

Spatio-Temporal Forecasts for Bike Availability in Dockless Bike Sharing Systems

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Lucas van der Meer

✉ luukvandermeer@live.nl

⌚ <https://github.com/luukvdmeer>

Supervised by:

Edzer Pebesma

Institute for Geoinformatics

University of Münster

Co-supervised by:

Jorge Mateu

Department of Mathematics

Universidade Jaume I

Co-supervised by:

Joel Silva

Information Management School

Universidade Nova de Lisboa



ifgi
Institut für Geoinformatik
Universität Münster



Declaration of Academic Integrity

I hereby confirm that this thesis on *Spatio-Temporal Forecasts for Bike Availability in Dockless Bike Sharing Systems* is solely my own work and that I have used no sources or aids other than the ones stated.

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I agree to have my thesis checked in order to rule out potential similarities with other works and to have my thesis stored in a database for this purpose.

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List of Acronyms

ACF	Autocorrelation Function
AIC	Aikake's Information Criterion
AR	Autoregressive
ARIMA	Autoregressive Integrated Moving Average
ARMA	Autoregressive Moving Average
DBAFS	Dockless Bike Availability Forecasting System
GPS	Global Positioning System
ID	Identification
KPSS	Kwiatkowski-Phillips-Schmidt-Shin
MA	Moving Average
MAE	Mean Absolute Error
MLE	Maximum Likelihood Estimation
NFS	Naïve Forecasting System
PACF	Partial Autocorrelation Function
PDT	Pacific Daylight Saving Time
PST	Pacific Standard Time
PBSS	Public Bike Sharing Systems
RMSE	Root Mean Squared Error
RMSLE	Root Mean Squared Logarithmic Error
SFMTA	San Francisco Municipal Transportation Agency
SQL	Structured Query Language
STL	Seasonal Trend decomposition procedure based on Loess
WGS84	World Geodetic System 1984

Abstract

Forecasting bike availability is of great importance when turning the shared bike into a reliable, pleasant and uncomplicated mode of transport. Several approaches have been developed to forecast bike availability in station-based bike sharing systems. However, dockless bike sharing systems remain fairly unexplored in that sense, despite their rapid expansion over the world in recent years. To fill this gap, this thesis aims to develop a generally applicable methodology for bike availability forecasting in dockless bike sharing systems, that produces automated, fast and accurate forecasts.

To balance speed and accuracy, an approach is taken in which the system area of a dockless bike sharing system is divided into spatially contiguous clusters that represent locations with the same temporal patterns in the historical data. Each cluster gets assigned a model point, for which an ARIMA(p,d,q) forecasting model is fitted to the deseasonalized data. Each individual forecast will inherit the structure and parameters of one of those pre-build models, rather than building a new model on its own.

The proposed system was tested through a case study in San Francisco, California. The results showed that the proposed system outperforms simple baseline methods. However, they also highlighted the limited forecastability of dockless bike sharing data.

Keywords: dockless bike sharing systems, bike availability, forecasting, time series analysis, sustainable transport

Chapter 1

Introduction

1.1 Context

Over the past decades, the world has been urbanizing at a rapid pace. Where in 1950, 30% of the world's population lived in urban areas, this grew to 55% by 2018. It is a development of which the end is not yet in sight. By 2050, the urban population is projected to have increased to 68% (United Nations, 2018). Managing the urban growth in a sustainable manner, balancing economical, social and environmental factors, forms a tremendous challenge. One of the cores of this challenge relates to transportation. Nowadays, urban transport policies still have a strong focus on the private car as leading transportation mode. However, neither from the economical, social nor environmental perspective, this is sustainable. Air pollution, resource depletion, fuel costs, congestion, noise, accidents and space requirements are among the elements that set limits to a car-oriented urban environment (Hickman & Banister, 2014). Therefore, on our way towards more sustainable cities, with a high quality of life, a drastic shift of focus is required, which includes the integration of transport modes that provide feasible alternatives to car usage. Although changing travel behaviours is a complex and slow process, more and more cities across the world are acknowledging this need, and start acting upon it.

As argued by Pucher & Buehler (2017), the most sustainable and functional mode of transport in urban areas, is probably the bicycle. It can be used for short and medium distance trips, that form a large part of everyday city travel. Since it causes no air pollution, is healthy, has low usage and infrastructure costs, and requires little space, cycling is sustainable in the economical, social and environmental sense. Not for nothing, it receives increasing attention in cities all over the world. The share of trips done by bicycle, has risen sharply in recent years, also in cities without a cycling tradition, and investments are made to improve the bicycle infrastructure. Furthermore, urban cycling is becoming a hot topic in academia as well, with a strong growth in the number of publications related to this topic over the last few years (Fishman, 2016; Pucher & Buehler, 2017).

Public bike sharing systems (PBSS) form an important part of the shift towards more cycling-oriented cities. They are build on the concept of a shared utilization of bicycle fleets, in

which individuals can use bicycles whenever they need them, eliminating the costs and responsibilities that come with private bike ownership (Shaheen, Guzman, & Zhang, 2010). Especially in cities without a cycling tradition, PBSS can normalize the image of cycling as a legitimate mode of everyday transport (Goodman, Green, & Woodcock, 2014). Furthermore, the flexibility of PBSS make them a suitable way to improve the first and last mile connection to other transit modes (X.-H. Yang et al., 2018).

The number of PBSS worldwide grew from 5 in 2005 to 1571 in 2018 (C. Schmidt, 2018). Although this extraordinary growth is a relatively recent development, PBSS have been around for much longer. Already in 1965, the first one started in Amsterdam. This system, known as *Witte Fietsen* (White Bikes), consisted of fifty permanently unlocked, white painted bikes that were scattered throughout the city, could be freely used, and left in any location. However, due to theft and vandalism, the experiment became a failure, and the system was shut down within days. It took 25 years before a new generation of PBSS entered the stage, in Denmark, 1991. In these systems, bikes had to be picked up and dropped off at designated docking stations, and payments were done with coin deposits. Because of the anonymity of the users, theft remained an issue. This lead to the third generation PBSS, which really took hold when Lyon's Velo'v system was introduced in 2005. Third generation PBSS used more advanced technologies, including electronic docking stations, information tracking, and electronic, dynamic payments with smartcards (DeMaio, 2009; Shaheen et al., 2010). Over time, this evolved into the station-based bike sharing systems as we know them now, with the smartcard being replaced by mobile applications.

The modern, station-based systems are organized and well manageable. However, the accessibility of docking stations forms a large barrier for its usage: either there are no docking stations close enough to the desired trip origin, either there are no docking stations close enough to the desired trip destination (Fishman, Washington, Haworth, & Mazzei, 2014). The possibilities of increasing the number of docking stations are generally limited, due to high costs and space requirements. As an answer to these inconveniences, so-called *dockless bike sharing systems*, in some literature also referred to as *free floating bike sharing systems* or *flexible bike sharing systems*, have rapidly gained popularity in the last few years. In 2018, an estimated 16 to 18 million dockless shared bikes were in use, compared to 3.7 million station-based shared bikes (C. Schmidt, 2018).

