n}{2}} (\det(\Sigma_n))^{-\frac{1}{2}} \exp\left(-\frac{1}{2} (\mathbf{Y} - X\beta)^\top \Sigma_n^{-1} (\mathbf{Y} - X\beta)\right)$$

Where the covariance matrix  $\Sigma_n(\theta, \phi, \sigma_w^2)$  is parametrized by the coefficients  $\theta, \phi, \sigma_w^2$ , which define the ARMA process assumed for  $(E_t : t \in \{1, 2, \dots, n\})$ . Assuming an ARMA(2,3) process we can implement this approach in R using the nlme library (Box, Jenkins, and Reinsel) :

```
library(nlme)
cs <- corARMA(from = ~t, p=2, q=3)
fit.gls <- gls(y ~ t + cos(2 * pi * f * t) + sin(2 * pi * f * t), corr=cs)
```

### 3.2.2 Sandwich Estimation

The second approach is to fit an OLS regression first and correct the estimated covariance matrix of the regression coefficients  $\Psi$  with a sandwich estimator. In the presence of autocorrelation one usually estimates  $\Phi = \frac{1}{n}X^\top \Sigma X$ , the covariance matrix of the scores or estimating functions  $V_i(\beta) = x_{t_i}(y_{t_i} - x_{t_i}^\top \beta)$ , which can then be used to derive  $\Psi$ :

$$\Psi = \text{Var}(\hat{\beta}_{OLS}) = (X^\top X)^{-1} X^\top \Sigma X (X^\top X)^{-1} = \left(\frac{1}{n}X^\top X\right)^{-1} \frac{1}{n} \Phi \left(\frac{1}{n}X^\top X\right)^{-1} \quad (3.2.2.1)$$

The general form of the estimators for  $\Phi$  is:

$$\hat{\Phi} = \frac{1}{n} \sum_{i,j=1}^n w_{|i-j|} \hat{V}_i \hat{V}_j^\top \quad (3.2.2.2)$$

where  $w = [w_0, \dots, w_{n-1}]^\top$  is a weight vector and  $\hat{V}_i = V_i(\hat{\beta}_{OLS})$ .

Plugging  $\hat{\Phi}$  into the equation 3.2.2.1 one obtains the heteroskedasticity and autocorrelation consistent (HAC) covariance estimate  $\hat{\Psi}_{HAC}$ .

Newey and West, Andrews and others have suggested different approaches for calculating the weights  $w$ . They all yield decreasing weights with increasing lag  $l = |i - j|$ . The R sandwich package implements some of these methods to estimate  $\hat{\Psi}_{HAC}$ . An introduction to the sandwich package and how it can be used for inference is described by Zeileis.

### 3.2.3 Extension to Irregularly Spaced Time Series

Although literature and "ready to use" implementations only exist for the equispaced case, both of the approaches described above could probably be extended to the case of irregularly spaced time series. For the Maximum-Likelihood approach the parametrization of the covariance matrix  $\Sigma_n$  as described in 3.2.1 would need to be adapted, such that the covariance of the errors at different time points depends on the actual time difference rather than the lag. Similarly for the sandwich estimator, the weights in 3.2.2.2 should depend on the time difference rather than on the lag.

### 3.2.4 Confidence Intervals for the Mean Function

The objective, as described in the introduction, is not only to estimate the mean function  $\mu(t)$  of the time BP time series but also to find confidence intervals for it. The model for the BP time series described in 3.1 has the following mean function:

$$\mu(t) = x_t^\top \beta$$

with  $x_t = [1, t, \cos(2\pi ft), \sin(2\pi ft)]^\top$

Hence, we may also write  $\mu(x_t)$  and its  $1 - \alpha$  confidence interval is:

$$x_t^\top \hat{\beta} \pm qt_{n-p}(1 - \frac{\alpha}{2}) \sqrt{x_t^\top \Psi x_t}$$

where  $\Psi = Var(\hat{\beta})$  is the covariance matrix of the estimated regression coefficients and  $qt_{n-p}(1 - \frac{\alpha}{2})$  denotes the  $1 - \frac{\alpha}{2}$  quantile of the student's t-distribution of  $n - p$  degrees of freedom.

As the CI for  $\mu(t)$  is based on the variance of the estimated global model parameters  $\Psi$ , it cannot adapt to the local observation density. Even if we were able to derive realistic confidence interval for the mean function of the irregularly spaced time series, the uncertainty due to the lack of data in the proximity of a time point can still not be reflected.

