

**An R Package for
Change Point Detection**

Thales Mello

DISSERTAÇÃO APRESENTADA
AO
INSTITUTO DE MATEMÁTICA E ESTATÍSTICA
DA
UNIVERSIDADE DE SÃO PAULO
PARA
OBTENÇÃO DO TÍTULO
DE
MESTRE EM CIÊNCIAS

Programa: Mestrado em Estatística

Orientador: Florencia Leonardi

São Paulo, 24 de Setembro de 2019

An R Package for Change Point Detection

Esta versão da dissertação contém as correções e alterações sugeridas pela Comissão Julgadora durante a defesa da versão original do trabalho, realizada em 30 de Agosto de 2019. Uma cópia da versão original está disponível no Instituto de Matemática e Estatística da Universidade de São Paulo.

Comissão Julgadora:

- Profa. Dra. Florencia Leonardi
- Prof. Dr. André Fujita
- Prof. Dr. Jesús Enrique Garcia

Acknowledgements

I thank Bruno M. Castro and Florencia Leonardi, for their work in the paper that inspired this project. I also thank specially Hadley Wickham, for his work in several R packages and his tutorial on the development of R packages, and Yihui Xie for his work in the bookdown package. Without their contributions to the R community, none of this would be possible.

Resumo

Mello, Thales. **Um pacote R para detectar pontos de mudança**. 2019. 67 f. Dissertação (Mestrado) - Instituto de Matemática e Estatística, Universidade de São Paulo, São Paulo, 2019.

Esta dissertação explora o desenvolvimento de um pacote da linguagem de programação R com o objetivo de detectar pontos de mudança em um conjunto de dados a ser analisado. Os pontos de mudança são estimados com base em uma função de custo de segmentos, a qual é escolhida de acordo com o tipo de problema que se deseja analisar. Os casos de uso abordados neste trabalho são (i) segmentos como blocos independentes de variáveis aleatórias discretas e (ii) segmentos como blocos de variáveis aleatórias com mesmo parâmetro de regressão, sendo demonstrado um exemplo com regressão linear e outro com a média dos valores numéricos do segmento.

Neste trabalho são descritos os algoritmos de busca implementados pelo pacote (exato, hierárquico e misto), em que cada um possui características de performance e exatidão das estimativas próprios de cada algoritmo.

Por fim, são exploradas algumas aplicações de uso do pacote, bem como algumas tentativas de otimização de performance, explorando implementação de trechos críticos do código em linguagens de baixo nível, bem como se valendo também do uso de computação paralela.

Palavras-chave: segment, change-point, cost, R-package.

Abstract

Mello, Thales. **An R Package for Change Point Detection**. 2019. 67 f. Dissertação (Mestrado) - Instituto de Matemática e Estatística, Universidade de São Paulo, São Paulo, 2019.

This dissertation explores the development of a package for the R programming language that allows the user to detect change points in a given data set. The change points are estimated using a segment cost function, which is chosen to suit the type of problem analyzed. The use cases mentioned in this work are (i) segments as blocks of independent discrete variables; and (ii) segments of random variables with a common regression parameter, for which a case of linear regression blocks and a case of Bernoulli distribution blocks are exemplified in this work.

This work also describes the search algorithms implemented by the package (exact, hierarchical and mixed), each one having characteristics of performance and quality of the results distinct from the others.

Finally, we explore some use-cases for the package, as well as some attempts at performance optimization, exploring the implementation of critical sections of code in low-level programming languages, as try to make use of parallel computing.

Keywords: segment, change-point, cost, R-package.

Contents

List of Figures	ix
List of Tables	xi
1 Introduction	1
1.1 Related Work	1
2 Main Definition	3
2.1 A sequence of random variables and its segments	3
2.2 The segmentation problem	4
2.3 The Hausdorff distance	5
3 Solution Estimation	7
3.1 Exact Algorithm	7
3.2 Hierarchical Algorithm	8
3.3 Hybrid algorithm	8
4 Simulations	11
4.1 Segments of Independent Variables	11
4.2 Segments with similar averages	12
4.3 Accuracy of algorithms using different algorithms	14
5 Real Data Examples	17
5.1 Understanding the data	17
5.2 Building the cost function	17
5.3 Penalizing the cost function	20
5.4 Reducing granularity	23
5.5 Accuracy of estimates for the Berlin dataset	26
5.6 A non-usual cost function	27
6 Considerations on performance	31
6.1 Benchmark the code	31
6.2 Native Code	31
6.3 Parallelization	32
7 Conclusion	35

A Package Usage	37
A.1 Installation	37
A.2 Usage	37
B Support Code	39
Bibliography	53

List of Figures

5.1	Average daily temperature over time as measured by different stations in Berlin . . .	18
5.2	Manual segmentation of the weather data picked according to intuition	18
5.3	Berlin weather data segmented using a non-penalized cost function	21
5.4	Example curve of the penalty function for $C_1 = C_2 = 1$, $s_1 = s_2 = 0.3$ and $L = 100$.	22
5.5	Berlin weather data segmented using an auto-penalized cost function	22
5.6	Berlin weather data segmented using an adjusted penalized cost function	24
5.7	Average monthly temperature over time as measured by different stations in Berlin .	25
5.8	Downsampled Berlin monthly weather data segmented using an auto penalized cost function	25
5.9	Rescaled segments estimated for a downsampled monthly weather data of the Berlin data set using an auto penalized cost function	26
5.10	Berlin daily weather data segmented using an auto-penalized R-squared cost function	28
5.11	Berlin daily weather data segmented using an adjusted penalized R-squared cost function	28
5.12	Subset of Berlin daily weather data segmented using an auto-penalized R-squared cost function	30

List of Tables

4.1	Sample values of the correlated random variables defined in (4.1).	12
4.2	Segment tables as defined in (4.1).	12
4.3	Results of segmentation using a non-penalized multivariate cost	13
4.4	Results of segmentation by applying the cost function defined in (4.5) to a sample of size 10 of the model defined in (4.6).	14
4.5	Comparison of solutions of different algorithms to segment the data set described in (4.1), measuring how far each solution is from the ideal solution using the Hausdorff distance.	14
4.6	Comparison of solutions of different algorithms to segment the data set described in (4.6), measuring how far each solution is from the ideal solution using the Hausdorff distance.	15
5.1	First and last columns of the ‘berlin‘ dataset	19
5.2	Expected values to be found when segmenting the Berlin dataset	19
5.3	Sample values of the squared residual cost function for different sizes of segment candidates	20
5.4	Results of the segmentation algorithm using a non-penalized cost function	20
5.5	Results of the segmentation algorithm using an auto-penalized cost function	23
5.6	Results of the segmentation algorithm using an adjusted penalized cost function	23
5.7	Results of the segmentation algorithm using an auto-penalized cost function over downsampled berlin data	24
5.8	Results of the segmentation algorithm using an auto-penalized cost function over downsampled berlin data, but rescaled to fit the original data dimensions	26
5.9	Hausdorff distance for different segmentation attempts over the Berlin weather data set	27
5.10	Sample values of the R-squared cost function for different sizes of segment candidates	27
5.11	Results of the segmentation algorithm using an auto-penalized R-squared cost function over Berlin data	29
5.12	Results of the segmentation algorithm using an adjusted penalized R-squared cost function over Berlin data	29
5.13	Results of the segmentation algorithm using an auto-penalized R-squared cost function over a subset of Berlin data	30
6.1	Execution time comparison between native C++ and interpreted R code	32

6.2	Execution time comparison between parallel and single-threaded computation with a data set of 100 samples and 10 columns	32
6.3	Execution time comparison between parallel and single-threaded computation with a data set of 5 samples and 100 columns	33

Chapter 1

Introduction

[Castro *et al.*, 2018] describe a method of segmenting a data set of a finite alphabet into blocks of independent variables. This work expands on that by minimizing a cost function rather than maximizing a likelihood function, such the cost is the opposite of the likelihood. We show this generalization can be used for other use-cases, e.g. segments with homogeneous values (see Chapter 4.2), segments that have the same linear regression trend 5.

This work was developed as an R Programming Language [R Core Team, 2018] package. The packaging of the code into redistributable software was based on instructions provided by [Wickham, 2015], and the final code is made available as an R package [Mello e Leonardi, 2019]. The goal was to make it as easy as possible for researchers and R programmers to use this software. The source code for the package is also available as an open-source software Mello [2019]. Finally, as a special implementation for the use case described by [Castro *et al.*, 2018] of segmenting finite alphabets, a specialized version of the multivariate likelihood function is implemented in native code using Rcpp [Eddelbuettel e François, 2011].

1.1 Related Work

[Maidstone *et al.*, 2017] also talks about optimally segmenting a data set with the minimization of a given cost function. In their paper, they discuss search path algorithms different than the ones shown in this work. In their case, if the cost function satisfies certain conditions, the `fpop` and `snip` search algorithms can prune the search path in a mathematically optimal way. They claim the algorithms presented in their work provide better results than previous work.

Notice that, because the approach used by [Maidstone *et al.*, 2017] is different than the one used by [Castro *et al.*, 2018], the `fpop` and `snip` algorithms couldn't be investigated and validated in time to be implemented in the `segmentr` package. However, if in future work those algorithms provide good results estimation and performance compared to the currently implemented algorithms, they can be included in the `segmentr` package. That will allow users to use the newly implemented algorithms with minimal code modification, by changing a single parameter.

Chapter 2

Main Definition

In this chapter, we explain the problem by providing definitions of concepts and build equations that gradually help us explain the problem and make the case for our solution.

2.1 A sequence of random variables and its segments

As shown in defined in (2.1), let $X = (X_1, \dots, X_m)$, be a vector of random variables whose elements X_j belong to a set S . The equation also shows all random variables X_j have probability distribution F , each with parameter Θ_j , such that $X_j \sim F(\Theta_j)$. A segment is defined as a sequence of indices for which $\Theta_a = \Theta_{a+1} = \dots = \Theta_b$ such that $1 \leq a \leq b \leq m$, for a and b as the first and last indices of the segment, respectively. We also define a change point c as being an index for which there is a change in the probability distribution parameters, i.e. $\Theta_{c-1} \neq \Theta_c$, for $c \geq 2$.

$$\begin{aligned} X &= (X_1, \dots, X_m) \\ X_j &\in S, \text{ for } 1 \leq j \leq m \text{ and } j \in \mathbb{Z} \\ X_j &\sim F(\Theta_j) \end{aligned} \tag{2.1}$$

Putting it all together in (2.2), a data set X with t change points has each segment represented by the sequence $S_k = X_{c_k}, \dots, X_{c_{k+1}-1}$, with c_k each representing a change point when $k \leq t$. In order to simplify equations, let $c_0 = 1$ and $c_{t+1} = m + 1$, even though they are not change points. With it we say $S_{c_0} = S_1$ represents the first segment of the data set, even though c_0 is not a change point.

$$\begin{aligned} c_0 &= 1 \\ c_{t+1} &= m + 1 \\ 1 &< c_1 < \dots < c_k < \dots < c_t < m + 1 \\ &, \text{ for } 0 \leq k \leq t \text{ and } k \in \mathbb{Z} \\ \Theta_{c_k} &= \Theta_{c_k+1} = \dots = \Theta_{c_{k+1}-1} \\ \Theta_{c_{k-1}} &\neq \Theta_{c_k}, \text{ for } 1 \leq k \leq t \text{ and } k \in \mathbb{Z} \\ S_k &= X_{c_k}, \dots, X_{c_{k+1}-1} \end{aligned} \tag{2.2}$$

2.2 The segmentation problem

As defined in (2.3), let D be a $n \times m$ matrix with elements $x_{i,j}$, with row and column indices i and j , respectively. Each of the n rows in the data matrix D is a sample of the vector of random variables X , i.e. any row element with column index j is a sample of the random variable X_j . In (2.4), let C is the set of change points in the data set. Considering all random variables within a segment have the same probability function parameter, let K be a cost function that calculates the cost value for a segment S_k with estimated parameter Θ_k , i.e. the calculated cost is minimal when the estimated Θ_k is optimal for the segment S_k . Therefore, a common definition for K is the opposite of the maximum value of a log-likelihood function, illustrated in (2.5).

$$D = \begin{bmatrix} x_{11} & \dots & x_{1j} & \dots & x_{1m} \\ \dots & \dots & \dots & \dots & \dots \\ x_{i1} & \dots & x_{ij} & \dots & x_{im} \\ \dots & \dots & \dots & \dots & \dots \\ x_{n1} & \dots & x_{nj} & \dots & x_{nm} \end{bmatrix}_{n \times m} \quad (2.3)$$

$$C = \{c_1, \dots, c_t\} \quad (2.4)$$

$$\Theta_k = \arg \max \{L(\Theta|S_k)\} \quad (2.5)$$

Let the total cost of the segments T , i.e. the sum of all segment costs, as illustrated in (2.6). So, the segmentation problem is defined as estimating the optimal set of change points C that minimize the total cost T , as described in (2.7).