The dockless systems build on the philosophy behind the first generation PBSS, with bikes that can be picked up and dropped off at any location in the city. They are, however, supported by new technologies that limit the risk of theft and vandalism. The bicycles generally have integrated GPS tracking and an electronic lock. Usage is simple and convenient. Users download a mobile application and create a profile, which they link to their credit card, or charge with money from their bank account. On the app, they find an available bike, which they can unlock with their smartphone, usually by scanning a QR code. The ride can be ended anywhere, and a mobile payment is made, with the price depending on the travel time (Shen, Zhang, & Zhao, 2018).

The revival of dockless bike sharing systems started in 2015, when two Chinese start-up companies, Mobike and Ofo, introduced them to several cities in China (Sun, 2018). Since that moment, the expansion evolved extremely fast. Within one year, Mobike was present

in eighteen Chinese cities with more than a million bikes in total, and other bike sharing start-ups emerged to follow their example (Van Mead, 2017). From 2017 on, the systems spread across the world. In most cases, they were not welcomed with open arms by the local authorities and inhabitants, since regulations did not exist, and the companies simply dumped bikes throughout the cities, fighting for the highest market share, and not putting any effort into frequently maintaining and rebalancing the bikes. *BBC* talked about the dockless bikes that are ‘flooding the world’ (Belton, 2018), *The New York Times* named it ‘the bike sharing explosion’ (Larmer, 2017), and *The Guardian* even used the term ‘bike war’ (Collinson, 2018).

Currently, the peak of the storm seems to have passed, and more and more cities have defined rules to control the dockless bike sharing expansion. These include requirements for operators to obtain a permit before entering the market, designated ‘system areas’ in which the bikes can be used, limits to the fleet size and restrictions to allowed parking spots (Deighton-Smith, 2018). Thus, cities embrace dockless bike sharing in a well balanced way, take advantage of its convenience, and make it an important part of the strive to a more sustainable urban environment.

1.2 Objective

In order to become a serious alternative for motorized transport, PBSS need to be organized and reliable. For station-based systems, this means that situations in which a user either can not start a trip at the desired time and location because of an empty docking station, or can not end a trip at the desired time and location because of a full docking station, should be avoided. In dockless bike sharing systems, the latter is not an issue, since bikes can be left anywhere and anytime. The first, however, remains a challenge. A user does not have the certainty of finding an available bike near the desired trip origin, at the desired time of departure.

Accurate, short-term forecasts of the distribution of available bikes both over space and time, enable system operators to anticipate on imbalances between supply and demand, such that the occurrence of situations as described above is limited to a minimum. Furthermore, users can take advantage of these forecasts also in a direct way, to plan their trips effectively, and reduce the time spent on searching for a bike. Hence, forecasting bike availability is of great importance when turning the shared bike into a reliable, pleasant and uncomplicated mode of transport.

Several approaches have been developed to forecast the bike availability in station-based bike sharing systems. However, dockless bike sharing systems remain fairly unexplored in that sense, since their rapid expansion only started very recently, and in contradiction to the station-based system, large historical data sets are not widely and openly available.

Furthermore, the spatio-temporal nature of dockless bike sharing data brings additional challenges to the forecasting task. In station-based systems, forecasts are only required at fixed spatial locations, and although some works include spatio-temporal relationships between stations, they can mostly be treated as distinct entities, with different forecasting

models for each station. In dockless bike sharing systems, however, available bikes can be at any spatial location inside the system area. Besides, the bike availability not only has a spatial dependence, with more bikes being available in certain areas, and a temporal dependence, with more bikes being available at certain times, but those dependencies are also linked to each other. That is, temporal patterns may differ over space, and vice versa.

The objective of this thesis is to deal with those challenges, and develop a generally applicable methodology for bike availability forecasting in dockless bike sharing systems.

1.3 Related work

Pal, Zhang, & Kwon (2018) define two main categories in which publications related to PBSS can be classified. The first category involves the studies whose primary objective is to forecast the system's future bike availability, bike demand, or similar. The second category involves the studies whose primary objective is to understand and describe the system, so that either its service level can be improved or the system can be expanded. Since this thesis aims to forecast bike availability, publications of the first category are the ones of interest. In essence, they all deal with time series analysis, and a wide range of forecasting methods has already been applied, primarily focused on station-based PBSS. These are covered in Section 1.3.1, while the first attempts targeting dockless PBSS are reviewed in Section 1.3.2.

1.3.1 Forecasting in station-based systems

One of the first works on bike availability forecasting was published ten years ago, by Froehlich, Neumann, & Oliver (2009). The study had an exploratory approach, focused on gaining a better understanding of the spatio-temporal patterns in station-based bike sharing systems and the factors that influence forecasts of those patterns. Some forecasting models were selected, ranging from very simple (e.g. a Last Value Predictor) to slightly more complex (e.g. a Bayesian Network). The most accurate forecasts were made at stations with a low usage, where the variability in the data was small. The Bayesian Network started outperforming the simpler methods at stations with a higher usage, and a corresponding large variability in the data. Usage intensity did not only vary over space, but also over time. The same conclusions were drawn in this sense, with the most accurate forecasts during the night, and the highest difference between simple and advanced methods during peak hours. Furthermore, the length of the forecasting window influenced forecasts, with higher forecast errors at larger forecasting windows. Using more historical data generally increased forecast accuracies, but recent observations were found to have a considerably higher influence than distant ones. External variables such as weather and special events were not considered.

Although the conclusions of Froehlich et al. (2009) seem obvious now, they formed an important basis for further research, with more advanced forecasting methods. Kaltenbrunner, Meza, Grivolla, Codina, & Banchs (2010) fitted Auto Regressive Integrated Moving Average (ARIMA) models to the historical bike availability data of each docking station in Barcelona's *Bicing* system, incorporated information from neighbouring stations into these

models, and forecasted the amount of available bicycles up to one hour ahead. Won Yoon, Pinelli, & Calabrese (2012) used a similar approach, but included recurring seasonal patterns in the ARIMA models. Borgnat et al. (2011), instead, split the forecasting task in two: linear regression, with weather, usage intensity and specific conditions like holidays as explanatory variables, was used to forecast a non-stationary amplitude for a given day, while an autoregressive (AR) model forecasted the hourly fluctuations in the data.

Rixey (2013) created linear regression models to forecast the number of monthly rentals per docking station. Explanatory variables such as demographic and built environment factors were extracted from a circular buffer with a radius of 400 meters around each station. D. Singhvi et al. (2015) did a comparable study, but on a macroscopic level, arguing that aggregating stations in neighbourhoods can substantially improve predictions.