TODO: Prediction interval  $1 - \alpha$  prediction interval is:

$$x_t^\top \hat{\beta} \pm qt_{n-p}(1 - \frac{\alpha}{2}) \sqrt{\sigma^2 + x_t^\top \Psi x_t}$$

with  $\sigma^2 = \Sigma_{11}$

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## Chapter 4

# Gaussian Process Regression

We again consider a regression problem of mapping the input  $x$  to an output  $f(x)$ . In order to solve such a problem one usually needs some additional constraints on the  $f(x)$ . In 3 we restricted ourselves to the class of linear functions. Another approach is to assign a prior probability to every possible function, where higher probabilities are assigned to functions that are assumed to be more likely. Inference in this Bayesian setting is then based on the posterior distribution of these functions given some potentially noisy observations of  $f(x)$ .

This chapter first provides a definition of a Gaussian Process and then describes how it can be used to solve a regression problem. The argument presented in this chapter is based on the textbook of [Rasmussen and Williams](#).

### 4.1 Gaussian Process Definition

A Gaussian process (GP) can be viewed as a gaussian distribution over functions or as an infinite set of random variables representing the values of the function  $f(x)$  at location  $x$ . The Gaussian process is thus a generalization of the Gaussian distribution and a formal definition is given by [Rasmussen and Williams](#) :

**Definition 4.1.0.1** (Gaussian Process). *A Gaussian process is a collection of random variables, any finite number of which have a joint Gaussian distribution.*

As a (multivariate) Gaussian distribution is defined by its mean and covariance matrix, a GP is uniquely identified by its mean  $m(x)$  and covariance (kernel) function  $k(x, x')$ .

We write

$$f(x) \sim GP(m(x), k(x, x'))$$

with

$$\begin{aligned} m(x) &= \mathbb{E}[f(x)] \\ k(x, x') &= \mathbb{E}[(f(x) - m(x))(f(x') - m(x')))] \end{aligned}$$

If we assume  $X$  to be the index set or set of possible inputs of  $f$ , then there is a random variable  $F_x := f(x)$  such that for a set  $A \subset X$  with  $A = x_1, \dots, x_n$  it holds that:

$$F_A = [F_{x_1}, \dots, F_{x_n}] \sim \mathcal{N}(\mu_A, K_{AA})$$

for

$$K_{AA} = \begin{bmatrix} k(x_1, x_1) & k(x_1, x_2) & \dots & k(x_1, x_n) \\ \vdots & & \ddots & \vdots \\ k(x_n, x_1) & k(x_n, x_2) & \dots & k(x_n, x_n) \end{bmatrix} \text{ and } \mu_A = \begin{bmatrix} \mu(x_1) \\ \vdots \\ \mu(x_n) \end{bmatrix} \quad (4.1.0.1)$$

The finite marginals  $F_{x_1}, \dots, F_{x_n}$  of the GP thus have a multivariate gaussian distribution. In our running example we might consider  $X$  to be the time interval  $T_0 = [0, T]$  however it could be higher dimensional.

Note that a GP with finite index set and hence with joint gaussian distribution is just a specific case of GP. If we assume an ARMA process with gaussian innovations for the blood pressure time series, one can view the time series as a collection of multivariate normally distributed random variables and thus as a GP.

If we consider the linear regression case from chapter 3 and assume a prior distribution on  $\beta$ , i.e.  $\beta \sim \mathcal{N}(0, I)$  then the predictive distribution over  $\mu = X\beta$  is Gaussian:

$$\mu \sim \mathcal{N}(0, XX^\top)$$

This is equivalent to a GP with mean function  $m(x) = 0$  and kernel function  $k(x, x') = x^\top x'$ . This special case of gaussian process regression with this specific kernel function is known as Bayesian linear regression and will be presented in the next section.

## 4.2 Bayesian Linear Regression

Predictions in the Bayesian regression setting is finding the posterior distribution of  $f^* := f(x^*)$  at some input  $x^*$ , given some potentially noisy observations of  $f(x)$ . This is made possible by employing a prior distribution over the function  $f(x)$ . As shown in section 4.1, a GP is essentially assuming a Gaussian distribution over functions. This section however still stays in the domain of parametric models, in which case we assume a distribution over the parameters of the function  $f(x)$ , rather than over the function itself. In Bayesian linear regression we are thus assuming a distribution over the regression coefficients  $\beta$ .

Recall the linear regression model from chapter 3. However, we are assuming a more general setting, where the data generating process does not need to be a time series process. The function is denoted with  $f(x)$  instead of  $\mu(t)$  and  $Y_i$  is again a noisy observation of  $f(x_i)$ , where the additive error  $E_i$  does not necessarily need to be from a time series process ( $E_t : t \in \{t_1, t_2, \dots, t_n\}$ ). We obtain the following data generating model:

$$f(x_i) = x_i^\top \beta, \quad Y_i = f(x_i) + E_i, \quad (i = 1, \dots, n)$$

with  $x_i \in \mathbb{R}^p$  being again the input vector and  $\beta \in \mathbb{R}^p$  is the vector with the regression coefficients.