Notice that, in (2.6) and in (2.7), the cost function K and the data set D are parameters to the segmentation problem, which will ultimately be used to search for the set of change points C using dynamic programming. So, let $s(K, D) = C$ be the segmentation function whose output is the estimation of change points, as illustrated in (2.7). The `segmentr` package implements a few different segmentation function algorithms, which are described in this work.

$$T = \sum_{k=0}^t K(S_k) \quad (2.6)$$

$$C = \arg \min \{T\} = \arg \min \left\{ \sum_{k=0}^t K(S_k) \right\} \quad (2.7)$$

In summary, `segmentr` is a generalization of the work described in [Castro *et al.*, 2018], in which the random variables of X are taken from finite alphabets and L is the multivariate estimate of discrete variables. In this work, with the difference that we minimize a cost function rather than maximize a cost function, we solve the same problem proposed by [Castro *et al.*, 2018], with the difference the cost function concept can be applied to many other use cases as well, e.g. segments with changes in the mean of columns, segments with different linear regression parameters. These cases are discussed in 4 and 5.

2.3 The Hausdorff distance

As the solution estimated by the segmentation function is a set of points, a measure is made necessary to compare the estimations provided by the different estimation algorithms that will be presented in Chapter 3. The Hausdorff distance is commonly used as a measure of distance between two distinct sets, and will be used to compare change point sets with differing numbers of elements each.

[Munkres, 2000] defines the Hausdorff distance as a measure of how far two subsets from a metric space are from one another. It's defined as the biggest of all the distances from a point in one set to the closest point in the other set, which is expressed mathematically by the equation defined in (2.8), in which X and Y represent sets given as inputs to the function, $d(x, y)$ represents a distance function defined in the metric space S such that $x, y \in S$.

$$d_H(X, Y) = \max \left\{ \sup_{x \in X} \inf_{y \in Y} d(x, y), \sup_{y \in Y} \inf_{x \in X} d(x, y) \right\} \quad (2.8)$$

Since a set of change points is a subset of the column indices in a data set, we define the distance d as the absolute value of two given numbers for the use-cases analyzed in this paper.

Chapter 3

Solution Estimation

In this chapter, we discuss the process to solve (2.7) and explore a solution involving dynamic programming. Because the exact solution to this problem has quadratic complexity, we also discuss some alternatives that simplify the search path and provide an approximate solution.

3.1 Exact Algorithm

The first attempt to solve the equation would be to search for all the possible alternatives to find the correct minimal set of intervals that minimize the total cost of the system. It's done iteratively by:

- let D be the current data set we want to segment
- for each column index $i \in \{1, \dots, m\}$
 - for each column index $j \in \{i, \dots, m\}$
 - * compute $K_{i:j} = K(D_{i:j})$
 - * store the cost $K_{i:j}$ and the index j for the lowest value of $K_{i:j}$ for later comparison

Finally, after computing all of the possible combinations of segment costs, the procedure to find the optimal solution is:

- let $j = m$
- while $j > 1$
 - search the stored values for $i = \arg \min(K_{i:j})$
 - store i in the set of change points $\overset{i}{C}$ if $i \neq 1$
 - let $j = i$ and repeat until $j = 1$

With the execution of the procedure described above, the estimated set of change points is stored in C . The solution will be exact precisely because it analyses all the possible combinations. However, that has a time complexity of $O(m^2)$ in the Big-O notation, for the number of columns m in the data set. Because the number of columns in data segmentation problems can be very large, computation time can be very prohibitive. For those situations, approximate solutions are described.

3.2 Hierarchical Algorithm

To try to simplify the search path of the algorithm, [Castro *et al.*, 2018] also proposes a technique that relies on the assumption of the data hierarchical, i.e. a segment can be sub-divided by reapplying the segmentation function recursively. The algorithm is described as:

- let D be the current data set we want to segment
- for each column i in the data set
 - compute the total cost $K_i = K(D_{1:i-1}) + K(D_{i:m})$ if $i \neq 1$
- find i for which K_i is minimum
- if $K_i > K(D_{1:m})$
 - return the empty set as the result of the current function call
- recursively find the set of change points C_L by calling the algorithm on the left segment $D_{1:i-1}$
- recursively find the set of change points C_R by calling the algorithm on the right segment $D_{i:m}$
- return $C = C_L \cup C_R \cup \{i\}$ as result of current function call

Implementing the algorithm described above will estimate the set of change points C with time complexity of $O(m \log(m))$, for the number of columns m in the data set. The reduction in time complexity is only possible because of the strong assumption the data set has a hierarchical cost behavior. However, that doesn't hold for many situations, as it will be seen in more detail in the next chapters. So, the usage of this algorithm should be considered with care.

3.3 Hybrid algorithm

The hybrid algorithm is a modified version of the hierarchical algorithm, in which it will start searching the segments using the hierarchical algorithm, and if the segments become smaller than a certain number of columns threshold, it will switch to the exact algorithm. The procedure would be as follow:

- let D be the current data set we want to segment
- if the number of columns of D is $m < k$, in which k is a predefined threshold
 - return the set of change points calculated by the exact algorithm.
- for each column i in the data set
 - compute the total cost $K_i = K(D_{1:i-1}) + K(D_{i:m})$ if $i \neq 1$
- find i for which K_i is minimum
- if $K_i < K(X_{1:p})$
 - return empty set as the result of the current function call
- recursively find the set of change points C_L by calling the algorithm on the left segment $K_{1:i-1}$
- recursively find the set of change points C_R by calling the algorithm on the right segment $K_{i:m}$

- return $C = C_L \cup C_R \cup \{i\}$ as result of current function call

The only difference between this and the hierarchical procedure is the presence of the conditional step is the beginning of the procedure that tests whether or not to use the hybrid algorithm. As will be shown in later chapters, the accuracy of this algorithm is shown not to be more advantageous than using the hierarchical or the exact algorithms directly, depending on the situation.

Chapter 4

Simulations

To exemplify the utility of this package, a handful of hypothetical data will be presented, together with a proposal of an appropriate cost function that is expected to segment the data.

4.1 Segments of Independent Variables

To show compatibility with the work presented in [Castro *et al.*, 2018], we analyze the same problem presented in their work.

Let $N = (N_1, \dots, N_6)$ be a sequence of independent random variables with standard normal distributions and let $X = (X_1, \dots, X_{15})$ be another sequence of random variables dependent on N , with relationships described in (4.1). From the relationships, it's possible to see the first segment X_1, \dots, X_5 depend on N_1, N_2 , the second segment X_6, \dots, X_{10} depend on N_3, N_4 and the third and last segment X_{11}, \dots, X_{15} depend on X_4, X_5 . Therefore, the set of change points for X is $C = 6, 11$.

$$\begin{aligned} X_1 &= N_1 \\ X_2 &= N_1 - N_2 \\ X_3 &= N_2 \\ X_4 &= N_1 + N_2 \\ X_5 &= N_1 \\ X_6 &= N_3 \\ X_7 &= N_3 - N_4 \\ X_8 &= N_4 \\ X_9 &= N_3 + N_4 \\ X_{10} &= N_3 \\ X_{11} &= N_5 \\ X_{12} &= N_5 - N_6 \\ X_{13} &= N_6 \\ X_{14} &= N_5 + N_6 \\ X_{15} &= N_5 \end{aligned} \tag{4.1}$$

Given D , illustrated in 4.1, a sample data set of the sequence of random variables X , the

Table 4.1: *Sample values of the correlated random variables defined in (4.1).*

X1	X2	X3	X4	X5	X6	X7	X8	X9	X10	X11	X12	X13	X14	X15
1	-1	2	3	1	2	0	2	4	2	1	-1	2	3	1
1	0	1	2	1	1	-1	2	3	1	2	0	2	4	2
1	-1	2	3	1	1	-1	2	3	1	2	0	2	4	2
1	-1	2	3	1	1	-1	2	3	1	2	0	2	4	2
2	1	1	3	2	2	1	1	3	2	1	0	1	2	1
1	0	1	2	1	1	-1	2	3	1	1	-1	2	3	1

Table 4.2: *Segment tables as defined in (4.1).*

Segment no.	First index	Last index
1	1	5
2	6	10
3	11	15

multivariate likelihood function L [Park, 2017] can be used to estimate the likelihood of a given segment in the discrete data set, as described in (4.2). The `multivariate()` is a fast native-code implementation of that function that is available in the `segmentr` package. We then use that likelihood function to define a penalized cost K in (4.3) with an extra term to penalize segments that are too large, based on the number of columns $\text{ncol}(D)$ of the segment.

$$\log(L(X|D)) = \sum_{k=0}^t P(X_{c_k:c_{k+1}-1} = D_{c_k:c_{k+1}-1}) \quad (4.2)$$

$$K(D) = -\log(L(D)) + \text{ncol}(D) \quad (4.3)$$

Therefore, the cost function K applied over a sample D , shown in of X provides the same set of expected change points C , as Table 4.2 show. Notice it's important to use a penalized cost function because the original likelihood function tends to favor bigger segments. An estimate of the segments using an unpenalized cost is shown in Table 4.3.

4.2 Segments with similar averages

[Ceballos *et al.*, 2018] describes a process on how to find windows of contiguous homozygosity, i.e. segments in the genetic data in which the alleles are of the same type. This is of interest to a researcher investigating diseases. Considering this problems scenario, `segmentr` can be used to segment random variables X_1, \dots, X_m that represent genetic data, encoded as zero for homozygosity and one for heterozygosity, i.e. 0 when the alleles are the same and 1 when different.

So, to use `segmentr` to solve this problem, it's necessary to find a cost function that favors the homogeneity of a given segment. That problem is approached by proposing a heterogeneity cost function, i.e. a function that penalized the segments whose elements are far from the segment average. One such function is defined in (4.4). Notice, however, the cost function proposed favors single column segments, as it's the size for which all the elements approximate the segment average the most. To counter this undesirable behavior, we penalized the function by adding a constant to it, as described in (4.5). The constant factor has the effect of adding up when too many segments

Table 4.3: *Results of segmentation using a non-penalized multivariate cost*

Segment no.	First index	Last index
1	1	15

are considered in the estimation process, making it so wider segments end being picked up in the estimation process.

In order to observe how the proposed function behaves, consider the simple example defined in (4.6), in which X_i for $i \in \{1, \dots, 20\}$ represent each a column indexed by i of a data set D , and $\text{Bern}(p)$ representing the Bernoulli distribution with probability p . The result for applying (4.5) over (4.6) is shown in Table 4.4.

$$K(D) = \sum_i (D_i - E[D])^2 \quad (4.4)$$

$$K_p(D) = K(D) + 1 \quad (4.5)$$

$$\begin{aligned}
X_1 &\sim \text{Bern}(0.9) \\
X_2 &\sim \text{Bern}(0.9) \\
X_3 &\sim \text{Bern}(0.9) \\
X_4 &\sim \text{Bern}(0.9) \\
X_5 &\sim \text{Bern}(0.9) \\
X_6 &\sim \text{Bern}(0.1) \\
X_7 &\sim \text{Bern}(0.1) \\
X_8 &\sim \text{Bern}(0.1) \\
X_9 &\sim \text{Bern}(0.1) \\
X_{10} &\sim \text{Bern}(0.1) \\
X_{11} &\sim \text{Bern}(0.1) \\
X_{12} &\sim \text{Bern}(0.1) \\
X_{13} &\sim \text{Bern}(0.1) \\
X_{14} &\sim \text{Bern}(0.1) \\
X_{15} &\sim \text{Bern}(0.1) \\
X_{16} &\sim \text{Bern}(0.9) \\
X_{17} &\sim \text{Bern}(0.9) \\
X_{18} &\sim \text{Bern}(0.9) \\
X_{19} &\sim \text{Bern}(0.9) \\
X_{20} &\sim \text{Bern}(0.9)
\end{aligned} \quad (4.6)$$

Table 4.4: Results of segmentation by applying the cost function defined in (4.5) to a sample of size 10 of the model defined in (4.6).

Segment no.	First index	Last index
1	1	5
2	6	15
3	16	20

Table 4.5: Comparison of solutions of different algorithms to segment the data set described in (4.1), measuring how far each solution is from the ideal solution using the Hausdorff distance.