In 2014, Kaggle, a well-known online community for data scientists, hosted a machine learning competition, in which participants were asked to combine historical usage patterns with weather data, and forecast bike demand in the station-based PBSS of Washington D.C. (Kaggle, 2014). The competition increased the academic interest in bike availability forecasting with machine learning methods, and new publications on this topic followed rapidly. Giot & Cherrier (2014) compared Ridge Regression, Adaboost Regression, Random Forest Regression, Gradient Tree Boosting Regression and Support Vector Regression by predicting Washington's city-wide bike sharing usage up to one day ahead, inputting recent observations, time features (e.g. season, day of the week, hour of the day) and weather features (e.g. temperature, wind speed). Ridge Regression and Adaboost Regression turned out to be the best performing methods. Y. Li, Zheng, Zhang, & Chen (2015) used Gradient Tree Boosting Regression with time and weather features. However, they first grouped the docking stations into distinct, spatially contiguous clusters, and forecasted the bike usage per cluster. Dias, Bellalta, & Oechsner (2015) attempted to simplify the task, by using a Random Forest Regressor to forecast only if a docking station will be either completely full, completely empty, or anything in between.

Later, spatial relations between individual docking stations were incorporated into the machine learning approaches, which resulted in more sophisticated forecasting methods. Z. Yang et al. (2016) proposed a probabilistic spatio-temporal mobility model that considered previous check-out records at other stations and expected trip durations to estimate the future check-ins at each station. Subsequently, check-outs at each station were estimated with a Random Forest Regressor, that also took weather forecasts into account. L. Lin, He, & Peeta (2018) modelled station-based PBSS as a graph, with each station being a node. Then, they applied a Convolutional Neural Network in a form generalized for graph-structured data, to forecast hourly bike demand. Lozano, Paz, Villarrubia, De La Iglesia, & Bajo (2018) created an automated multi-agent bike demand forecasting system for the Salamanca's *SalenBici* system, with digital 'agents' that collect different types of data, such as calendar events, weather forecasts and historical usage. These data were combined, and used to forecast check-ins and check-outs separately for each station, with a Random Forest Regressor.

The Random Forest and Convolutional Neural Network approaches were compared by Ruffieux, Spycher, Mugellini, & Khaled (2017). Furthermore, they differentiated themselves

by forecasting bike availability in six different cities, instead of only one. The outcomes showed that the Random Forest Regressor works better for short-term forecasts, while Convolutional Neural Networks are more suitable for long-term forecasts. B. Wang & Kim (2018) compared the Random Forest approach to two of the latest machine learning innovations, Long Short Term Memory Neural Networks and Gated Recurrent Units, but found no substantial improvements in the results.

All discussed academic publications related to bike availability forecasting in station-based PBSS are listed in Table 1.1, in chronological order. It can be seen that machine learning methods have received a lot of attention in recent years, compared to traditional statistical forecasting methods such as ARIMA. The two serve the same goal, but have a different philosophy and model development process. Traditional statistical methods assume a functional form in advance, concern inference and estimation, and aim at providing models that offer insights on the data. Machine learning methods approximate the functional form via learning inside a ‘black box’, do not require specifications of the model and the error distribution, and aim solely at providing an efficient forecast (Ermagun & Levinson, 2018).

Studies in the field of bike availability forecasting that make valuable comparisons between traditional time series forecasting and machine learning methods, are scarce. Y. Li et al. (2015) and Z. Yang et al. (2016) included ARIMA in their baseline methods, but only in a form that does not take any seasonal component into account, while Dias et al. (2015) compared a seasonal ARIMA model with their proposed Random Forest Regressor, but without using the same amount of data for both methods. In spatio-temporal transportation forecasting in general, there is no clear consensus on which method is ‘better’. Despite the strong increase in publications that use machine learning, Ermagun & Levinson (2018) state that “there is not a certain superiority when machine learning methods are compared with advanced statistical methods such as autoregressive integrated moving average.”

Table 1.1: Publications regarding forecasts in station-based bike sharing systems, known to the author

Authors	Year	Main forecasting method	Spatial unit of analysis	Case study
Froehlich, Neumann, and Oliver	2009	Bayesian Network	Docking station	Barcelona
Kaltenbrunner et al.	2010	Spatial ARIMA	Docking station	Barcelona
Borgnat et al.	2011	Linear regression and AR	Docking station	Lyon
Won Yoon, Pinelli, and Calabrese	2012	Spatial, seasonal ARIMA	Docking station	Dublin
Rixey	2013	Linear regression	Docking station	Washington DC, Minneapolis and Denver

Table 1.1: Publications regarding forecasts in station-based bike sharing systems, known to the author
(continued)

Authors	Year	Main forecasting method	Spatial unit of analysis	Case study
Giot and Cherrier	2014	Ridge regression, Adaboost regression, Random Forest regression, Gradient Tree Boosting regression and Support Vector regression	City	Washington DC
D. Singhvi et al.	2015	Linear regression	Neighbourhood	New York
Y. Li et al.	2015	Gradient Tree Boosting regression	Cluster	Washington DC
Dias, Bellalta, and Oechsner	2015	Random Forest regression	Docking station	Barcelona
Z. Yang et al.	2016	Probabilistic mobility model and Random Forest regression	Docking station	Hangzhou
Ruffieux et al.	2017	Random Forest regression and Convolutional Neural Network	Docking station	Namur, Essen, Glasgow, Budapest, Vienna and Nice
Lin, He, and Peeta	2018	Graph Convolutional Neural Network	Docking station	New York
Lozano et al.	2018	Random Forest regression	Docking station	Salamanca
B. Wang and Kim	2018	Long Short Term Memory Neural Networks and Gated Recurrent Units	Docking station	Suzhou

1.3.2 Forecasting in dockless systems

Publications regarding bike availability forecasting in dockless PBSS can be counted on the fingers of one hand. In addition to them, a small number of similar studies have been done in the field of dockless car sharing, which is based on the same principles as dockless bike sharing.

Those few attempts can be divided in two groups of approaches, which are labeled here as the *grid based approach* ad the *distance based approach*. In the grid based approach, the system's operational area, i.e. the 'system area', is divided into distinct grid cells, which

may be regularly shaped, but do not have to be. For example, the cell boundaries may also correspond with administrative boundaries. Subsequently, each cell is treated as being a docking station. That is, from the historical data on locations of available vehicles, the number of vehicles in each cell is counted at several timestamps in the past, creating a time series of counts. Hence, for a given geographical point, the forecasted value will be the expected number of vehicles inside the cell that contains the point.

The distance based approach uses the historical data to calculate the distance from a given geographical location to the nearest available vehicle, for several timestamps in the past, creating a time series of real-valued distances. Hence, the forecasted value will be the expected distance from the given point to the nearest available vehicle, at a given timestamp in the future.

The grid based approach was taken by Caggiani, Ottomanelli, Camporeale, & Binetti (2017), who were among of the first to forecast bike availability in dockless PBSS. They did not use a regular grid, but defined the outline of the cells with a spatio-temporal clustering procedure, that worked as follows. Historical time series containing daily counts of available bikes were obtained for each zone, and clustered based on temporal patterns. Geographically connected zones that belonged to the same temporal cluster, were aggregated. The resulting clusters formed the spatial units of analysis, and for each of them, the number of available bikes was forecasted one day ahead with a Nonlinear Autoregressive Neural Network. However, at that time, they lacked data to test their methodology on. Instead, they used data from the station-based bike sharing system in London, pretending each docking station to be a cluster centroid.