In matrix from:

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

Where  $\mathbf{Y} = [Y_1, \dots, Y_n]^\top$  is the observed data,  $X = [x_1, \dots, x_n]^\top \in \mathbb{R}^{n \times p}$  is the design matrix. We assume again gaussian but potentially correlated errors  $\mathbf{E} = [E_1, \dots, E_n]^\top$ :

$$\mathbf{E} \sim \mathcal{N}(0, \Sigma_e)$$

If  $\mathbf{E}$  is an ARMA process, then every element of the time series  $E_i$  is itself a sum of innovations. Therefore,  $\mathbf{E}$  is gaussian as long as it has gaussian innovations.

The likelihood, i.e. the probability of the observations  $\mathbf{Y}$  given  $X$  and  $\beta$  is then:

$$p(\mathbf{Y}|X, \beta) = \frac{1}{(2\pi)^{n/2} \sqrt{\det(\Sigma_e)}} \exp\left(-\frac{1}{2}(y - X\beta)^\top \Sigma_e^{-1}(y - X\beta)\right) = \mathcal{N}(X\beta, \Sigma_e)$$

Until now the regression model is exactly the same as in chapter 3. The Bayesian approach is different in that we additionally assume a prior distribution over the regression coefficients  $\beta$ , based on what we believe are likely values for the coefficients. To stay in the realm of gaussian processes the prior has to be Gaussian and we choose:

$$p(\beta) = \mathcal{N}(0, \Sigma_p)$$

Note how the function  $f(x_i) = x_i^\top \beta$  is now no longer deterministic but a random function.

Given our observations  $\mathbf{Y}$  we can use Bayes' theorem to calculate the posterior distribution over  $\beta$ :

$$p(\beta|\mathbf{Y}, X) = \frac{p(\mathbf{Y}, \beta|X)}{p(\mathbf{Y}|X)} = \frac{p(\mathbf{Y}|X, \beta)p(\beta)}{p(\mathbf{Y}|X)}$$

One approach is to just plug in the expressions for  $p(\mathbf{Y}|X, \beta)$  and  $p(\beta|\mathbf{Y}, X)$  from above, with the marginal likelihood:

$$p(\mathbf{Y}|X) = \int p(\mathbf{Y}|X, \beta)p(\beta)d\beta = \mathcal{N}(0, X\Sigma_p X^\top + \Sigma_e)$$

Or it can be helpful to combine the coefficients and the observations into a single random vector with multivariate normal distribution:

$$\begin{bmatrix} \mathbf{Y} \\ \beta \end{bmatrix} = \begin{bmatrix} X \\ I_p \end{bmatrix} \beta + \begin{bmatrix} I_n \\ 0 \end{bmatrix} \mathbf{E} \sim \mathcal{N} \left( \begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix}, \begin{bmatrix} X\Sigma_p X^\top + \Sigma_e & X\Sigma_p \\ \hline \Sigma_p X^\top & \Sigma_p \end{bmatrix} \right) = p(\mathbf{Y}, \beta|X) \quad (4.2.0.1)$$

with  $\Sigma_p X^\top + \Sigma_e \in \mathbb{R}^{n \times n}$  and  $\Sigma_p X^\top \in \mathbb{R}^{p \times n}$ .

To find now the posterior distribution  $p(\beta | \mathbf{Y}, X)$  one can use the rules for deriving conditional distributions for multivariate Gaussian's presented in theorem 4.2.0.1.

**Theorem 4.2.0.1.** (*von Mises*)

Let  $A \sim \mathcal{N}(\mu_A, \Sigma_{AA})$  and  $B \sim \mathcal{N}(\mu_B, \Sigma_{BB})$  be Gaussian random vectors with the following joint distribution:

$$p(A, B) = \mathcal{N} \left( \begin{bmatrix} \mu_A \\ \mu_B \end{bmatrix}, \begin{bmatrix} \Sigma_{AA} & \Sigma_{AB} \\ \Sigma_{BA} & \Sigma_{BB} \end{bmatrix} \right)$$

Then the conditional distribution  $p(\mathbf{B} | \mathbf{A} = a)$  is also normally distributed with mean  $\bar{\mu}$  and covariance  $\bar{\Sigma}$  of the following form:

$$\bar{\Sigma} = \Sigma_{BB} - \Sigma_{BA} \Sigma_{AA}^{-1} \Sigma_{AB} \quad \bar{\mu} = \mu_B + \Sigma_{BA} \Sigma_{AA}^{-1} (a - \mu_A)$$