Description	Changepoints	Hausdorff Distance
Expected solution	6, 11	0
Exact algorithm estimate	6, 11	0
Hierarchical algorithm estimate	6, 8, 11	2
Hybrid algorithm estimate with threshold 50	6, 11	0
Hybrid algorithm estimate with threshold 4	6, 8, 11	2

4.3 Accuracy of algorithms using different algorithms

Given different solutions obtained by the `segment` function, it's often necessary to compare them with each other. For that, the Hausdorff distance, defined in Chapter 2.3, can be used to measure a distance between two sets of estimated change points.

We want to measure how well the different algorithms provided in the `segmentr` package find the segments in the example correlated columns simulated data set described in (4.1). Since the simulation was arbitrarily built, we know what the exact solution to the segmentation problem is.

Therefore, in Table 4.5 we can see the comparison of different algorithms with different parameters. We notice the “exact” algorithm manages to properly match the expected change points solution, whereas the “hierarchical” algorithm finds an extra segment, which causes the Hausdorff distance to be bigger than zero. The two “hybrid” algorithm cases are interesting in the sense it that it shows how the algorithm works by either adopting the exact or the hierarchical algorithm depending on the threshold and the size of the segment being analyzed. When the threshold argument is large, it applies the exact algorithm to the data set, whereas when the threshold is small, it applies the hierarchical algorithm instead.

Consider now the simulated data set of segments with similar averages described in equation (4.6). We do the same algorithm comparison with this data set in Table 4.6. In contrast with the previous experiment, all the algorithms manage to find the expected solution to the problem.

Table 4.6: Comparison of solutions of different algorithms to segment the data set described in (4.6), measuring how far each solution is from the ideal solution using the Hausdorff distance.

Description	Changepoints	Hausdorff Distance
Expected solution	6, 16	0
Exact algorithm estimate	6, 16	0
Hierarchical algorithm estimate	6, 16	0
Hybrid algorithm estimate with threshold 50	6, 16	0
Hybrid algorithm estimate with threshold 4	6, 16	0

Chapter 5

Real Data Examples

To exemplify how `segmentr` is used in real situations, an example of weather data is provided in this paper. The data was obtained using data found in [Wetterdienst, 2019].

`segmentr` is a package that implements a handful of algorithms to segment a given data set, by finding the change points that minimize the total cost of the segments according to an arbitrary cost function. So, the user of this package has to find an adequate cost for the segmentation problem to be solved, possibly having to penalize it to avoid either an over parametrized or under parameterized model, i.e. one with too many or too few change points, respectively. Also, it's important to consider the computation time of each algorithm and its trade-offs. This example walks through the main concepts regarding its usage, using historical temperature data from Berlin as an example.

5.1 Understanding the data

The `berlin` data set, provided in this package, contains daily temperature measurements from 7 weather stations in Berlin for every day in the years 2010 and 2011, i.e., a total of 730 days. Therefore, every element in the data set has a temperature data point with units in Celsius, such that each of the 730 columns corresponds to a date, and each of the 7 rows corresponds to the weather station the data point was measured at. In Table 5.1, it's possible to see the first three columns, as well as the last three columns, together with the respective stations.

To grasp the behavior of the weather data, in Figure 5.1 the daily average temperature of all the weather stations, i.e., the mean value of each column in the data set as a time series graph to observe how the average temperature of Berlin behaves over time.

In the graph, the daily temperatures points alternate in upwards and downwards trends, which suggests it's possible to fit linear regressions for each of the upwards or downwards trend segments. So, a cost that optimizes for linear regressions function is proposed, which should minimize when a linear regression fits in a given segment. By intuition, we expect the cost function to segment the dataset approximately to the way the vertical lines are placed in Figure 5.2. The indices picked to represent each segment are available in Table 5.2.

5.2 Building the cost function

An adequate cost function should be able to rank a given set of possible segments and pick the best one given the evaluation criteria. Since the goal is to select segments with a good linear

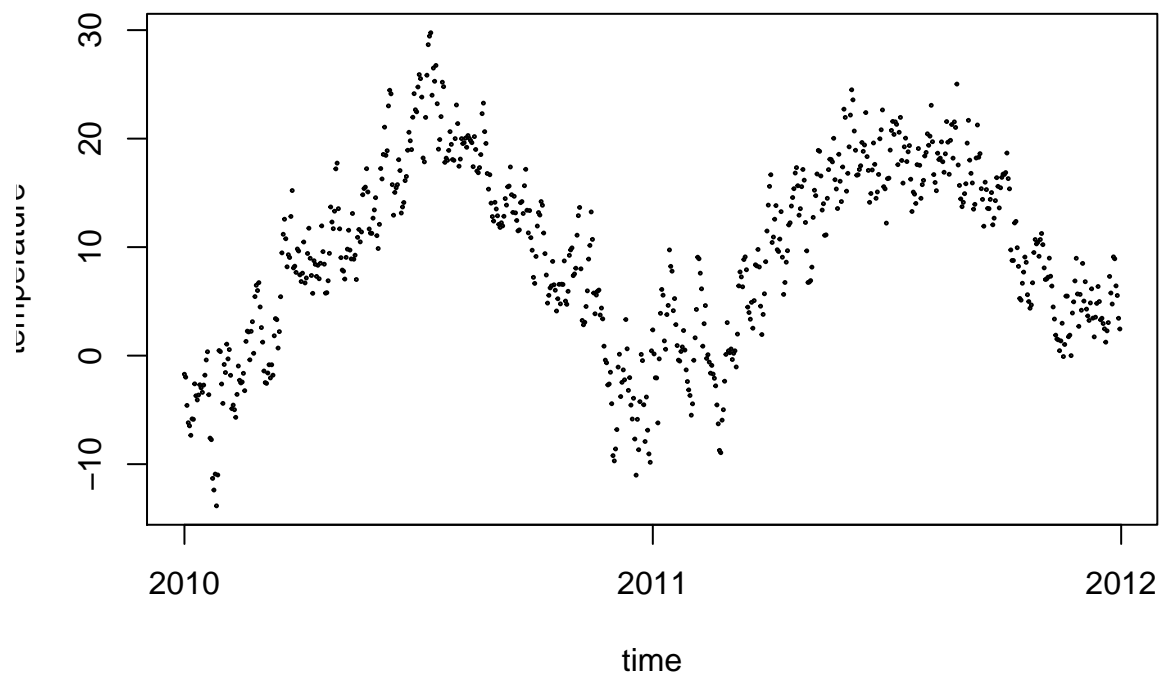


Figure 5.1: Average daily temperature over time as measured by different stations in Berlin

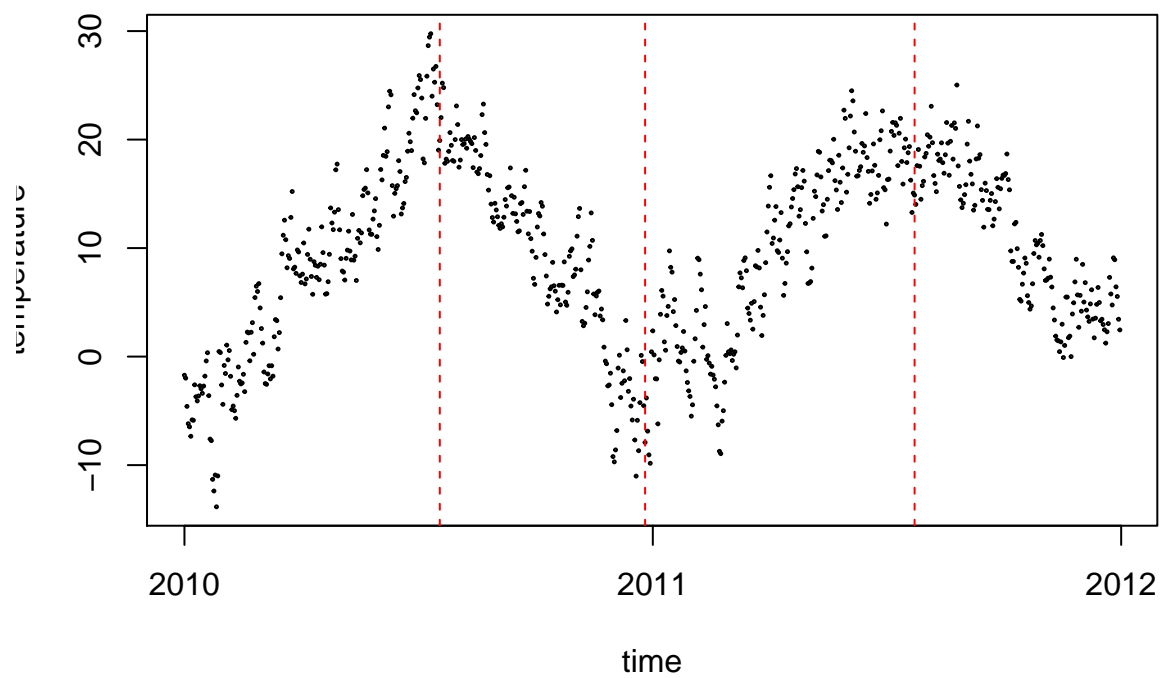


Figure 5.2: Manual segmentation of the weather data picked according to intuition

Table 5.1: *First and last columns of the ‘berlin’ dataset*

station	2010-01-01	2010-01-02	2010-01-03	..	2011-12-29	2011-12-30	2011-12-31
Berlin-Buch	-1.6	-1.9	-4.8	..	6.0	3.5	2.1
Berlin-Dahlem (FU)	-1.9	-2.3	-4.5	..	5.2	3.1	2.4
Berlin-Kaniswall	-1.9	-2.0	-4.6	..	5.2	3.3	1.9
Berlin-Marzahn	-1.8	-1.9	-4.8	..	5.7	3.7	2.6
Berlin-Schoenefeld	-1.9	-2.1	-4.6	..	5.0	3.3	2.4
Berlin-Tegel	-1.5	-2.0	-4.5	..	6.0	3.5	2.8
Berlin-Tempelhof	-1.4	-1.7	-4.3	..	5.7	3.7	3.0

Table 5.2: *Expected values to be found when segmenting the Berlin dataset*

Segment no.	First index	Last index
1	1	199
2	360	569
3	570	730

regression fit, the standard log-likelihood function for linear regressions is the negative of the squared sum of residuals, the squared sum of residuals is a good candidate for our segment cost function. So, the cost function K is shown in (5.1), with the set of points X that belong to the segment, x_i and y_i as the points that belong to X for each index i , and f is the best linear regression that fitted the X segment.

$$K(X) = \sum_{i=1}^n \frac{1}{n} (y_i - f(x_i))^2 \quad (5.1)$$

A cost argument for a segment () call requires a function which accepts a candidate segment matrix, i.e. a subset of the columns in the data set, and returns the cost for the given segment. Therefore, equation (5.1) is implemented as an R function called `residual_cost`, such that it obeys the argument contract by taking a matrix as argument and returning the mean of the squared residuals of a linear regression over the candidate segment. To get a sense of how the function behaves with the `berlin` data set, sample costs for a small, a medium, and a large segment are provided in 5.3.

With the cost function defined, it can now be applied to `segment()` to get the segments for the data set. Since the time complexity of the exact algorithm is $O(n^2)$ and the number of points in the data set is high, the execution time required for the computation is quite prohibitive. So, for demonstration purposes, we use the hierarchical algorithm, due to its $O(n \log(n))$ complexity. We point the hierarchical algorithm (generally suitable for the cost function based on multivariate likelihood) assumes the segments to be structured hierarchically, with a combination of two neighboring segments being selected as an intermediate step before evaluating the ideal change points of

Table 5.3: *Sample values of the squared residual cost function for different sizes of segment candidates*

Small Size	Medium Size	Large Size
0.0283673	12.18277	68.85185

Table 5.4: *Results of the segmentation algorithm using a non-penalized cost function*

Segment no.	First index	Last index
1	1	2
2	3	6
3	7	17
4	18	19
5	20	21
6	22	23
7	24	24
8	25	26
9	27	28
10	29	29
11	30	31
12	32	33
13	34	35
14	36	37
15	38	38
16	39	41
17	42	43
18	44	47
19	48	730

the data set. The segmentation results can be seen in Table 5.4, and they are also plotted together with the weather data in Figure 5.3.

In Figure 5.3, it's possible to see many very short segments, and a very large last segment. This is a result of the algorithm used, as well as the fact the `residual_cost` function tends to favor very short segments, as they usually have smaller residual error. So, to not get segments too short or too long, it's necessary to penalize the cost function for either extremely short or extremely long lengths.