Yi et al. (2018) did have access to a dataset of a dockless PBSS, in the Chinese city of Chengdu, and laid a regular grid with square cells over its systems area. Besides historical count data of available bikes in each grid cell, they included a categorical variable representing the time of day in their system. Forecasting was done with a recent machine learning method, named Convolutional Long Short Term Memory Network. J. Müller & Bogenberger (2015), in contradiction, used traditional statistical methods, and focused on forecasting the number of car bookings in a dockless car sharing system, for each ZIP-code area in Berlin. They compared a seasonal ARIMA model with a Holt Winters exponential smoothing model, and found acceptable and similar forecasting errors for both of them.

The only example of the application of the distance based approach, known to the author, is the work of Formentin, Bianchessi, & Savaresi (2015). Their methodology, focused on dockless car sharing systems, can be summarized as follows. For a set of given locations, evenly distributed over the city, historical location data is pre-processed into a time series of historical distance data. A strictly linear trend is subtracted from these time series, and if present, the seasonal component as well, using the classical time series decomposition method. AR models are fitted to the data that are left. Then, a model structure that is acceptable for all time series, is identified, and serves as the general forecasting model for the complete city. That is, for individual forecast requests, this general model structure will be used, no matter what the location of the request is. Only when a forecast request is located inside the city center, the corresponding historical distance data will be decomposed before forecasting, assuming a daily seasonal pattern. In that case, the seasonal component will

afterwards be added to the forecast produced by the general model. The general model is updated every month.

All discussed academic publications related to bike availability forecasting in dockless PBSS are listed in Table 1.2.

Table 1.2: Publications regarding forecasts in dockless vehicle sharing systems, known to the author

Authors	Year	Main forecasting method	Approach	Case study	Type
Formentin, Bianchessi, and Savares	2015	AR	Distance based	Milan	Car
Müller and Bogenberger	2015	ARIMA and Holt Winters ETS	Grid based	Berlin	Car
Caggiani et al.	2017	Nonlinear Autoregressive Neural Network	Grid based	London	Bike
Yi et al.	2018	Convolutional Long Short Term Memory Network	Grid based	Chengu	Bike

1.4 Approach

The bike availability forecasting system as proposed in this thesis extends the methodology proposed by Formentin et al. (2015), and uses the distance based approach, since it has the following advantages over the grid based approach.

- Forecasts will not be dependent on the chosen spatial resolution of the grid.
- Forecasts will not be made with count data, which would have limited the choice of suitable forecasting models.
- Forecasts can be interpreted in the same way at every location in space. This in contradiction to the grid based approach, where for a location at the edge of a grid cell, there might as well be closer bikes within the neighbouring cell.
- Forecasts give more freedom to the user, who can decide for themselves if they consider the forecasted distance acceptable or not. In the grid based approach, the cell size is fixed, and does not take into account that some people are willing to walk further than others.

By choosing the distance based approach, the proposed forecasting system will involve the analysis, modelling and forecasting of time series that each contain the distances from specific geographical locations to the nearest available bike, at several timestamps in the past. Hence, the data of interest are *spatio-temporal* in nature, and require a methodology that adequately deals with both their spatial and temporal dimension. In the proposed system, the spatio-temporal nature of the data is used as an advantage, and an approach is developed in

which the structures of time series forecasting models build at specific locations and specific timestamps, are inherited by forecast requests for nearby locations, and future timestamps. In that way, the need for separate models for each individual forecast, is taken out.

Throughout the thesis, the proposed forecasting system will be referred to as the **Dockless Bike Availability Forecasting System** (DBAFS). The focus will lay on the design of a general methodology for it, rather than on the creation of a fully configured, practical application. A forecast can be requested for any location within the system area of a dockless bike sharing system, and, theoretically, any timestamp in the future. However, short-term forecasts, up to one day ahead, form the target, and longer forecasting horizons will not be handled.

1.5 Outline

The rest of the document is structured as follows. Chapter 2 provides a theoretical background of the concepts used in this thesis, which are all linked to the field of time series analysis. In Chapter 3, the methodology of the proposed forecasting system is described into detail. Chapter 4 presents the data on which the system is tested, and describes the experimental setup. In Chapter 5, the results of the experiments are shown, interpreted, and discussed. Finally, Chapter 6 lists the conclusions of this thesis.

Chapter 2

Theoretical background

This chapter presents a brief introduction to the theory of time series analysis. It is meant to serve as a theoretical foundation of the concepts used in this thesis. Therefore, the focus is clearly on those specific concepts, and the chapter should to no means be considered a thorough overview of the complete field of study.

The chapter is divided into five sections. In the first section, a formal definition of time series is given. The second section discusses the main characteristics of time series. Section three describes the different components of time series data and presents methods to split a time series into these components. The fourth section introduces statistical models to forecast time series, in particular the *autoregressive integrated moving average* (ARIMA) class of models. Finally, the fifth section focuses on a specific niche within time series analysis that is used in this thesis, namely time series clustering.

2.1 Time series definition

According to Woodward, Gray, & Elliott (2017), a time series can be defined as follows:

Definition 1 A *time series* is a special type of a stochastic process. A stochastic process $\{Y(t); t \in T\}$ is a collection of random variables, where T is an index set for which all of the random variables are defined on the same sample space. When T represents time, the stochastic process is referred to as a time series. ■

Typically, observations are made at equally spaced time intervals, such as every hour, every day or every year. In such cases, T takes on a discrete set of values, and are known as *discrete-time time series*. On the other hand, *continuous-time time series* arise when T takes on a continuous range of values (Brockwell & Davis, 2002). In this thesis, only discrete-time time series are analyzed.

An observed realization of the stochastic process described in Definition 1, is referred to by Woodward et al. (2017) as a *realization of a time series*. Other works, such as Brockwell & Davis (2002), Shumway & Stoffer (2011) and Hyndman & Athanasopoulos (2018), use the term *time series* for both the data and the stochastic process of which it is a realization. In

this thesis, for the sake of simplicity, the latter approach is used, and no notational distinction is made.

Definition 2 A *time series* is a set of observed values $\{y_t\}$ of a stochastic process $\{Y(t); t \in T\}$, where T represents time. ■

From the context it will be clear whether the term time series refers to the process (Definition 1) or its realization (Definition 2). When clarification is needed, it is given locally.

2.2 Time series characteristics

2.2.1 Autocorrelation

Analyzing time series raises unique problems in statistical modelling and inference. In conventional statistics, methods rely on the assumptions of independent and identically distributed random variables. However, in time series analysis, observations made at nearby moments in time are likely to be related. That is, it is likely that there exist internal relationships within a time series. If these relationships are linear, they are called autocorrelation, as defined in Definition 3 (Shumway & Stoffer, 2011).