Using theorem 4.2.0.1 the posterior distribution over  $\beta$  is then given by:

$$\begin{aligned} p(\beta | \mathbf{Y} = y, X) &\sim \mathcal{N}(\bar{\mu}, \bar{\Sigma}), \\ \bar{\Sigma} &= \Sigma_p - \Sigma_p X^\top (X \Sigma_p X^\top + \Sigma_e)^{-1} X \Sigma_p, \\ \bar{\mu} &= \mu_\beta + \Sigma_p X^\top (X \Sigma_p X^\top + \Sigma_e)^{-1} y \end{aligned}$$

The expression for the posterior mean and covariance matrix can be further simplified using Woodbury matrix identity and we obtain:

$$\bar{\Sigma} = (X^\top \Sigma_e^{-1} X + \Sigma_p^{-1})^{-1} \quad \bar{\mu} = \bar{\Sigma} X^\top \Sigma_e^{-1} y \quad (4.2.0.2)$$

Since  $f(x) = x^\top \beta$ , one can use the posterior mean and covariance matrix from 4.2.0.2 to obtain the predictive distribution of  $f^* := f(x^*)$  at  $x^*$  given our observations:

$$p(f^* | \mathbf{Y}, X, x^*) = \mathcal{N}(x^{*\top} \bar{\mu}, x^{*\top} \bar{\Sigma} x^*) \quad (4.2.0.3)$$

One can also use the rules for conditioning to directly derive  $f^* | \mathbf{Y}, X, x^*$ . Similar to before we can write the joint distribution  $p(\mathbf{Y}, f^* | X, x^*)$ :

$$\begin{bmatrix} \mathbf{Y} \\ f^* \end{bmatrix} = \begin{bmatrix} X \\ x^* \end{bmatrix} \beta + \begin{bmatrix} I_n \\ 0 \end{bmatrix} \mathbf{E} \sim \mathcal{N} \left( \begin{bmatrix} 0 \\ \vdots \\ \vdots \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} X \Sigma_p X^\top + \Sigma_e & X \Sigma_p x^* \\ \text{---} & \text{---} \\ x^{*\top} \Sigma_p X^\top & \Sigma_p \end{bmatrix} \right) = p(\mathbf{Y}, f^* | X, x^*) \quad (4.2.0.4)$$

The expression in 4.2.0.3 can then be derived using theorem 4.2.0.1 on conditioning of multivariate Gaussian's.

The next section will extend the Bayesian approach to non-parametric models and illustrate how Bayesian linear regression is just a special case of GP regression.

### 4.3 Bayesian Linear Regression as Gaussian Process Regression

The linear model discussed so far, with a cyclic component represented by a cosine and a linear trend component, might be an evident first guess. However, it is unlikely that the BP values are exactly following this pattern. Instead of reducing the function space to this specific class of linear functions, we may use our domain knowledge to tell which functions of the infinite space of all functions are more likely to have generated our data. As these functions are not characterized with explicit sets of parameters, this approach belongs to the branch of non-parametric modelling. By abandoning the parameters  $\beta$ , Gaussian process regression directly aims for the predictive distribution of  $f^* := f(x^*)$  at an input  $x^*$  given our observations.

Starting with the Bayesian linear regression example from last section and transforming it into a GP regression problem, we recall that the distribution of  $F_X = [f(x_1) \dots f(x_n)]^\top$  with given  $X = [x_1 \dots x_n]^\top$  is:

$$F_X \sim \mathcal{N}(0, X \Sigma_p X^\top)$$

Alternatively this can be written as a distribution over the function  $f(x)$ :

$$f(x) \sim GP(0, k(x, x'))$$

where  $k(x, x')$  needs to be chosen such that for an input  $X$  we obtain  $K_{XX} = X \Sigma_p X^\top$ . Given  $\Sigma_p = \sigma_p I$ , we would choose  $k(x, x') = \sigma_p x^\top x'$ , with the input pairs  $x$  and  $x'$  only entering as a dot product.

Combining  $f^*$  and  $\mathbf{Y}$  into a single random vector we can use the theorem 4.2.0.1 to arrive at the same posterior predictive distribution  $p(f^* | \mathbf{Y}, X, x^*)$  as presented in 4.2.0.3. The joint distribution of  $f^*$  and  $\mathbf{Y}$  can be expressed as follows:

$$\begin{bmatrix} \mathbf{Y} \\ f^* \end{bmatrix} \sim \mathcal{N} \left( \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} K_{XX} + \Sigma_e & K_{Xx^*} \\ K_{x^*X} & K_{x^*x^*} \end{bmatrix} \right) = p(\mathbf{Y}, f^* | X, x^*) \quad (4.3.0.1)$$

where:

$$K_{XX} = \begin{bmatrix} k(x_1, x_1) & k(x_1, x_2) & \dots & k(x_1, x_n) \\ \vdots & & \ddots & \vdots \\ k(x_n, x_1) & k(x_n, x_2) & \dots & k(x_n, x_n) \end{bmatrix},$$

$$K_{Xx^*} = K_{x^*X}^\top = \begin{bmatrix} k(x_1, x^*) \\ \vdots \\ k(x_n, x^*) \end{bmatrix} \text{ and } K_{x^*x^*} = k(x^*, x^*)$$