5.3 Penalizing the cost function

To penalize a cost function in the `segment_r` context is to increase the return value of the cost function whenever unwanted segments are provided as an input. Typically, this involves penalizing the cost function whenever a very short or a very long segment is provided.

One such method is to add the output of the cost function with a penalty function which is a function of the length of the segment. We propose a penalty function in (5.2).

$$p(l) = C_1 e^{s_1(l - \frac{l}{2})} + C_2 e^{s_2(-l + \frac{l}{2})} \quad (5.2)$$

In equation (5.2), the penalty $p(l)$ is a function of the segment's length l and, for parametrization values $C_1 > 0$, $s_1 > 0$, $C_2 > 0$ and $s_2 > 0$, the penalty is high for values of l neighboring 0, as well as values of l in the order of the total length L of the data set. However, penalty is close to

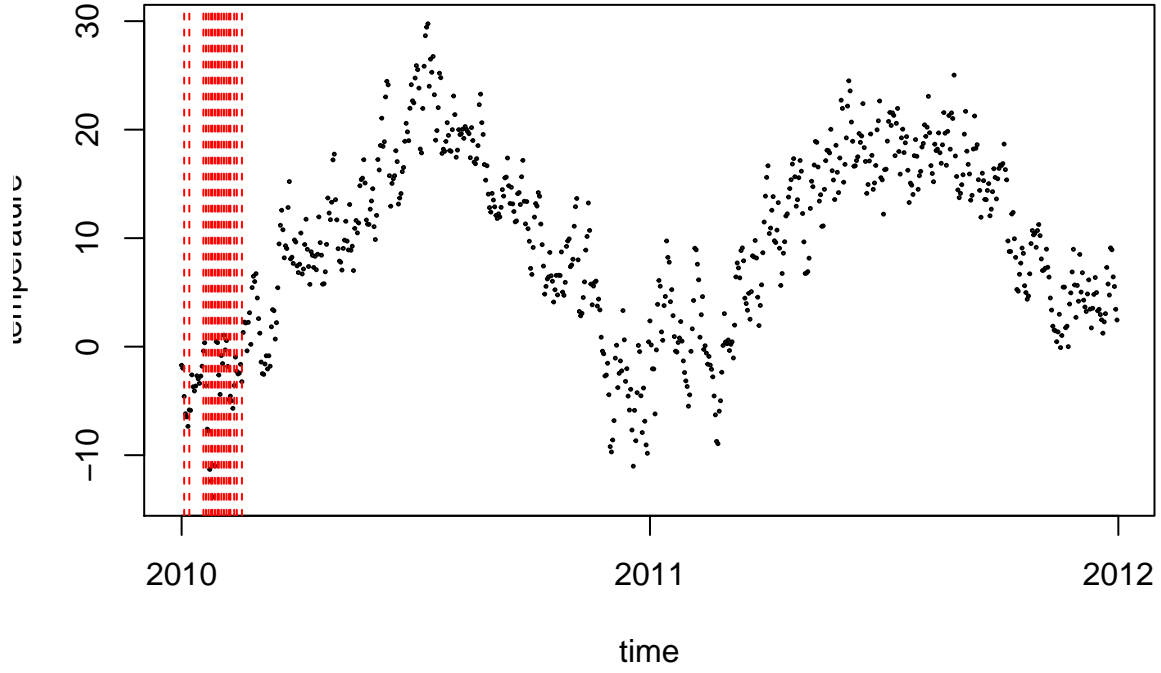


Figure 5.3: *Berlin weather data segmented using a non-penalized cost function*

its minimum for values of l neighboring $\frac{L}{2}$. To visualize, consider a sample penalty function, with $C_1 = C_2 = 1$, $s_1 = s_2 = 0.3$ and $L = 100$, plotted in Figure 5.4.

Given the penalty function general formula, it's necessary to adjust the parameters such as the penalty function has a scale compatible with the cost function. The `auto_penalize()` function, provided in the `segmentr` package, builds a penalized version of the cost function, by estimating parametrization values based on sample cost values for big and small segments of the data set provided. The estimated parameters are tunable by adjusting the `small_segment_penalty` and the `big_segment_penalty` parameters, depending on how much small or big segments, respectively, should be penalized, i.e. the higher the parameter, the more penalized the related type of segment size is.

Let P_s be the `small_segment_penalty`, P_b be the `big_segment_penalty`, μ_s be the average cost for the sampled small segments and μ_b be the average cost for the sample's big segments. The relationship between the parameters, as defined by the `auto_penalize()` function, is defined in (5.3).

$$\begin{aligned}
 C_1 &= \frac{\mu_b}{P_b} \\
 s_1 &= \frac{4 \log(P_b)}{L} \\
 C_2 &= \frac{\mu_s}{P_s} \\
 s_2 &= \frac{4 \log(P_s)}{L}
 \end{aligned} \tag{5.3}$$

So, a penalized cost version of the function is created with `auto_penalize()` and then used with `segment()`. The results of the segmentation can be seen in Table 5.5, and it's possible to the segments with the weather data in Figure 5.5.

We now get a reduced number of segments estimated by the new penalized cost function in Figure

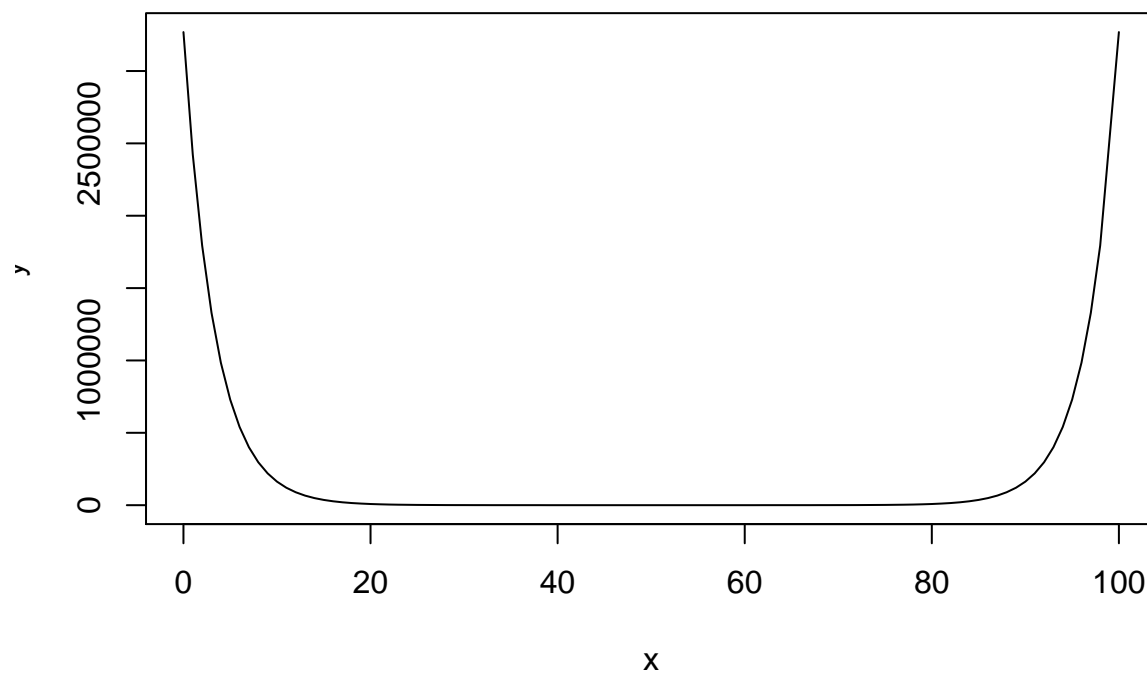


Figure 5.4: Example curve of the penalty function for $C_1 = C_2 = 1$, $s_1 = s_2 = 0.3$ and $L = 100$

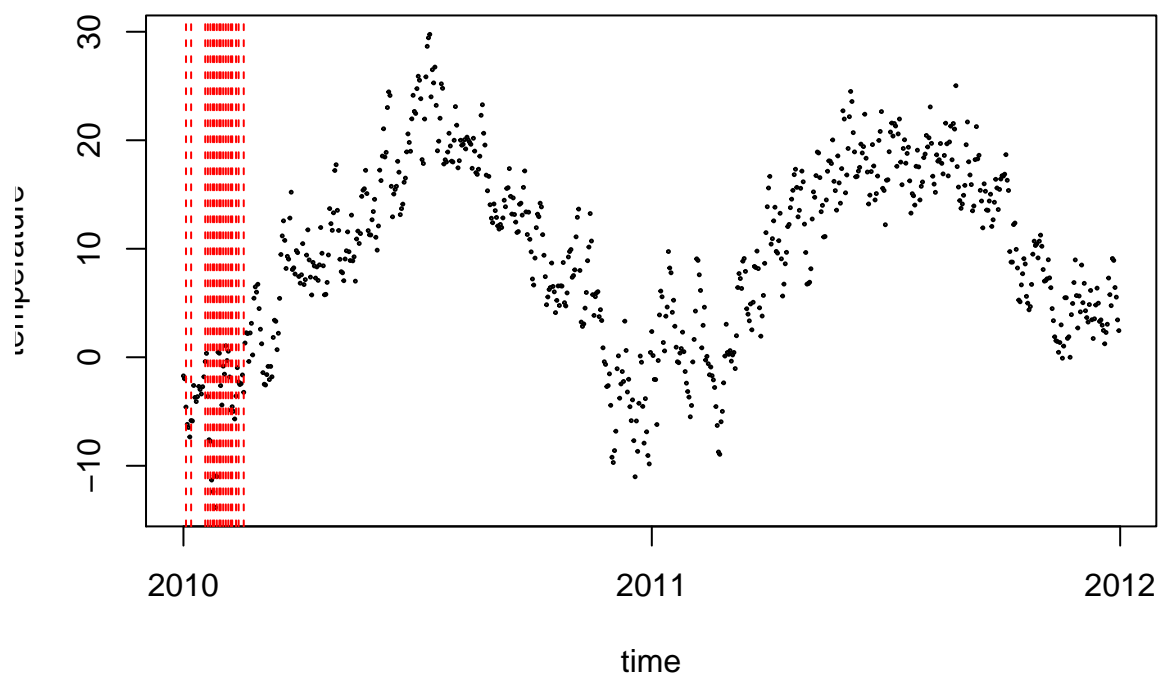


Figure 5.5: Berlin weather data segmented using an auto-penalized cost function

Table 5.5: *Results of the segmentation algorithm using an auto-penalized cost function*

Segment no.	First index	Last index
1	1	2
2	3	6
3	7	17
4	18	19
5	20	21
6	22	23
7	24	24
8	25	26
9	27	28
10	29	29
11	30	31
12	32	33
13	34	35
14	36	37
15	38	38
16	39	41
17	42	43
18	44	47
19	48	730

Table 5.6: *Results of the segmentation algorithm using an adjusted penalized cost function*

Segment no.	First index	Last index
1	1	237
2	238	453
3	454	730

5.5 found by the new penalized cost, though it's also over segmenting some downward trends. It suggests the `big_segment_penalty` argument needs to be decreased to allow for larger segments to be estimated by the solution. So, by decreasing it's value, from the default of 10, down to 2, we run the results again with the `segment()` function. The results can be seen in 5.6, and it's possible for the segments with the weather data in Figure 5.6.

Though we got a reduced number of segments in the new adjusted `penalized_cost`, the segments seen in Figure 5.6 still aren't similar to what we are looking for as shown in Figure 5.2. The reason behind this, as discussed earlier, is due to the incorrect assumption the data is hierarchical. So, to segment the data ideally, it's necessary to evaluate all of the possibilities.

The exact algorithm does precisely compute all of the possibilities, but its $O(n^2)$ time complexity is quite prohibitive to run the computation on the entire data set. So we can make the computation tolerable by reducing the granularity of the data, getting the monthly averages for each of the measurement stations.