Defintion 3 *Autocorrelation* measures the linear correlation between two points on the same time series observed at different times. ■

Given a sample $\{y_1, y_2, \dots, y_n\}$ of a time series, the degree of dependence in the data can be assessed by computing the *autocorrelation function* (ACF), for each lag h , as defined in Equation (2.1) (Brockwell & Davis, 2002).

$$\hat{\rho}(h) = \frac{\hat{\gamma}(h)}{\hat{\gamma}(0)}, \quad -n < h < n \quad (2.1)$$

Where $\hat{\gamma}(h)$ is the autocovariance function of the sample at lag h , defined in Equation (2.2).

$$\hat{\gamma}(h) = n^{-1} \sum_{t=1}^{n-|h|} (y_{t+|h|} - \bar{y})(y_t - \bar{y}), \quad -n < h < n \quad (2.2)$$

Where n is the length of the sample, y_t is the data value at time t , $y_{t-|h|}$ is the data value at time t minus $|h|$ time periods, and \bar{y} is the mean of the sample. Whenever a time series $\{Y_t\}$ is stationary, a concept that is introduced in the next section, the ACF of the sample $\{y_t\}$ can be used as an estimate for the ACF of $\{Y_t\}$. A time series without autocorrelation, with zero mean and finite variance, is called *white noise*.

Conventional statistical methods can not be appropriately applied to data that exhibit autocorrelation, since the independency assumption is violated. The primary objective of time series analysis, therefore, is to develop mathematical models that are appropriate to use for data with a temporal autocorrelation structure (Shumway & Stoffer, 2011). Furthermore, autocorrelation is in some cases an advantage, since an internal dependence structure implies that past observations can be used adequately to forecast future values.

2.2.2 Stationarity

In time series analysis, a key role is played by time series whose statistical properties do not vary with time (Brockwell & Davis, 2002). Such time series are called *stationary time series*. The most restrictive form of stationarity is defined in Definition 4 (Woodward et al., 2017).

Definition 4 A time series $\{Y(t); t \in T\}$ is *strictly stationary* if for any $t_1, t_2, \dots, t_k \in T$ and any $h \in T$, the joint distribution of $\{Y_{t_1}, Y_{t_2}, \dots, Y_{t_k}\}$ is identical to that of $\{Y_{t_1+h}, Y_{t_2+h}, \dots, Y_{t_k+h}\}$. ■

However, it is often too hard to mathematically establish the requirement of strict stationarity, since the involved distributions are not known. For most applications, a milder form of stationarity, which only imposes conditions on the first and second moment of a time series, is sufficient. This is officially known as *weak stationarity*, but, in time series analysis, usually just called *stationarity*, for the sake of simplicity. It is mathematically defined as in Definition 5 (Woodward et al., 2017).

Definition 5 A time series $\{Y(t); t \in T\}$ is *stationary* if

- 1) $E[Y_t] = \mu$ (constant for all t).
- 2) $Var[Y_t] = \sigma^2$ (constant for all t).
- 3) $\gamma(t_1, t_2)$ depends only on $t_2 - t_1$. ■

In words, this means that a time series is said to be stationary when the mean and variance are constant over time, and the autocovariance function only depends on the difference between two time points, and not on the time point itself. Note here that each time series that is strictly stationary (Definition 4), is, by definition, also stationary (Definition 5).

Stationarity is important, since in real-world problems, it is common that only one realization of a time series is available. That means that each random variable in the time series is represented by a single value. This makes it impossible to get an understanding of the underlying probability distributions of those random variables, unless it is assumed that their statistical properties are the same (i.e. the time series is stationary). In that case, the statistical properties of the whole sample can be used to estimate the statistical properties of each individual probability distribution. An understanding of the underlying probability distributions, in turn, is especially important when the goal is to forecast how the time series will behave at future time points. When the statistical properties of the time series have been constant over time in the past, one can simply predict that they will remain constant in the future.

In most practical applications, non-stationary time series are the rule rather than the exception. Luckily, by applying mathematical transformations, it often possible to render a non-stationary time series as, approximately, stationary. This process is referred to as *stationarizing* a time series (Nau, 2018). Stationarizing is used often in statistical forecasting methods, which are discussed in Section 2.4.

2.2.3 Spectral entropy

Often, two separate approaches to time series analysis are defined. The first, referred to as the *time domain*, deals primarily with the internal dependence structure in time series data, where current values can be explained in terms of a dependence on past values, as discussed in Section 2.2.1. The second, referred to as the *frequency domain*, works with a spectral representation of the time series, in which the original data is expressed as a weighted sum of sine and cosine waveforms, each with their own frequency. Named after the French mathematician Jean-Baptiste Joseph Fourier, such a representation is commonly known as a *Fourier representation* or *Fourier series*, and its corresponding sine and cosine terms as *Fourier terms*. Forecasting is inherently tied to the time domain of time series analysis, which will therefore be the focus of this thesis. However, there is no schism dividing the two approaches. That is, some frequency domain techniques can be useful even in the time domain, and vice versa (Shumway & Stoffer, 2011).

One of such techniques is the calculation of the spectral entropy of a time series, which describes the order and regularity of a time series, based on its Fourier representation. The spectral entropy of a time series can be calculated with Equation (2.3).

$$H = \int_{-\pi}^{\pi} \hat{f}(\lambda) \log \hat{f}(\lambda) d\lambda \quad (2.3)$$

Where $\hat{f}_y(\lambda)$ is the estimated spectral density function, which describes the importance of the different frequencies in the Fourier representation of the time series. Usually, H is normalized to the range of values between 0 and 1. For a detailed description of the calculations, see Goerg (2013).

Spectral entropy is useful in forecasting, since it can serve as a quantitative measure of the forecastability of a time series. Very smooth data, that are easy to forecast, will have a small value of H , while very noisy data, that are hard to forecast, will have a large value of H (T. S. Talagala, Hyndman, & Athanasopoulos, 2018).

2.3 Time series components

2.3.1 Definitions

A time series can consist of various underlying patterns. Each of those patterns is considered a distinct component of the time series, with its own properties and behaviour. Splitting a time series into its components, is known as *time series decomposition*. It enables a separate analysis of all the components, which helps to better understand the dynamics of a time series, but can also be useful in forecasting, as will be discussed later in this chapter.

Hyndman & Athanasopoulos (2018) define three main components of a time series: a trend-cycle component, a seasonal component, and a remainder component. For simplicity, the trend-cycle component is usually called just the trend component, which is done in this thesis as well.

Definition 4 The *trend component* is the combination of the trend and cyclical pattern of a time series. A trend exists when there is a long-term, not necessarily linear, increase or decrease in the data. A cyclical pattern occurs when the data exhibit rises and falls that are not of a fixed frequency. ■

Definition 5 The *seasonal component* contains the seasonal pattern of a time series. A seasonal pattern occurs when a time series is affected by seasonal factors such as the time of the year or the day of the week, and is always of a fixed and known frequency. ■

Definition 6 The *remainder component* is the remaining variation in a time series after the trend and seasonal components are removed. ■

There exist several methods for the decomposition of a time series. Most of them are based on the classical decomposition method, which is discussed in the next section. A more sophisticated approach is known as STL, and is covered in Section 2.3.3.