### 4.3.1 Time Series Gaussian Process Regression

Unlike in chapter 3,  $f(x)$  is no longer assumed to be a deterministic and parametric function. This way, GP regression allows us to treat  $\mathbf{E}$  not simply as an error term but an actual part of our signal which we can predict. If  $\mathbf{E}$  is not independent noise but for example a time series, where the elements of  $\mathbf{E}$  are correlated, we want to leverage the information we have about an unobserved time point given our observations. Hence, we are not interested in the posterior distribution of  $f^*$  only, but also of  $Y^* := Y(x^*) = f(x^*) + E(x^*)$ .

Recall the expression for the marginal likelihood  $p(\mathbf{Y}|X)$ :

$$\mathbf{Y}|X \sim \mathcal{N}(0, X\Sigma_p X^\top + \Sigma_e)$$

Alternatively, this can be expressed as a distribution over the function  $Y(x)$ :

$$Y(x) \sim GP(0, k(x, x'))$$

The kernel function  $k(x, x')$  needs to be chosen such that for an index set  $X$  we obtain  $K_{XX} = X\Sigma_p X^\top + \Sigma_e$ . One can then follow again the same procedure as before and combine  $Y^*$  and  $\mathbf{Y}$  into a single random vector:

$$\begin{bmatrix} \mathbf{Y} \\ Y^* \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} K_{XX} & K_{Xx^*} \\ K_{x^*X} & K_{x^*x^*} \end{bmatrix}\right) = p(\mathbf{Y}, Y^*|X, x^*) \quad (4.3.1.1)$$

The predictive distribution  $p(Y^*|\mathbf{Y}, X, x^*)$  is then again derived by conditioning.

One could also assume additional measurement noise on the time series  $f(x) + E(x)$ . We then have for the observed time series  $Y(x)$ :

$$Y(x) = f(x) + E(x) + \epsilon \quad \epsilon \sim \mathcal{N}(0, \sigma_n^2)$$

To be inline with the literature on Gaussian process regression, we will from now on consider our goal to find some function  $f(x)$ , which is a combination of the mean function, until now denoted by  $f(x)$ , and the stationary time series  $E(x)$ . The observed time series  $Y(x)$  will thus be equivalent to  $f(x)$  up to some additive independent noise term  $\epsilon$ . We can write:

$$Y(x) = f(x) + \epsilon \quad \epsilon \sim \mathcal{N}(0, \sigma_n^2)$$

Assuming the same linear model as before, we have for  $F_X = [f(x_1), \dots, f(x_n)]^\top$ :

$$F_X = X\beta + \mathbf{E}, \text{ with } \beta \sim \mathcal{N}(0, \Sigma_p) \text{ and } \mathbf{E} \sim \mathcal{N}(0, \Sigma_e)$$

Analogously we can write:

$$f(x) \sim GP(0, k(x, x')),$$

with  $k(x, x')$  such that for an input  $X = [x_1 \dots x_n]^\top$  we obtain  $K_{XX} = X\Sigma_p X^\top + \Sigma_e$ . Similarly  $Y(x) \sim GP(0, k(x, x') + \delta_{x, x'}\sigma_n)$ , where  $\delta_{x, x'}$  is the Kronecker delta which is one if  $x = x'$  and zero otherwise.

The joint distribution of  $\mathbf{Y}$  and  $f^* := f(x^*)$  is given by:

$$\begin{bmatrix} \mathbf{Y} \\ f^* \end{bmatrix} \sim \mathcal{N} \left( \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} K_{XX} + \sigma_n^2 I & K_{Xx^*} \\ K_{x^*X} & K_{x^*x^*} \end{bmatrix} \right) = p(\mathbf{Y}, f^* | X, x^*) \quad (4.3.1.2)$$

Also note how until now we have still assumed  $\Sigma_e$ , the covariance matrix of  $\mathbf{E}$ , to be known. However, deriving  $\Sigma_e$  for an ARMA process with irregularly spaced samples is not straight forward, as has already been shown in chapter 3. The next section will illustrate how choosing a specific kernel function solves this problem.

## 4.4 Mean Function

Incorporating Explicit Basis Functions [Rasmussen and Williams](#) p.27

## 4.5 Kernel Functions

In the last section we started of with a describing the prior distribution over  $\mathbf{Y}$  or  $F_X = [f(x_1) \dots f(x_n)]^\top$  and shoved that a kernel function  $k(x, x')$  needs to be chosen to match this distribution. However, in Gaussian process regression it generally goes the other way around. One would choose a prior distribution over  $f(x)$  or  $Y(x)$  first, which boils down to choosing a kernel function. The kernel function evaluated at your inputs  $X = [x_1 \dots x_n]^\top$  is then needed to calculate the predictive distribution of  $f^*$  or  $y^*$ .