5.4 Reducing granularity

The data set needs to be resampled to represent the monthly weather averages. It is done by computing the average temperature for each combination of the month and weather station. With

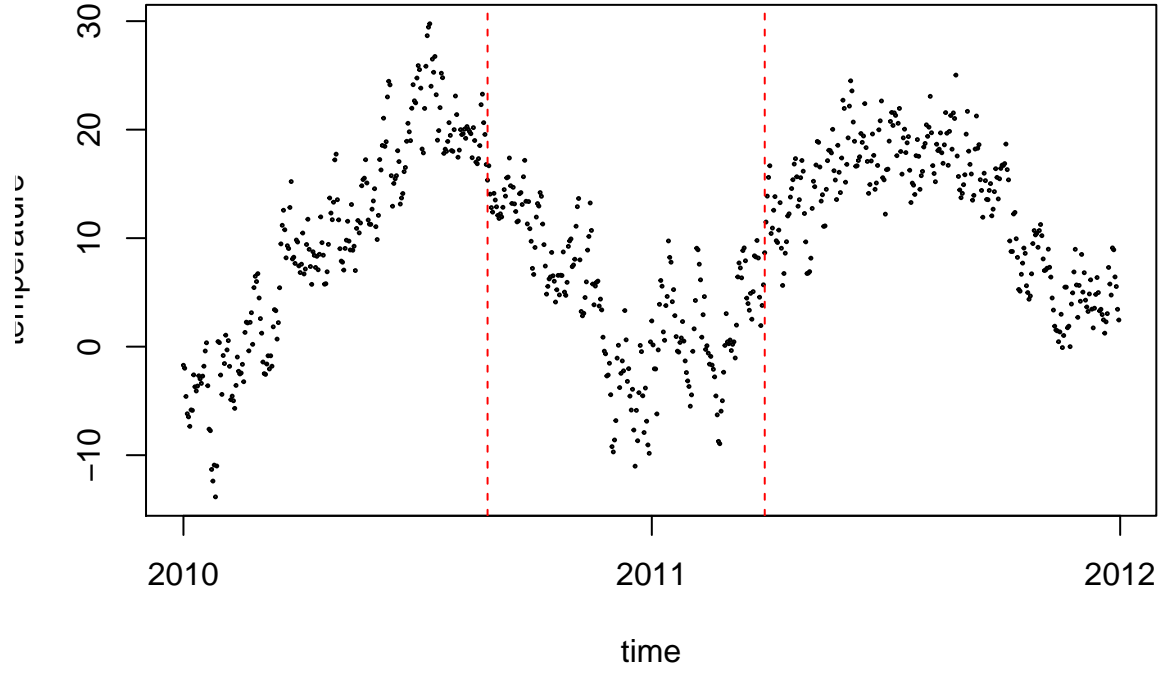


Figure 5.6: Berlin weather data segmented using an adjusted penalized cost function

Table 5.7: Results of the segmentation algorithm using an auto-penalized cost function over downsampled berlin data

Segment no.	First index	Last index
1	1	6
2	7	11
3	12	18
4	19	24

the granularity reduction, the data set will have 24 columns, one for each month in the two years comprehended. The plot of the monthly average temperature of the temperatures of all the data points is plotted in figure 5.7

A new `penalized_cost` function is then built and applied to the monthly data set using `segment()`, with the results being shown in Table 5.7, and with we also plot it with weather data in Figure 5.8.

To make the solution comparison clearer, it's possible to rescale the exact solution to the monthly sampled dataset to the daily sampled dataset by applying a linear transformation of multiplying all the change points for the number of columns in the daily dataset and dividing it by the number of columns in the monthly dataset, i.e. each rescaled change point C_i relates to the original change point c_i as described in equation (5.4), in which i is the index of each change point estimated with the monthly data set, N_M represents the number of columns in the monthly Berlin weather data set and N_B represents the number of columns in the daily Berlin data set, in the original form provided by the `segmentr` package.

$$C_i = \left\lceil c_i \frac{N_B}{N_M} \right\rceil \quad (5.4)$$

After applying that transformation, the results can be seen in Table 5.8, as well as the plot

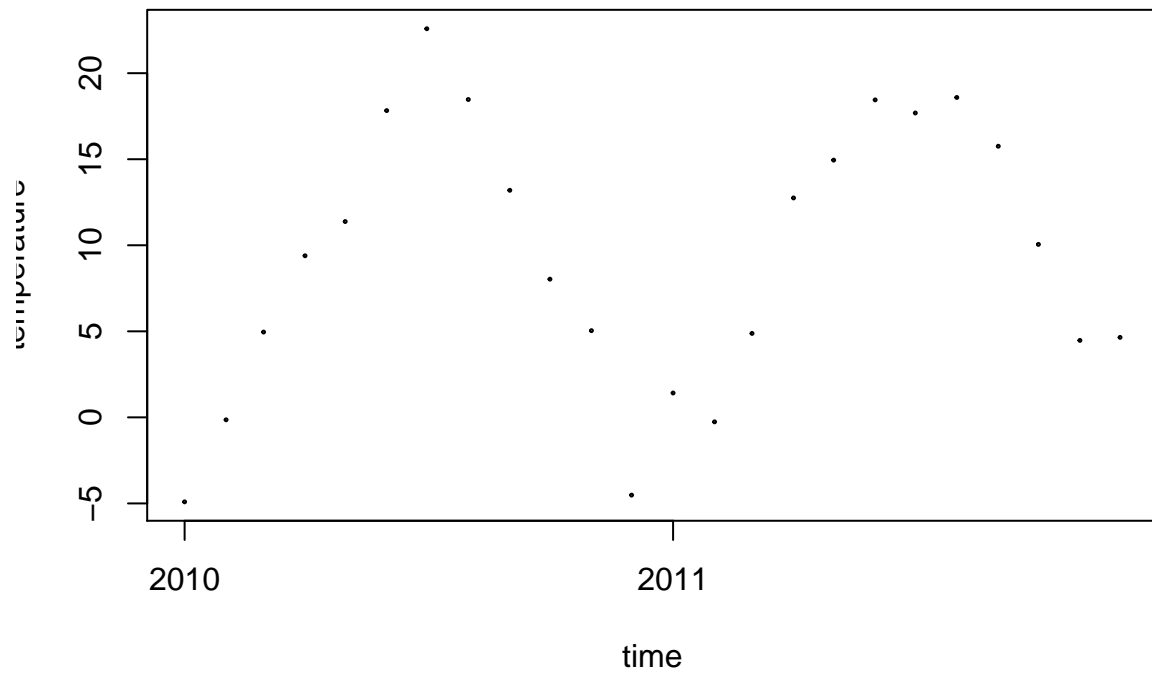


Figure 5.7: *Average monthly temperature over time as measured by different stations in Berlin*

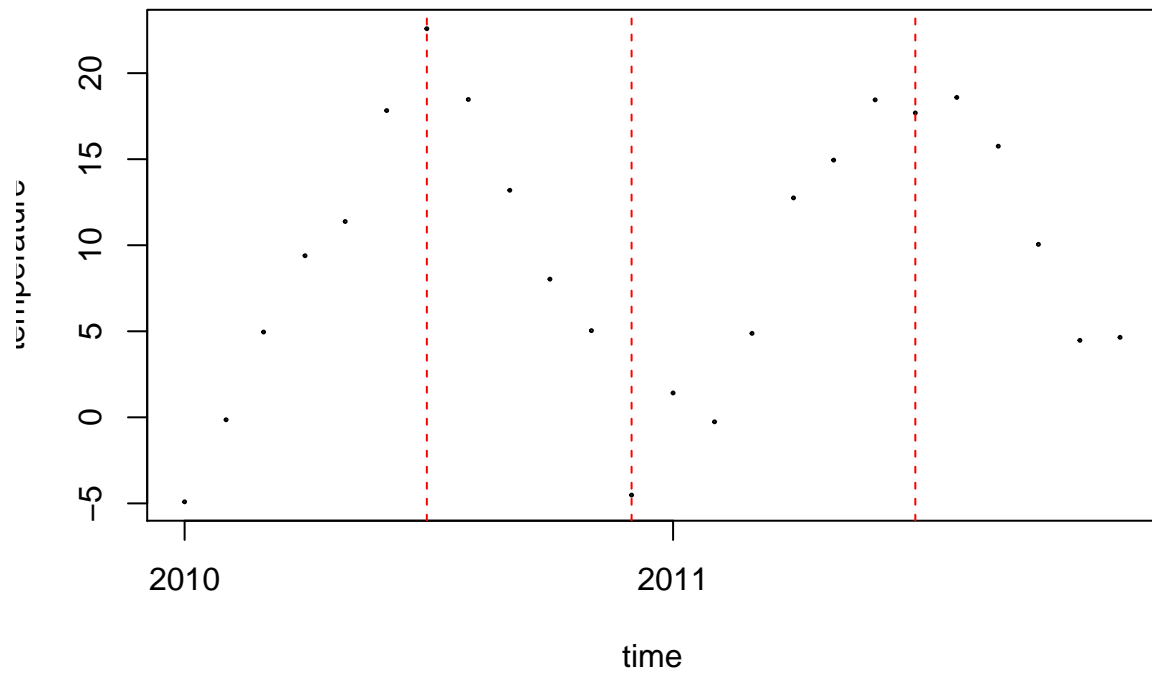


Figure 5.8: *Downsampled Berlin monthly weather data segmented using an auto penalized cost function*

Table 5.8: Results of the segmentation algorithm using an auto-penalized cost function over downsampled berlin data, but rescaled to fit the original data dimensions

Segment no.	First index	Last index
1	1	212
2	213	364
3	365	577
4	578	730

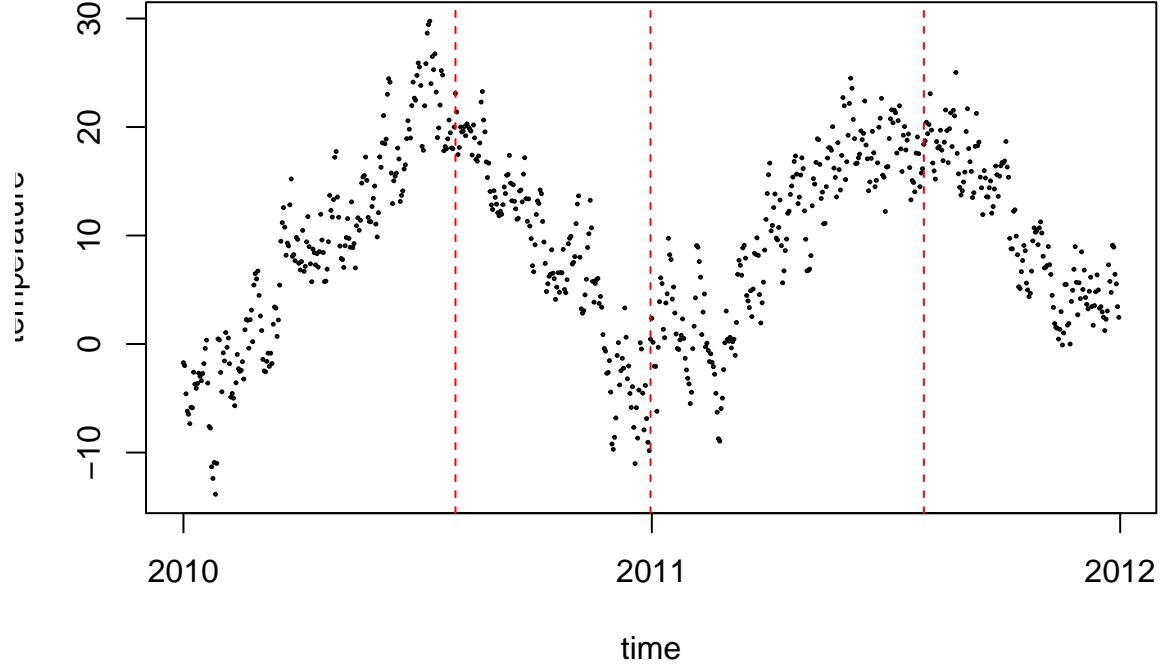


Figure 5.9: Rescaled segments estimated for a downsampled monthly weather data of the Berlin data set using an auto penalized cost function

along with the daily graph in Figure 5.9

With the exact solution, made possible with the granularity reduction, we noticed the data set is segmented closer to what the ideal solution would be, as the algorithm is able to evaluate all of the possibilities.

5.5 Accuracy of estimates for the Berlin dataset

In this chapter, the data set of weather temperatures in Berlin was presented, and there was a walkthrough on different ways to use `segmentr` to find a good estimate set of segments for it. Table 5.2 lists the considered solution considered ideal to the problem, at the same time as different solutions were found in Tables 5.4, 5.5 and 5.7. Considering this, the Hausdorff distance can be used to measure how far each estimate is from the ideal solution described in Table 5.2. In Table 5.9 we can see the results of the comparison, in which we can see the distance of each estimate calculated.

In Table 5.9 we can see the distance to the ideal is gradually decreased more adequate parameters are used to compute the segment estimates for the segmentation estimate. This improvement reflects the progress that can be observed in gradually in Figures 5.3, 5.5, 5.6 and 5.9.