2.3.2 Classical decomposition

The oldest and simplest method for the decomposition of a time series is referred to as classical decomposition by Hyndman & Athanasopoulos (2018). They present a stepwise approach for the use of the method, which is summarized in this section. Classical decomposition can be applied in two different forms. In the additive form, a time series is assumed to be the sum of its components, as shown in Equation (2.4).

$$y_t = T_t + S_t + R_t \quad (2.4)$$

In the multiplicative form, a time series is assumed to be the product of its components, as shown in Equation (2.5).

$$y_t = T_t \times S_t \times R_t \quad (2.5)$$

Where, for both Equation (2.4) and Equation (2.5), y_t is the data, T_t is the trend component, S_t is the seasonal component and R_t is the remainder component.

Additive decomposition is used in cases when the amplitude of the variation around the trend is relatively constant. On the other hand, when the amplitude of the variation around the trend changes with the level of the trend, multiplicative decomposition should be used.

In both the additive and multiplicative form of classical decomposition, the first step is to estimate the trend component. This is done by smoothing the data with a symmetric moving average filter of order m , where m is a non-negative integer. That is, the estimate of the trend component at time t is the average of all the data values within a window of m time periods centered at t , as shown in Equation (2.6). Usually, m is set to be equal to the seasonal period of the time series, which, in turn, is the number of observations per seasonal cycle. For example, when working with daily data that show a weekly seasonal pattern, the seasonal period is 7.

$$\hat{T}_t = \frac{1}{m} \sum_{j=-k}^k y_{t+j} \quad (2.6)$$

Where $k = (m - 1)/2$.

The detrended time series data are then calculated by removing the estimated trend component from the original data. In the case of additive decomposition by subtraction, $y_t - \hat{T}_t$, and in the case of multiplicative decomposition by division, y_t / \hat{T}_t .

The seasonal component is estimated by averaging the detrended data values per season, as shown in Equation (2.7). Using again the example of daily data with a weekly seasonal pattern, that would mean that the estimated seasonal component for a specific Monday is the average value of all Monday observations in the data set, the estimated seasonal component for a specific Tuesday is the average value of all Tuesday observations in the data set, and so on.

$$\hat{S}_t = \frac{1}{n_t} \sum_{i=1}^{n_t} (\omega_t)_i \quad (2.7)$$

Where ω_t is a vector containing all the detrended values belonging to the same season as y_t , and n_t is the length of ω_t . Usually, the estimated seasonal component values for each season are adjusted such that they add up to 0 in the case of additive decomposition and 1 in the case of multiplicative decomposition.

Finally, the remainder component is estimated by removing both the estimated trend component and the estimated seasonal component from the original time series. For additive decomposition, this is done by applying Equation (2.8).

$$\hat{R}_t = y_t - \hat{T}_t - \hat{S}_t \quad (2.8)$$

For multiplicative decomposition, Equation (2.9) is used.

$$\hat{R}_t = \frac{y_t}{\hat{T}_t \hat{S}_t} \quad (2.9)$$

Classical decomposition is generally praised for its simplicity, but has several disadvantages compared to some of the more modern decomposition methods (Hyndman & Athanasopoulos, 2018). As a consequence of the use of a symmetric moving average filter, there are no trend component estimates available for the first few and last few observations of the time series. Therefore, also the remainder component estimate lacks these values. An unknown current value of a time series, is mainly problematic when forecasting, as is shown in Section 2.4. Furthermore, the seasonal component stays constant over all the seasonal cycles, and cannot capture slight changes over time. Especially when working with longer time series, this may be an inappropriate representation of the truth. Finally, classical decomposition is not robust to extreme values in the data.

2.3.3 STL decomposition

A widely used method that is based on classical decomposition, but deals with many of the limitations mentioned above, is known as STL. It stands for *A Seasonal-Trend decomposition procedure based on Loess*, and was developed by R. B. Cleveland, Cleveland, McRae, & Terpenning (1990). In this section, their methodology is summarized. STL estimates all three components for every observation in a time series, and can also handle missing values in the

data. Both the trend and seasonal component are robust and not distorted by extreme values. Furthermore, the seasonal component is not fixed, but can vary slightly over time.

As its name already implies, STL is based on loess, also known as locally-weighted regression. Loess was developed by Cleveland & Devlin (1988), and is a non-parametric regression technique, often used for smoothing, that fits weighted least squares regression curves to local subsets of a data set. Joining them together forms the loess regression curve $\hat{g}(x)$. More specifically, for each value of x , $\hat{g}(x)$ is computed in the following way. First, a positive integer q is chosen, which defines the neighbourhood width. That is, the q observations that are closest to x are selected as neighbours of x . Each of these observations is given a weight based on its distance to x , in a way that the closest observations get the highest weight. Let W be the tricube weight function as defined in Equation (2.10).

$$W(u) = \begin{cases} (1 - u^3)^3 & 0 \leq u < 1 \\ 0 & u \geq 1 \end{cases} \quad (2.10)$$

Subsequently, the neighbourhood weight for each observation x_i is calculated with Equation (2.11).

$$v_i = W\left(\frac{|x_i - x|}{\lambda_q(x)}\right) \quad (2.11)$$

Where $\lambda_q(x)$ is the distance of the q th farthest observation from x . Then, $\hat{g}(x)$ is calculated by fitting a polynomial regression of degree d to x , using weighted least squares with the neighbourhood weights v_i . Usually, d is either 1 or 2, corresponding respectively to a locally-linear regression and a locally-quadratic regression. Since the loess regression curve is smooth, there is no need to compute $\hat{g}(x)$ at all possible values of x . In general, the computation of $\hat{g}(x)$ as described above is only performed at a finite set of locations, and interpolated elsewhere.

STL uses loess for several smoothing operations, that, when performed on a time series, lead to estimations of the trend, seasonal and remainder components of the data. The method is build up of two loops: an inner loop nested inside an outer loop. In the inner loop, the estimates of the seasonal and trend component are updated once, in a stepwise manner, which is described below.

Step 1. The inner loop starts with computing the detrended time series data $y_t - \hat{T}_t$ from the original time series data y_t . In the initial pass through the inner loop, there is no estimation of T_t yet, and \hat{T}_t is set equivalent to 0. That is, it is assumed there is no trend at all. This may be a rather poor estimate, but inside the loop, it will soon be updated to something more reasonable. In all successive passes through the loop, the estimated trend component that resulted from the previous loop is used.

Step 2. In the second step, the detrended time series is split up into subsets, with each subset containing all the data belonging to one specific season. That is, there will be n_p different subsets, where n_p is the number of observations per seasonal cycle. Each of those subsets is smoothed by loess, with $q = n_s$ and $d = 1$. n_s is referred to as the seasonal smoothing parameter and its value must be chosen by the analyst. It basically determines

how much the seasonal component is allowed to change over time. High values of n_s allow little variation, while low values can lead to overfitting. The smoothed values of all the subsets are then binded back together into a temporary seasonal component C_t . Each end of C_t is extended n_p positions, such that C_t has $2 \times n_p$ observations more than the original time series.