The choice of kernel function depends on the assumptions about correlation in your output given arbitrary input pairs  $x$  and  $x'$ .

### 4.5.1 Stationary Covariance Function

Does only depend on  $\tau = x - x'$ .

#### The Matérn Class of Covariance Functions

A expression for the Matérn covariance function is given by [Rasmussen and Williams](#):

$$k_\nu(\tau) = \sigma^2 \frac{2^{1-\nu}}{\Gamma(\nu)} \left( \frac{\sqrt{2\nu}\tau}{l} \right)^\nu K_\nu \left( \frac{\sqrt{2\nu}\tau}{l} \right)$$

where  $\nu$  and  $l$  are positive parameters,  $K_\nu$  is a modified Bessel function and  $\sigma^2 = k_\nu(0)$

For  $\nu = r + 1/2, r \in \mathbb{N}$  the expression for the Matérn covariance function can be simplified:

$$k_{\nu=r+1/2}(\tau) = \sigma \exp\left(-\frac{\sqrt{2r+1}\tau}{l}\right) \frac{r!}{(2p)!} \sum_{i=0}^r \frac{(r+i)!}{i!(r-i)!} \left(\frac{2\sqrt{2r+1}\tau}{l}\right)^{r-i} \quad (4.5.1.1)$$

Setting  $\nu = 1/2$  with input domain  $X \subset \mathbb{R}$  gives rise to a continuous-time AR(1) process, also called Ornstein-Uhlenbeck process. With  $\nu = 1/2$ , i.e.  $r = 0$ , the Matérn covariance function is given by:

$$k(\tau) = \sigma^2 \exp(-\tau/l) \quad (4.5.1.2)$$

The autocovariance function of an Ornstein-Uhlenbeck (OU) process can be derived by solving the stochastic differential equation (SDE) that defines the process.

Starting with the SDE for an OU process:

$$dX_t = \theta(\mu - X_t)dt + \sigma_w dW_t,$$

where  $X_t$  is the value of the process at time  $t$ ,  $\theta$  is a positive constant that determines the speed of mean reversion,  $\mu$  is the long-term mean of the process,  $\sigma_w$  is the standard deviation of the random shocks, and  $W_t$  is a standard Wiener process or Brownian motion.

Let  $Y_t = X_t - \mu$ , then we have:

$$\begin{aligned} dY_t &= dX_t \\ &= \theta(\mu - X_t)dt + \sigma_w dW_t \\ &= \theta(-Y_t)dt + \sigma_w dW_t \end{aligned}$$

This is a linear stochastic differential equation with constant coefficients, which can be solved using the method of integrating factors. We multiply both sides of the equation by  $e^{\theta t}$  and integrate from 0 to  $t$ :

$$\int_0^t e^{\theta s} dY_s = - \int_0^t \theta e^{\theta s} Y_s ds + \int_0^t \sigma_w e^{\theta s} dW_s$$

Using the fact that  $\int_0^t \sigma_w e^{\theta s} dW_s$  is a Gaussian random variable with mean 0 and variance  $\frac{\sigma_w^2}{2\theta}(1 - e^{-2\theta t})$ , we can solve for  $Y_t$  and get:

$$Y_t = e^{-\theta t} Y_0 + \frac{\sigma_w}{\sqrt{2\theta}} \int_0^t e^{-\theta(t-s)} dW_s$$

where  $Y_0 = X_0 - \mu$ .

Now, we can use the definition of covariance to find the autocovariance function of the OU process:

$$\begin{aligned} Cov(X_t, X_{t-k}) &= E[(X_t - \mu)(X_{t-k} - \mu)] \\ &= E[(Y_t + \mu)(Y_{t-k} + \mu)] \\ &= E[Y_t Y_{t-k}] + \mu^2 \end{aligned}$$



Substituting the expression for  $Y_t$  and  $Y_{t-k}$  from the above equation, we get:

$$\text{Cov}(X_t, X_{t-k}) = e^{-\theta k} \text{Var}(Y_0) = \frac{\sigma_w^2}{2\theta} e^{-\theta k}$$

where we have used the fact that  $\text{Var}(Y_0) = \frac{\sigma_w^2}{2\theta}$ .

Therefore, the autocovariance function of an OU process is given by  $\text{Cov}(X_t, X_{t-k}) = \frac{\sigma_w^2}{2\theta} e^{-\theta k}$ , where  $k \geq 0$  and  $\theta > 0$ . The process is covariance stationary if  $\theta > 0$ .