Table 5.9: *Hausdorff distance for different segmentation attempts over the Berlin weather data set*

Results referenced	Estimated Changepoints	Hausdorff Distance to Ideal
Table 5.2	200, 360, 570	0
Table 5.4	3, 7, 18, 20, 22, 24, 25, 27, 29, 30, 32, 34, 36, 38, 39, 42, 44, 48	522
Table 5.5	3, 7, 18, 20, 22, 24, 25, 27, 29, 30, 32, 34, 36, 38, 39, 42, 44, 48	522
Table 5.6	238, 454	116
Table 5.8	213, 365, 578	13

Table 5.10: *Sample values of the R-squared cost function for different sizes of segment candidates*

Small Size	Medium Size	Large Size
-0.982116	-0.7601494	-0.0328304

5.6 A non-usual cost function

Notice the only requirement on the cost function is for it to be able to rank segments in a desired manner. Therefore, there's freedom to pick a non-conventional cost function. For example, the R-squared statistic of the linear regression in each segment is conventionally used to infer how well the linear model fits the points in the data. It ranges from zero to one and the closer it is to one, the better it predicts the points in the data. Therefore, we propose the implementation of a `rsquared_cost`, which fits a linear regression against the data set received as input in the function and then returns the opposite R-squared statistic as the “cost” value of the segment. The defined function is applied against different segment sizes of the `berlin` data set, analogous to Table 5.3, and the results are shown in 5.10.

From what is observed in Table 5.10, and similar to the previous case, the new `rsquared_cost` has the lowest values for small segments. Therefore, it needs to be penalized with the `auto_penalize` function. We then go on and apply the results of the penalized function and show them in Table 5.11. The plot with the weather data can be seen in Figure 5.10.

The default penalized `rsquared_cost` split the data set in three segments, roughly the same size each. It makes sense because the penalty applied by the default `auto_penalize` function has the lowest penalty for segments of sizes closer to about half the total length. So, increasing the `big_penalty_segment` argument will not affect solution estimation anymore. In contrast, smaller segments are being over penalized. Because of this, it's necessary to reduce the `small_segment_penalty` segment, which we decrease to 1.5, from the default of 10. The results of the new segmentation can be seen in Table 5.12, and the plot in Figure 5.11.

With the adjusted parameters, we see the `rsquared_penalized` was able to segment the data in Figure 5.11 in a seemingly accurate manner, despite the nature of the hierarchical algorithm. As discussed previously, we point the hierarchical algorithm is not adequate for the squared residual cost, as the grouping of neighboring segments under a macro-segment, an intermediate segment state under the hierarchical algorithm, has an unattractive cost value, due to the presence of alternating trends. Because of this, the macro-segment is never picked by the algorithm during the computation process, and so the ideal change points are never picked at their ideal positions. To see it more clearly, take the first 547 data points of the Berlin data set, roughly one year and a half. The results of the

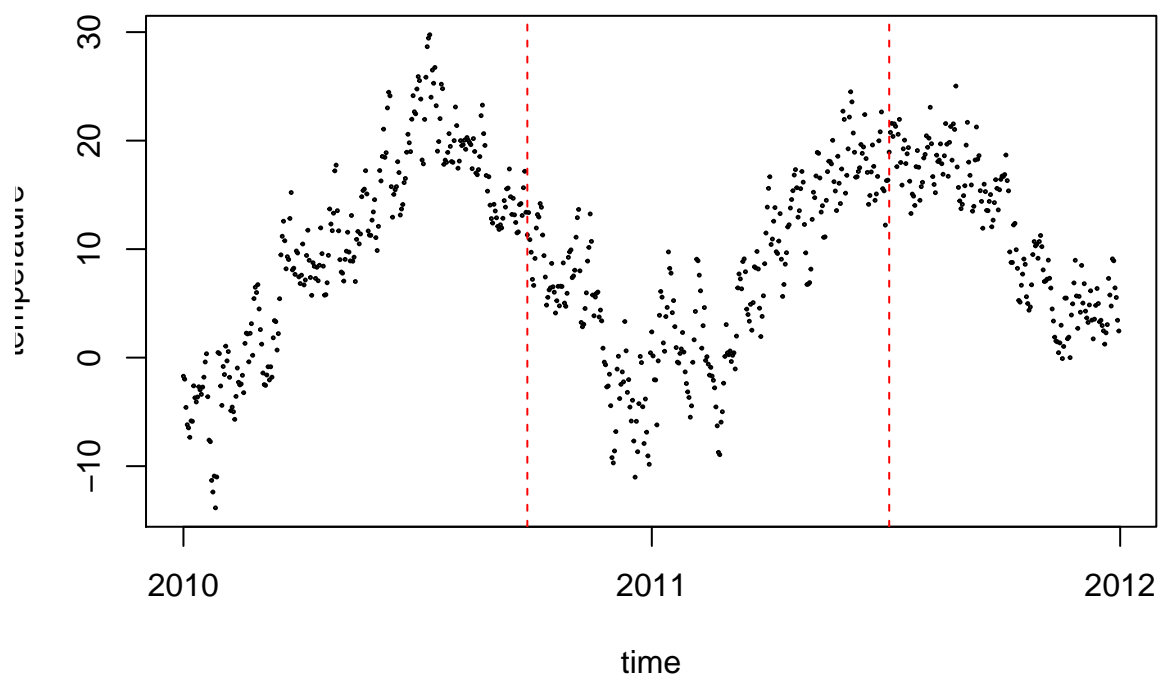


Figure 5.10: *Berlin daily weather data segmented using an auto-penalized R -squared cost function*

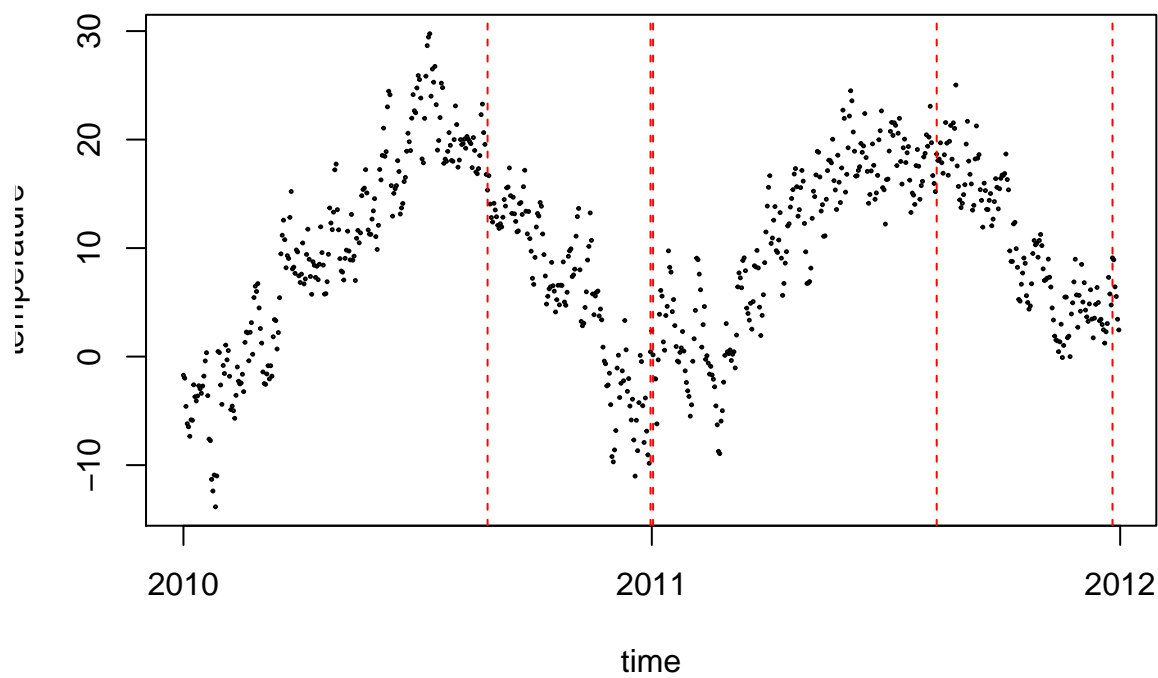


Figure 5.11: *Berlin daily weather data segmented using an adjusted penalized R -squared cost function*

Table 5.11: *Results of the segmentation algorithm using an auto-penalized R -squared cost function over Berlin data*

Segment no.	First index	Last index
1	1	268
2	269	550
3	551	730

Table 5.12: *Results of the segmentation algorithm using an adjusted penalized R -squared cost function over Berlin data*

Segment no.	First index	Last index
1	1	237
2	238	364
3	365	366
4	367	587
5	588	724
6	725	730

segmentation with that portion of the `berlin` data set can be seen in Table 5.13, and the plot can be seen in Figure 5.12.

In Figure 5.12, we can see the segments do not match our expectations, as the algorithm is not able to bisect a macro-segment before finding the ideal segments in the next algorithm iteration.

Table 5.13: Results of the segmentation algorithm using an auto-penalized R -squared cost function over a subset of Berlin data

Segment no.	First index	Last index
1	1	178
2	179	282
3	283	547

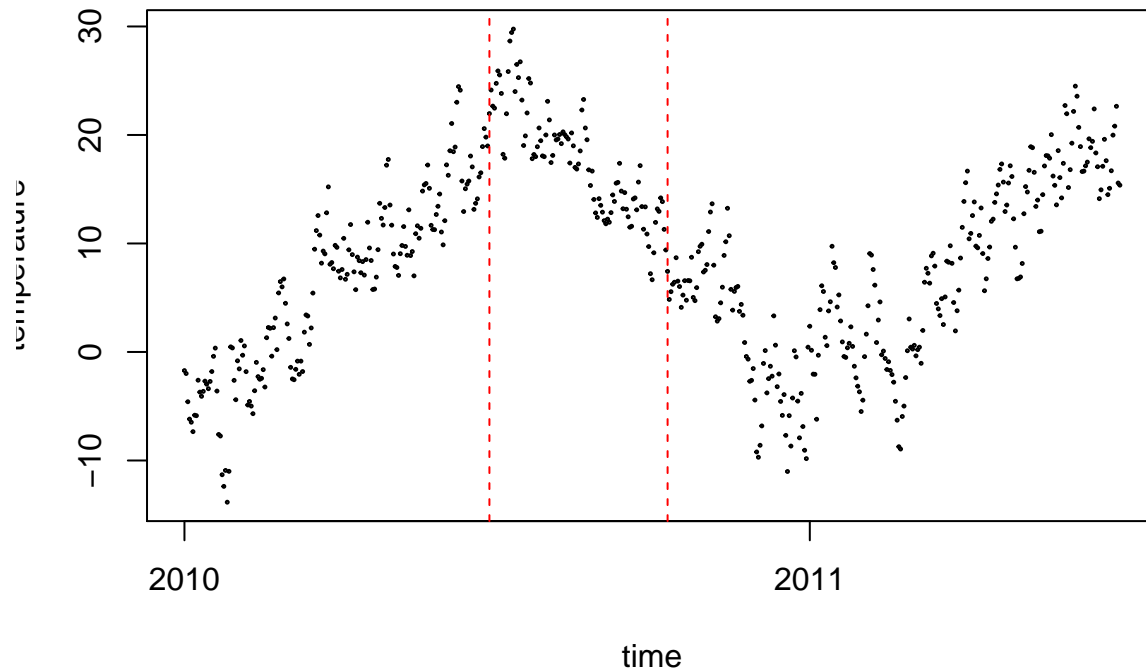


Figure 5.12: Subset of Berlin daily weather data segmented using an auto-penalized R -squared cost function

Chapter 6

Considerations on performance

This code shows a handful of attempts that were made in actually trying to execution time of the algorithms implemented by the package.

6.1 Benchmark the code

The package `microbenchmark` allows us to execute the code and compare different run-times. Therefore it's going to be used in this package to compare the performance of different code snippets.

6.2 Native Code

In the algorithms chapter, we discussed the time complexity of the different types of algorithms. In that scenario, the most relevant variable is the number of columns in the data set, which dictates whether the computation of the exact algorithm will be prohibitive or not. However, the number of samples does influence the computation time linearly. Given the most performed operation in any of the algorithms described in the chapter is the cost function, it's, in essence, the bottleneck of the whole computation. Therefore, real performance gains can be obtained depending on the performance of the application.

In R statistical programming, it's commonplace to use the functions provided by the programming environment, which are usually performant algorithms implemented in compiled programming languages such as C. However, there are times the programmer must implement a custom function in R, which in turn is a dynamically, and typically slower execution environment.

Therefore, in a first attempt to make the code execution run faster, and compare different results, `segmentr` implements the `[multivariate()]` likelihood function (used to calculate the cost) in compiled C++ programming language, as well as it implements `[r_multivariate()]` which implements the same algorithm in the R programming environment.