Step 3. In the third step, any trend that may have contaminated C_t is identified. This is done by applying a sequence of smoothers, called a low-pass filter, to C_t . It starts with a moving average of length n_p , followed by another moving average of length n_p , followed by a moving average of length 3, followed by a loess smoothing with $q = n_l$ and $d = 1$. Just as earlier with n_s , the low-pass filter smoothing parameter n_l should be chosen by the analyst. The output of the third step is called L_t . Since moving averages are used, the first n_p observations and the last n_p observations of C_t will not have a smoothed value in L_t . However, this was already accounted for by extending C_t in step 2. That is, L_t is again of the same length as the original time series.

Step 4. In the fourth step, the seasonal component is estimated by detrending the temporary seasonal component. That is, $\hat{S}_t = C_t - L_t$.

Step 5. In the fifth step, the deseasonalized time series data $y_t - \hat{S}_t$ are computed from the original time series data y_t .

Step 6. In the sixth and last step of the inner loop, the estimation of the trend component, \hat{T}_t , is calculated by loess smoothing the deseasonalized time series with $q = n_t$ and $d = 1$. The trend smoothing parameter n_t should be chosen by the analyst.

The outer loop of STL starts with n_i iterations of the inner loop. The estimations of the trend and seasonal components that follow from the passes through the inner loop, are used to estimate the remainder component with Equation (2.12).

$$\hat{R}_t = y_t - \hat{T}_t - \hat{S}_t \quad (2.12)$$

For each observation in the time series, a robustness weight is calculated. This weight reflects how extreme the value of the remainder component of that observation is, in a way that an extreme value is given a very low, or even zero, weight. Let B be the bisquare weight function as defined in Equation (2.13).

$$B(u) = \begin{cases} (1 - u^2)^2 & 0 \leq u < 1 \\ 0 & u \geq 1 \end{cases} \quad (2.13)$$

Then, the robustness weight at time point t is calculated with Equation (2.14).

$$\rho_t = B\left(\frac{|R_t|}{6\text{median}(|R_t|)}\right) \quad (2.14)$$

After the first pass through the outer loop, the next iteration starts again with n_i passes through the inner loop. However, in the loess smoothing in step 2 and step 6, each neighbourhood weight v_t is now multiplied by its corresponding robustness weight ρ_t , such that

extreme values have less influence on the estimates of the trend and seasonal components. Also, the estimated trend component that resulted from the last inner loop in the previous outer loop, is now used as first value of \hat{T}_t , rather than 0. In total, the outer loop is carried out n_o times.

STL is designed for additive decomposition. However, a multiplicative version can be obtained by first log transforming the data, and finally back-transforming the components. This is based on the logarithm product rule, which states that $\log(a) + \log(b)$ is equivalent to $\log(a \times b)$ (Hyndman & Athanasopoulos, 2018).

The complete methodology of STL as described above is summarized in Figure 2.1.

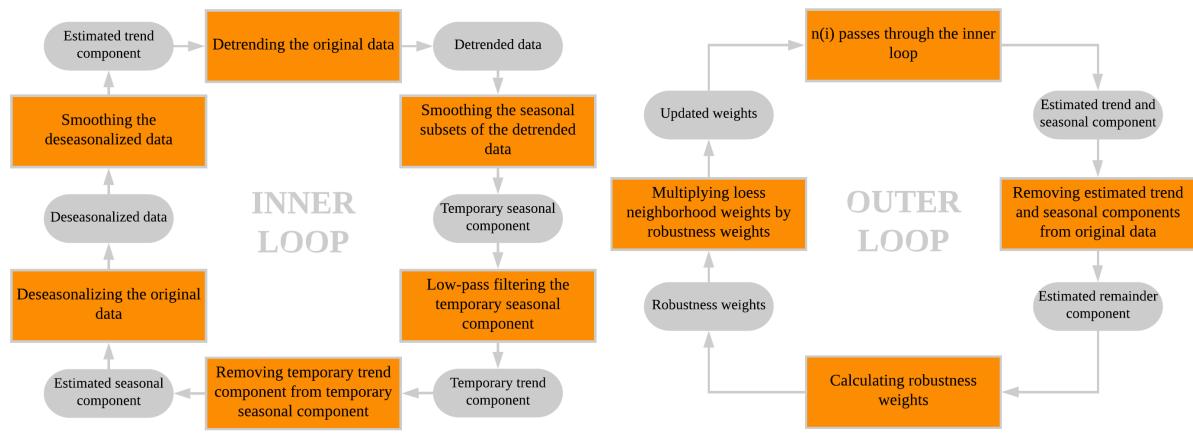


Figure 2.1: Summary of the STL methodology

2.4 Time series forecasting

2.4.1 Forecasting models

Often, the main aim of time series analysis is to forecast future values of a time series. In some cases, this can be done by using external exploratory variables. One could for example try to forecast the profit of ice cream sales by using air temperature as an exploratory variable in a linear regression model. However, there are several reasons not to forecast time series in this way, as summed up by Hyndman & Athanasopoulos (2018). Firstly, the underlying system of the forecasted time series may not be sufficiently understood, and even if it is, the relations with exploratory variables may be too complex. Secondly, when forecasting future values of a time series, also the future values of the exploratory variables should be known, which means that each exploratory variable should be forecasted separately before the response variable can be forecasted. This may be too difficult to do accurately, and even when it is possible, it remains a very time consuming task. Especially when the only aim is to know what will happen, and not why it will happen, it is not worth the effort. Finally, modelling a time series with conventional statistical method like linear regression will likely

result in model errors that exhibit autocorrelation, which implies that such models are not able to capture all the dynamics of the data. Thus, produced forecast are not as efficient, and, probably, not as accurate as can be.

Instead, in time series analysis, the internal dependence structure of a time series is used to forecast future values as a function of the current and past values (Shumway & Stoffer, 2011). Obviously, this primarily requires a good understanding of that structure, which is obtained by describing the process that generated the data with a time series model, as defined in Definition 7, adapted from Brockwell & Davis (2002).

Definition 7 A *time series model* for an observed realization $\{y_t\}$ of a time series $\{Y_t\}$ is a specification of the joint distributions, or possibly only the means, variances and covariances, of the random variables that $\{Y_t\}$ comprises. ■

One of the most famous and widely used groups of time series models is known as the *autoregressive integrated moving average* (ARIMA) class of models, developed by Box & Jenkins (1970). In this thesis, ARIMA is used as well. The next section gives a summary of its theory, based on Brockwell & Davis (2002), Chapter 5, Shumway & Stoffer (2011), Chapter 3, and Hyndman & Athanasopoulos (2018), Chapter 3 and 8.

2.4.2 ARIMA

2.4.2.1 Structure

An ARIMA model is a combination of an *autoregressive* (AR) and *moving average* (MA) model, preceded by a differencing operation on the original data. An autoregressive model of order p , commonly referred to as an AR(p) model, is based on the assumption that the current value of a time series is a linear combination of p previous values, as showed in Equation (2.15).

$$y_t = \phi_1 y_{t-1} + \phi_2 y_{t-2} + \dots + \phi_p y_{t-p} + \epsilon_t \quad (2.15)$$

Where y_t is the current value of the time series at time period t , ϵ_t is the random error (i.e. white noise) at time t , and ϕ_1, \dots, ϕ_p are model parameters.