This is the same expression as we have obtained in 4.5.1.2, where  $k(0) = \sigma^2 = \frac{\sigma_w^2}{2\theta}$  and  $l = 1/\theta$

More generally a continuous AR(p) process has Matérn covariance function with  $\nu = p - 1/2$ .

TODO: different kernels, stationary kernels, link to power spectral density, with plots

A more detailed description of covariance functions and their property can be found in [Rasmussen and Williams](#) (chapter 4).

## 4.6 Model Selection - Choosing Hyperparameters

[Rasmussen and Williams](#) p.113.

Hyperparameters  $\theta$

Use marginal likelihood (or evidence):

$$\log p(\mathbf{Y}|\mathbf{X}, \theta) = -\frac{1}{2} \mathbf{Y}^\top K_{XX}^{-1}(\theta) \mathbf{Y} - \frac{1}{2} \log \det K_{XX}(\theta) - \frac{n}{2} \log 2\pi \quad (4.6.0.1)$$

Additionally one can combine valid covariance functions,  $k_1$  and  $k_2$  into new covariance functions based on the following rules:

•

TODO One could hence also assume additional measurement noise:

$$Z(x) = Y(x) + \epsilon = f(x) + E(x) + \epsilon \quad \epsilon \sim \mathcal{N}(0, \sigma_n^2)$$



## Chapter 5

# First Chapter

### 5.1 To include a picture

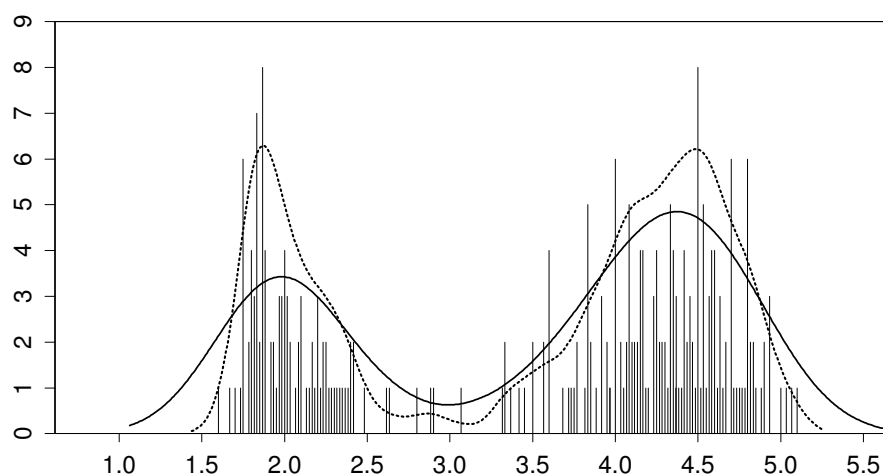


Figure 5.1: Old Faithful Geyser eruption lengths,  $n = 272$ ; binned data and two (Gaussian) kernel density estimates ( $\times 10$ ) with  $h = h^* = .3348$  and  $h = .1$  (dotted).

Or also with `includegraphics`:

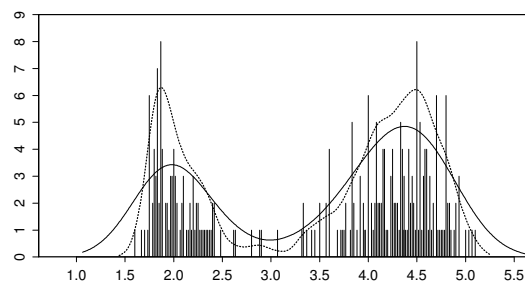


Figure 5.2: Old Faithful Geyser eruption lengths,  $n = 272$ ; binned data and two (Gaussian) kernel density estimates ( $\times 10$ ) with  $h = h^* = .3348$  and  $h = .1$  (dotted).

## 5.2 To make a proof

*Proof.*  $1 + 1 = 2$

□

## 5.3 To include R code

See information in Appendix [A](#).

## 5.4 Other information

Put a text between quotes: make sure to use nice quotes, such as “quote”.

Cite an article or book you refer shortly here, and then listed in the bibliography. Or mention that [Robinson](#) (a person) (two persons) have already done quite a bit work.

[Marvasti and Wolf](#)

Referencing a different part of your work: please refer to Appendix [A](#).

## Chapter 6

# Summary

Summarize the presented work. Why is it useful to the research field or institute?

### 6.1 Future Work

Possible ways to extend the work.



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## Appendix A

# Complementary information

Additional material. For example long mathematical derivations could be given in the appendix. Or you could include part of your code that is needed in printed form. You can add several Appendices to your thesis (as you can include several chapters in the main part of your work).