In the scenario above, we notice performance improvements in the native `[multivariate()]` function, with the biggest performance improvement taking place in the `exact` algorithm results. Therefore, whenever the resources are available, it's recommended to implement the cost function (or portions of it) directly in a native programming language such as C++. We recommend the `Rcpp` package, which makes it easy to implement functions that interface easily with the R programming environment.

Table 6.1: *Execution time comparison between native C++ and interpreted R code*

expr	time (ms)
segment(data, cost = function(x) -r_multivariate(x), algorithm = "exact")	50089.348
segment(data, cost = function(x) -multivariate(x), algorithm = "hierarchical")	30.187
segment(data, cost = function(x) -r_multivariate(x), algorithm = "hierarchical")	83.770
segment(data, cost = function(x) -multivariate(x), algorithm = "exact")	7241.269

Table 6.2: *Execution time comparison between parallel and single-threaded computation with a data set of 100 samples and 10 columns*

expr	time (ms)
segment(data, cost = function(x) -multivariate(x), algorithm = "hierarchical", allow_parallel = TRUE)	34.924
segment(data, cost = function(x) -multivariate(x), algorithm = "hierarchical", allow_parallel = FALSE)	19.859
segment(data, cost = function(x) -multivariate(x), algorithm = "exact", allow_parallel = TRUE)	261.536
segment(data, cost = function(x) -multivariate(x), algorithm = "exact", allow_parallel = FALSE)	145.575

6.3 Parallelization

Given the increasing trend of parallel programming in the past few years, it's natural to try to take advantage of that by parallelizing the algorithm execution. In the algorithms implemented in this paper, parallelization is a bit complicated because a lot of the execution steps in the algorithm iterations depend on values computed in previous steps, and the golden rule of parallel computing is that faster results are generally obtained when computation steps are independent from one another, i.e. no dependency between the task, hence they can be performed in parallel. Yet, there are a few steps of the computation that can be performed in parallel, and its parallelization was implemented with the help of the `foreach` package.

Therefore, whether or not the computation will be performed depends on whether there is a parallel cluster registered in the R session with packages such as `doMC`, and whether the `allow_parallel` argument is true or false. With that in mind, a few comparisons are evaluated.

Analyzing the results above, we notice good improvements, especially for the “exact” algorithm. However, in a situation in which the number of rows isn't very large in comparison with the number of columns, the results of the parallel computation are a lot more modest. Consider the following case.

In the result above, parallelization achieved the opposite effect, actually making the computation slower, as there is now a lot of work done synchronizing necessary information between all the processes in the cluster. That takes more time than is saved by running the algorithm in parallel.

Taking all of that into consideration, the decision of whether or not to use parallelization relies on the user after evaluating the nature of the data set. For data sets with few samples and many columns, parallelization is not recommended. In the case there are lots of samples, parallelization

Table 6.3: *Execution time comparison between parallel and single-threaded computation with a data set of 5 samples and 100 columns*

expr	time (ms)
segment(data, cost = function(x) -multivariate(x), algorithm = "exact", allow_parallel = FALSE)	5892.208
segment(data, cost = function(x) -multivariate(x), algorithm = "hierarchical", allow_parallel = TRUE)	39.549
segment(data, cost = function(x) -multivariate(x), algorithm = "exact", allow_parallel = TRUE)	6329.687
segment(data, cost = function(x) -multivariate(x), algorithm = "hierarchical", allow_parallel = FALSE)	49.665

might give better computation times.

An alternative not developed in this project would be to use a genetic algorithm approach to the optimal set estimation, which is a probabilistic process that converges to the result after enough computation time has passed. The main advantage of such a method is that computations can be more easily parallelized. Such development might be explored in future developments in this package.

Chapter 7

Conclusion

This work describes the segmentation problem, provides a theoretical model to work with the segmentation of data, and goes on to describe a few algorithms to try to estimate the set of points that optimally segment a given data set, explaining the differences between them.

Then we proceed and describe the actual implementation of such algorithms in an actual R package, in an attempt to make its use easier for researchers. We provide a few applications with simulated data, and also provide a real analysis with a real weather data set. Finally, performance considerations are taken into consideration when trying to have the code run faster.

In summary, there are a lot of decisions involved in the problem of segmentation, such as picking the right cost function for the evaluation, which algorithm to pick, and whether or not parallelization can help in running the computation faster. By providing a common set of tools, we hope to make the life of the researcher easier.

Appendix A

Package Usage

The purpose of this work is to have the `segmentr` to be as accessible as possible. Because of that, extra care was put into making it easy to install and use.

A.1 Installation

Given the algorithms and their applications discussed in [Castro *et al.*, 2018], the `segmentr` package for R is proposed to help researchers segment their data sets. Installation can be done using the default `install.packages` command, as shown below.

```
install.packages("segmentr")
```

A.2 Usage

The package can be used with `[segment()]`. It takes a `data` argument containing a bi-dimensional matrix in which the rows represent different samples and the columns represent the comprehension of the data set we wish to segment. The function also accepts an `algorithm` argument, which can be `exact`, `hierarchical` or `hybrid`, that specifies the type of algorithm will be used when exploring the data set. Finally, it's also necessary to specify a `cost` function as an argument, as it is used to compare and pick segments that are better fit according to the given cost's chosen criteria.

```
library("segmentr")

data <- rbind(
  c(1, 1, 0, 0, 0, 1023, 134521, 12324),
  c(1, 1, 0, 0, 0, -20941, 1423, 14334),
  c(1, 1, 0, 0, 0, 2398439, 1254, 146324),
  c(1, 1, 0, 0, 0, 24134, 1, 15323),
  c(1, 1, 0, 0, 0, -231, 1256, 13445),
  c(1, 1, 0, 0, 0, 10000, 1121, 331)
)
```

```
segment (  
  data,  
  algorithm = "exact",  
  cost = function(X) -multivariate(X) + 0.01*exp(ncol(X))  
)
```

```
## Segments (total of 6):  
##  
## 1:1  
## 2:2  
## 3:3  
## 4:4  
## 5:5  
## 6:8
```

Also, a vignette version of Chapter 5 is provided, and the user of the package can open it directly in R with embedded code examples and follow along with the analysis of the data set.

Appendix B

Support Code

```
library(knitr)
library(kableExtra)
library(segmentr)
library(tibble)
library(magrittr)
library(purrr)
knitr::opts_chunk$set(
  cache=TRUE,
  echo=FALSE
)
source("helper.R")
n <- 100
N1 <- sample(1:2, n, replace = TRUE)
N2 <- sample(1:2, n, replace = TRUE)
N3 <- sample(1:2, n, replace = TRUE)
N4 <- sample(1:2, n, replace = TRUE)
N5 <- sample(1:2, n, replace = TRUE)
N6 <- sample(1:2, n, replace = TRUE)

X1 <- N1
X2 <- N1 - N2
X3 <- N2
X4 <- N1 + N2
X5 <- N1
X6 <- N3
X7 <- N3 - N4
X8 <- N4
X9 <- N3 + N4
X10 <- N3
X11 <- N5
X12 <- N5 - N6
```

```

X13 <- N6
X14 <- N5 + N6
X15 <- N5
D_example <- cbind(X1, X2, X3, X4, X5, X6, X7, X8,
                  X9, X10, X11, X12, X13, X14, X15)
head(D_example) %>%
  kable(caption="Sample values of the correlated random
           variables defined in (4.1).")
multivariate_cost = function(X) -multivariate(X) + 2 ^ ncol(X)

results_multivariate_penalized <- segment(
  D_example,
  cost = multivariate_cost,
  algorithm = "exact"
)

print_results_table(
  results_multivariate_penalized,
  caption="Segment tables as defined in
(4.1).")
)
segment(D_example,
  cost = function(X) -multivariate(X),
  algorithm = "exact") %>%
  print_results_table(
    caption="Results of segmentation using a non-penalized
            multivariate cost")
heterogeneity_cost <- function(X) {
  mean_value <- mean(X, na.rm = T)
  if (is.na(mean_value)) {
    0
  } else {
    sum((X - mean_value)^2)
  }
}

penalized_heterogeneity_cost <- function(X) heterogeneity_cost(X) + 1

make_segment <- function(n, p) {
  matrix(rbinom(100 * n, 1, p), nrow = 100)
}

D_genetic <- cbind(

```

```

    make_segment(5, 0.9),
    make_segment(10, 0.1),
    make_segment(5, 0.9)
)

segment(
  D_genetic,
  cost = penalized_heterogeneity_cost,
  algorithm = "hierarchical"
) %>%
  print_results_table(
    caption="Results of segmentation by applying the
            cost function defined in
            (4.5) to a sample of size
            10 of the model defined in (4.6).
            ")
expected_multivariate_example <- c(6, 11)

deviation <- partial(
  segment_distance,
  changepoints2=expected_multivariate_example
)

exact_multivariate_changepoints <- segment(
  D_example,
  cost = multivariate_cost,
  algorithm = "exact"
)$changepoints

hierarchical_multivariate_changepoints <- segment(
  D_example,
  cost = multivariate_cost,
  algorithm = "hierarchical"
)$changepoints

hybrid_multivariate_changepoints <- segment(
  D_example,
  cost = multivariate_cost,
  algorithm = "hybrid"
)$changepoints

hybrid_multivariate_changepoints_threshold <- segment(
  D_example,

```

```

    cost = multivariate_cost,
    algorithm = "hybrid",
    threshold = 4
) $changepoints

tribble(
  ~`Description`,
  ~`Changepoints`,
  ~`Hausdorff Distance`,
  "Expected solution",
  comma_format(expected_multivariate_example),
  deviation(expected_multivariate_example),
  "Exact algorithm estimate",
  comma_format(exact_multivariate_changepoints),
  deviation(exact_multivariate_changepoints),
  "Hierarchical algorithm estimate",
  comma_format(hieralg_multivariate_changepoints),
  deviation(hieralg_multivariate_changepoints),
  "Hybrid algorithm estimate with threshold 50",
  comma_format(hybrid_multivariate_changepoints),
  deviation(hybrid_multivariate_changepoints),
  "Hybrid algorithm estimate with threshold 4",
  comma_format(hybrid_multivariate_changepoints_threshold),
  deviation(hybrid_multivariate_changepoints_threshold)
) %>%
  kable(caption="Comparison of solutions of different algorithms
to segment the data set described in (4.1),
measuring how far each solution is from the ideal
solution using the Hausdorff distance.")
expected_mean_example <- c(6, 16)

deviation <- partial(
  segment_distance,
  changepoints2=expected_mean_example
)

exact_mean_changepoints <- segment(
  D_genetic,
  cost = penalized_heterogeneity_cost,
  algorithm = "exact"
) $changepoints

hieralg_mean_changepoints <- segment(

```



```

D_genetic,
cost = penalized_heterogeneity_cost,
algorithm = "hierarchical"
)$changepoints

hybrid_mean_changepoints <- segment(
  D_genetic,
  cost = penalized_heterogeneity_cost,
  algorithm = "hybrid"
)$changepoints

hybrid_mean_changepoints_threshold <- segment(
  D_genetic,
  cost = penalized_heterogeneity_cost,
  algorithm = "hybrid",
  threshold = 4
)$changepoints

tribble(
  ~`Description`,
  ~`Changepoints`,
  ~`Hausdorff Distance`,
  "Expected solution",
  comma_format(expected_mean_example),
  deviation(expected_mean_example),
  "Exact algorithm estimate",
  comma_format(exact_mean_changepoints),
  deviation(exact_mean_changepoints),
  "Hierarchical algorithm estimate",
  comma_format(hieralg_mean_changepoints),
  deviation(hieralg_mean_changepoints),
  "Hybrid algorithm estimate with threshold 50",
  comma_format(hybrid_mean_changepoints),
  deviation(hybrid_mean_changepoints),
  "Hybrid algorithm estimate with threshold 4",
  comma_format(hybrid_mean_changepoints_threshold),
  deviation(hybrid_mean_changepoints_threshold)
) %>%
  kable(caption="Comparison of solutions of different algorithms
to segment the data set described in (4.6),
measuring how far each solution is from the ideal
solution using the Hausdorff distance.")
library(segmentr)