### A.1 Including R code with verbatim

A simple (rather too simple, see [A.2](#)) way to include code or *R* output is to use `verbatim`. It just prints the text however it is (including all spaces, “strange” symbols,...) in a slightly different font.

```
## loading packages
library(RBGL)
library(Rgraphviz)
library(boot)
```

```
## global variables
X_MAX <- 150
```

```
    This allows me to put as many s p a c e s as I want.
I can also use \ and ' and & and all the rest that is usually only
accepted in the math mode.
```

```
I can also make as
                many
            line
        breaks as
I want... and
                where I want.
```

But really recommended, much better is the following:

However, it is much nicer to use the *listings* package to include R code in your report. It allows you to number the lines, color the comments differently than the code, and so on. All the following is produced by simply writing `\lstinputlisting{Pictures/picture.R}` in your L<sup>A</sup>T<sub>E</sub>X “code”:

```
or \lstinputlisting{/u/maechler/R/Pkgs/sfsmisc/R/ellipse.R} :
```

[illegible]

### A.3 Using Sweave (or knitr) to include R code (and more) in your report

The easiest (and most elegant) way to include R code and its output (and have all your figures up to date with your report) is to use Sweave—or the **knitr** R package with even more possibilities.

Search the web to find lots of intro material on how to use Sweave or **knitr** ([on Wikipedia](#)).



## Appendix B

# Yet another appendix....

### B.1 Description

**Something** details.

**Something else** other definition.

### B.2 Tables

Refer to Table [B.1](#) to see a left justified table with caption on top.

Table B.1: Results.

<b>Student</b>	<b>Grade</b>
Marie	6
Alain	5.5
Josette	4.5
Pierre	5



## Appendix C

# 2nd Appendix: More sophisticated R code listing

Chapter-wise listing of parts of R code, using

- `firstline=n1`
- `lastline=n2`
- `title=<text>`

e.g., for the first example below

```
\lstinputlisting[firstline=1,lastline=20,  
                  title= \texttt{ellipse.R}]{ellipse.R}
```

and the second example

```
\lstinputlisting[firstline=20,lastline=40,  
                  title=\texttt{ellipse.R}]{ellipse.R}
```

### C.1 Chapter 5

```
1 ellipsePoints ← function(a,b, alpha = 0, loc = c(0,0), n = 201,  
2                           keep.ab.order = FALSE)  
3 {  
4   ## Purpose: ellipse points, radially equispaced, given geometric par.s  
5   ## -----  
6   ## Arguments: a, b : length of half axes in (x,y) direction  
7   ##              alpha: angle (in degrees) for rotation  
8   ##              loc  : center of ellipse  
9   ##              n    : number of points  
10  ## -----  
11  ## Author: Martin Maechler, Date: 19 Mar 2002  
12  
13  stopifnot(is.numeric(a), is.numeric(b))  
14  reorder ← a < b && keep.ab.order  
15  B ← min(a,b)  
16  A ← max(a,b)  
17  ## B <= A  
18  d2 ← (A-B)*(A+B) ## = A^2 - B^2  
19  phi ← 2*pi*seq(0,1, len = n)  
20  sp ← sin(phi)
```

---

ellipse.R

```
1  sp <- sin(phi)
2  cp <- cos(phi)
3  r <- a*b / sqrt(B^2 + d2 * sp^2)
4  xy <- r * if(reorder) cbind(sp, cp) else cbind(cp, sp)
5  ## xy are the ellipse points for alpha = 0 and loc = (0,0)
6  al <- alpha * pi/180
7  ca <- cos(al)
8  sa <- sin(al)
9  xy %*% rbind(c(ca, sa), c(-sa, ca)) + cbind(rep(loc[1],n),
10                                              rep(loc[2],n))
11 }
```

ellipse.R



# Epilogue

A few final words.



# Declaration of Originality

The signed declaration of originality is a component of every semester paper, Bachelor's thesis, Master's thesis and any other degree paper undertaken during the course of studies, including the respective electronic versions.

Lecturers may also require a declaration of originality for other written papers compiled for their courses.

I hereby confirm that I am the sole author of the written work here enclosed and that I have compiled it in my own words. Parts excepted are corrections of form and content by the supervisor .

**Title of work** (in block letters):

**Authored by** (in block letters):

*For papers written by groups the names of all authors are required.*

**Name(s):**

**First name(s):**

Muster	Student

With my signature I confirm that

- I have committed none of the forms of plagiarism described in the Citation etiquette information sheet.
- I have documented all methods, data and processes truthfully.
- I have not manipulated any data.
- I have mentioned all persons who were significant facilitators of the work .
- I am aware that the work may be screened electronically for plagiarism.
- I have understood and followed the guidelines in the document *Scientific Works in Mathematics*.

**Place, date:**

**Signature(s):**

Zurich August 19th 2009	bla

*For papers written by groups the names of all authors are required. Their signatures collectively guarantee the entire content of the written paper.*