```

```

library(tidyr)
library(tibble)
library(dplyr)
library(lubridate)
library(magrittr)
library(purrr)
library(knitr)
library(kableExtra)
data(berlin)
as_tibble(berlin, rownames="station") %>%
  mutate(`..`="..") %>%
  select(station, `2010-01-01`:`2010-01-03`,
          `..`, `2011-12-29`:`2011-12-31`) %>%
  kable(caption="
    First and last columns of the `berlin` dataset
  ") %>%
  column_spec(1, width="5em")
berlin %>%
  colMeans() %>%
  enframe("time", "temperature") %>%
  mutate_at(vars(time), ymd) %>%
  with(plot(time, temperature, cex=0.2))
expected_berlin <- list(
  changepoints=c(200, 360, 570),
  segments=list(1:199, 360:569, 570:ncol(berlin))
)

plot_results(expected_berlin, berlin)
print_results_table(
  expected_berlin,
  caption="Expected values to be found when segmenting
    the Berlin dataset"
)

residual_cost <- function (data) {
  fit <- t(data) %>%
    as_tibble() %>%
    rowid_to_column() %>%
    gather(station, temperature, -rowid) %>%
    with(lm(temperature ~ rowid))

  mean(fit$residuals ^ 2)
}

```

```

tibble(
  `Small Size` = residual_cost(berlin[, 2:3]),
  `Medium Size` = residual_cost(berlin[, 1:150]),
  `Large Size` = residual_cost(berlin)
) %>%
  kable(
    caption="Sample values of the squared residual cost
    function for different sizes of segment
    candidates"
  )
results_non_penalized <- segment(
  berlin,
  cost = residual_cost,
  algorithm = "hierarchical"
)

print_results_table(
  results_non_penalized,
  caption="Results of the segmentation algorithm
  using a non-penalized cost function"
)

plot_results(results_non_penalized, berlin)

plot_curve(~ exp(0.3*(. - 50)) + exp(0.3 * (-. + 50)),
  from = 0, to = 100, type="l")
penalized_cost <- auto_penalize(berlin,
  cost = residual_cost)
results_auto_penalized <- segment(
  berlin,
  cost = residual_cost,
  algorithm = "hierarchical"
)

print_results_table(
  results_auto_penalized,
  caption="Results of the segmentation algorithm
  using an auto-penalized cost function"
)

plot_results(results_auto_penalized, berlin)
penalized_cost <- auto_penalize(
  berlin,
  cost = residual_cost,
  big_segment_penalty = 2

```

```

)
results_adjusted_penalized <- segment(
  berlin,
  cost = penalized_cost,
  algorithm = "hierarchical"
)
print_results_table(
  results_adjusted_penalized,
  caption="Results of the segmentation algorithm
using an adjusted penalized cost function"
)
plot_results(results_adjusted_penalized, berlin)
monthly_berlin <- berlin %>%
  as_tibble(rownames = "station") %>%
  gather(time, temperature, -station) %>%
  mutate(month = floor_date(ymd(time), "month")) %>%
  group_by(station, month) %>%
  summarize(temperature = mean(temperature)) %>%
  spread(month, temperature) %>% {
    stations <- .$station
    result <- as.matrix(.[, -1])
    rownames(result) <- stations
    result
  }

monthly_berlin %>%
  colMeans() %>%
  enframe("time", "temperature") %>%
  mutate_at(vars(time), ymd) %>%
  with(plot(time, temperature, cex=0.2))
penalized_cost <- auto_penalize(
  monthly_berlin,
  cost = residual_cost,
  small_segment_penalty = 100
)

results_downscaled <- segment(
  monthly_berlin,
  cost = penalized_cost,
  algorithm = "exact"
)

print_results_table(

```

```

results_downscaled,
caption="Results of the segmentation algorithm
      using an auto-penalized cost function over
      downsampled berlin data"
)
plot_results(results_downscaled, monthly_berlin)
rescaled_changepoints <- round(
  results_downscaled$changepoints
  * ncol(berlin) / ncol(monthly_berlin)
)

results_rescaled <- with_segments(
  changepoints=rescaled_changepoints,
  len=ncol(berlin)
)

print_results_table(
  results_rescaled,
  caption="Results of the segmentation algorithm
        using an auto-penalized cost function over
        downsampled berlin data, but rescaled to fit the
        original data dimensions"
)
plot_results(results_rescaled, berlin)
deviation <- partial(
  segment_distance,
  changepoints2=expected_berlin$changepoints
)

tribble(
  ~`Results referenced`,
  ~`Estimated Changepoints`,
  ~`Hausdorff Distance to Ideal`,
  "Table 5.2",
  comma_format(expected_berlin$changepoints),
  deviation(expected_berlin$changepoints),
  "Table 5.4",
  comma_format(results_non_penalized$changepoints),
  deviation(results_non_penalized$changepoints),
  "Table 5.5",
  comma_format(results_auto_penalized$changepoints),
  deviation(results_auto_penalized$changepoints),
  "Table 5.6",

```

```

    comma_format(results_adjusted_penalized$changepts),
    deviation(results_adjusted_penalized$changepts),
    "Table 5.8",
    comma_format(results_rescaled$changepts),
    deviation(results_rescaled$changepts)
) %>% kable(
  caption="Hausdorff distance for different
  segmentation attempts over the Berlin weather data set"
) %>% column_spec(2, width="15em")
rsquared_cost <- function (data) {
  as_tibble(t(data)) %>%
    rowid_to_column() %>%
    gather(station, temperature, -rowid) %>%
    with(lm(temperature ~ rowid)) %>%
    summary %>%
    .$adj.r.squared %>%
    { -. }
}

tibble(
  `Small Size` = rsquared_cost(berlin[, 2:3]),
  `Medium Size` = rsquared_cost(berlin[, 1:150]),
  `Large Size` = rsquared_cost(berlin)
) %>%
  kable(
    caption="Sample values of the R-squared
    cost function for different sizes of segment
    candidates"
  )
penalized_cost <- auto_penalize(
  berlin,
  cost = rsquared_cost
)
results <- segment(
  berlin,
  cost = penalized_cost,
  algorithm = "hierarchical"
)

print_results_table(
  results,
  caption="Results of the segmentation algorithm
  using an auto-penalized R-squared cost function over

```

```

    Berlin data"
  )
  plot_results(results, berlin)
  penalized_cost <- auto_penalize(
    berlin,
    cost = rsquared_cost,
    small_segment_penalty = 1.5
  )
  results <- segment(
    berlin,
    cost = penalized_cost,
    algorithm = "hierarchical"
  )
  print_results_table(
    results,
    caption="Results of the segmentation algorithm
            using an adjusted penalized R-squared cost
            function over Berlin data"
  )
  plot_results(results, berlin)
  sub_berlin <- berlin[, 1:547]
  penalized_cost <- auto_penalize(
    sub_berlin,
    cost = rsquared_cost
  )
  results <- segment(
    sub_berlin,
    cost = penalized_cost,
    algorithm = "hierarchical"
  )
  print_results_table(
    results,
    caption="Results of the segmentation algorithm
            using an auto-penalized R-squared cost
            function over a subset of Berlin data"
  )
  plot_results(results, sub_berlin)
  source("helper.R")
  library(microbenchmark)
  data <- makeRandom(20, 100)

  bench <- microbenchmark(
    segment(data,

```

```

        cost = function(x) -multivariate(x),
        algorithm = "exact"),
  segment(data,
    cost = function(x) -r_multivariate(x),
    algorithm = "exact"),
  segment(data,
    cost = function(x) -multivariate(x),
    algorithm = "hierarchical"),
  segment(data,
    cost = function(x) -r_multivariate(x),
    algorithm = "hierarchical"),
  times = 1
)

print_benchmark(
  bench,
  caption="Execution time comparison
  between native C++ and interpreted R code"
)

data <- makeRandom(100, 10)
doMC::registerDoMC(4)
bench <- microbenchmark(
  segment(data,
    cost = function(x) -multivariate(x),
    algorithm = "exact",
    allow_parallel = FALSE),
  segment(data,
    cost = function(x) -multivariate(x),
    algorithm = "exact",
    allow_parallel = TRUE),
  segment(data,
    cost = function(x) -multivariate(x),
    algorithm = "hierarchical",
    allow_parallel = FALSE),
  segment(data,
    cost = function(x) -multivariate(x),
    algorithm = "hierarchical",
    allow_parallel = TRUE),
  times = 1
)

print_benchmark(
  bench,
  caption="Execution time comparison

```



```

    between parallel and single-threaded computation
    with a data set of 100 samples and 10 columns"
)
data <- makeRandom(5, 100)
doMC::registerDoMC(4)
bench <- microbenchmark(
  segment(data,
    cost = function(x) -multivariate(x),
    algorithm = "exact",
    allow_parallel = FALSE),
  segment(data,
    cost = function(x) -multivariate(x),
    algorithm = "exact",
    allow_parallel = TRUE),
  segment(data,
    cost = function(x) -multivariate(x),
    algorithm = "hierarchical",
    allow_parallel = FALSE),
  segment(data,
    cost = function(x) -multivariate(x),
    algorithm = "hierarchical",
    allow_parallel = TRUE),
  times = 1
)

print_benchmark(
  bench,
  caption="Execution time comparison
  between parallel and single-threaded computation
  with a data set of 5 samples and 100 columns"
)
install.packages("segmentr")
library("segmentr")

data <- rbind(
  c(1, 1, 0, 0, 0, 1023, 134521, 12324),
  c(1, 1, 0, 0, 0, -20941, 1423, 14334),
  c(1, 1, 0, 0, 0, 2398439, 1254, 146324),
  c(1, 1, 0, 0, 0, 24134, 1, 15323),
  c(1, 1, 0, 0, 0, -231, 1256, 13445),
  c(1, 1, 0, 0, 0, 10000, 1121, 331)
)

```

```
segment (  
  data,  
  algorithm = "exact",  
  cost = function(X) -multivariate(X) + 0.01*exp(ncol(X))  
)  
vignette("segmentr")
```

Bibliography

- Castro et al.(2018)** Bruno M. Castro, Renan B. Lemes, Jonatas Cesar, Tábita Hünemeier e Florencia Leonardi. A model selection approach for multiple sequence segmentation and dimensionality reduction. *Journal of Multivariate Analysis*, 167:319 – 330. ISSN 0047-259X. doi: <https://doi.org/10.1016/j.jmva.2018.05.006>. URL <http://www.sciencedirect.com/science/article/pii/S0047259X18302331>. Citado na página.
- Ceballos et al.(2018)** Francisco Ceballos, Peter Joshi, David W. Clark, Michèle Ramsay e James F. Wilson. Runs of homozygosity: Windows into population history and trait architecture. *Nature Reviews Genetics*, 19. doi: 10.1038/nrg.2017.109. Citado na página.
- Eddelbuettel e François(2011)** Dirk Eddelbuettel e Romain François. Rcpp: Seamless R and C++ integration. *Journal of Statistical Software*, 40(8):1–18. doi: 10.18637/jss.v040.i08. URL <http://www.jstatsoft.org/v40/i08/>. Citado na página.
- Maidstone et al.(2017)** Robert Maidstone, Toby Hocking, Guillem Rigai e Paul Fearnhead. On optimal multiple changepoint algorithms for large data. *Statistics and Computing*, 27(2): 519–533. ISSN 1573-1375. doi: 10.1007/s11222-016-9636-3. URL <https://doi.org/10.1007/s11222-016-9636-3>. Citado na página.
- Mello(2019)** Thales Mello. Segmentr: An r package to segment data with minimal total cost (aka change points). <https://github.com/thalesmello/segmentr>, 2019. Citado na página.
- Mello e Leonardi(2019)** Thales Mello e Florencia Leonardi. *segmentr: Segment Data Minimizing a Cost Function*, 2019. URL <https://CRAN.R-project.org/package=segmentr>. R package version 0.1.1. Citado na página.
- Munkres(2000)** J.R. Munkres. *Topology*. Featured Titles for Topology Series. Prentice Hall, Incorporated. ISBN 9780131816299. URL <https://books.google.com.br/books?id=XjoZAAIAIAAJ>. Citado na página.
- Park(2017)** K.I. Park. *Fundamentals of Probability and Stochastic Processes with Applications to Communications*. Springer International Publishing. ISBN 9783319680743. URL <https://books.google.com.br/books?id=cd2SswEACAAJ>. Citado na página.
- R Core Team(2018)** R Core Team. R: A language and environment for statistical computing, 2018. URL <https://www.R-project.org/>. Citado na página.
- Wetterdienst(2019)** Deutscher Wetterdienst. Climate data center - ftp server. https://www.dwd.de/EN/climate_environment/cdc/cdc.html, 2019. Citado na página.
- Wickham(2015)** Hadley Wickham. *R Packages*. O'Reilly Media, Inc., 1st edição. ISBN 1491910593, 9781491910597. URL <http://r-pkgs.had.co.nz/>. Citado na página.