A moving average model of order q , commonly referred to as an MA(q) model, is based on the assumption that the current value of a time series is a linear combination of q previous errors, as showed in Equation (2.16).

$$y_t = \epsilon_t + \theta_1 \epsilon_{t-1} + \theta_2 \epsilon_{t-2} + \dots + \theta_q \epsilon_{t-q} \quad (2.16)$$

Where y_t is the current value of the time series at time period t , ϵ_t is the error at time period t , which is assumed to be white noise, and $\theta_1, \dots, \theta_q$ are model parameters.

AR(p) and MA(q) models can be combined into an autoregressive moving average model of order (p, q) , commonly referred to as ARMA(p, q). That is, in such a model, the current value of a time series is a linear combination of both p previous values and q previous errors, as showed in Equation (2.17).

$$y_t = \phi_1 y_{t-1} + \dots + \phi_p y_{t-p} + \theta_1 \epsilon_{t-1} + \dots + \theta_q \epsilon_{t-q} + \epsilon_t \quad (2.17)$$

ARMA(p, q) models require the forecasted time series to be stationary. When working with non-stationary time series, it is often possible to stationarize the series by differencing it one or more times. The first order difference of a time series is the series of changes from one time period to the next, as shown in Equation (2.18).

$$\nabla y_t = y_t - y_{t-1} \quad (2.18)$$

Where ∇y_t is the first order difference of y_t . When the first order difference is still non-stationary, the second order difference $\nabla^2 y_t$ can be computed by taking again the first order difference of ∇y_t , and so on.

The original non-stationary time series that needed to be differenced in order to get stationary, is called an *integrated* version of the stationary series. That is why a model that first stationarizes the data by applying a d -th order difference, before fitting an ARMA(p, q) model, is called an autoregressive integrated moving average model of order (p, d, q) , commonly referred to as ARIMA(p, d, q). That is, in such a model, the current value of the d -th order difference of a time series is a linear combination of both p previous values and q previous errors, as showed in Equation (2.19).

$$\nabla^d y_t = \phi_1 \nabla^d y_{t-1} + \dots + \phi_p \nabla^d y_{t-p} + \theta_1 \epsilon_{t-1} + \dots + \theta_q \epsilon_{t-q} + \epsilon_t \quad (2.19)$$

Where $\nabla^d y_t$ is the d -th order difference of y_t . Note here that ARIMA(p, d, q) is a general form of all the other models discussed earlier in this section. For example, an AR(1) model can also be written as ARIMA(1,0,0), an ARMA(2,1) as ARIMA(1,0,2), and so on.

The process of finding an appropriate ARIMA(p, d, q) model that represents a time series is known as the Box-Jenkins modelling procedure and consists of three stages, named model selection, parameter estimation and model checking. All these stages are described separately in the next three subsections.

2.4.2.2 Model selection

In the model selection stage, p , d and q are chosen. In this process, d is selected first, such that the choice of p and q will be based on a stationary time series. An appropriate value for d can be found by inspecting the plotted data y_t , with time on the x-axis, and define visually if the data are stationary. If not, then difference the data once, and inspect the plot of ∇y_t . If ∇y_t does not seem stationary either, take the second-order difference $\nabla^2 y_t$, and so on. In general, however, it is not recommended to difference more than two times.

As an addition to the time plots, plotting the sample autocorrelation function of the data can help to identify stationarity. Non-stationary data show a slow decay in autocorrelation as the time lag increases, while for stationary data, the autocorrelation will drop to zero relatively fast.

Once d has been set, either p or q can be selected by inspecting the autocorrelation function plot and the partial autocorrelation function plot of the differenced data, which respectively plot the sample autocorrelation function (ACF), defined in Equation (2.1), and the sample partial autocorrelation function (PACF), for several lags h . The PACF is the relationship

between an observation at time t and an observation at time $t - k$, removing the effects of all time lags in between, i.e. $1, 2, \dots, k - 1$. Then, appropriate values for either p or q are found with the following rules of thumb:

- The PACF plot of an ARIMA($p, d, 0$) process cuts off after lag p ; the ACF plot tails off.
- The ACF plot of an ARIMA($0, d, q$) process cuts off after lag q ; the PACF plot tails off.

When dealing with ARIMA(p, d, q) processes where both $p > 0$ and $q > 0$, the ACF plot and PACF plot will both tail off, and finding appropriate values for p and q turns into a trial-and-error approach, where models with different combinations of p and q are compared.

The methodology as described above is used often, but involves a lot of manual interventions. This makes it a rather subjective way of working, that is labour intensive, especially when a large number of time series needs to be modelled, and requires expert knowledge. Therefore, several automated approaches to select p , d and q have been proposed. One of them is the Hyndman-Khandakar algorithm, which methodology is summarized below, in a simplified way. For the full details, see Hyndman & Khandakar (2008).

Step 1. To define d , the Hyndman-Khandakar algorithm uses the Kwiatkowski-Phillips-Schmidt-Shin (KPSS) test, which is a statistical test used to determine stationarity of a time series. Only if there is enough statistical evidence, the null hypothesis that the time series is stationary will be rejected, and the time series is instead considered to be non-stationary. The detailed mathematics underlying the test can be found in Kwiatkowski, Phillips, Schmidt, & Shin (1992).

Using the KPSS test, first, the original data y_t are tested for stationarity. When y_t are considered stationary, $d = 0$, and when considered non-stationary, the first-order differenced data ∇y_t are tested for stationarity. Again, when ∇y_t are considered stationary, $d = 1$, and when considered non-stationary, the second-order differenced data $\nabla^2 y_t$ are tested for stationarity. This process is repeated until a stationary series is obtained.

Step 2. In the second step, four models are fitted to the d -times differenced data.

- An ARIMA(0, d , 0) model.
- An ARIMA(1, d , 0) model.
- An ARIMA(0, d , 1) model.
- An ARIMA(2, d , 2) model.

The model with the lowest AIC is selected. AIC, which stands for Akaike's Information Criterion, is a measure for the goodness-of-fit of a model, and can be calculated with Equation (2.20).

$$AIC = -2 \log(L) + 2k \quad (2.20)$$

Where L is the Gaussian likelihood of the data, and k is the number of free parameters in the model. In this case, $k = p + q + l + 1$, where $l = 1$ when a non-zero constant is included, and $l = 0$ otherwise. The '+1' term is included, since the variance of the residuals is also a parameter. To find the best fitting model, AIC should be minimized. The idea behind AIC is the following. The likelihood monotonically increases when more parameters are added to the model, and therefore, only maximizing the likelihood would favor a model that overfits

the data. AIC prevents such overfitting, by penalizing the likelihood with a term that is proportional to the number of parameters used in the model.

Step 3. In the third step, several variations of the model that was selected in step 2, are fitted to the d -times differenced data. These variations include:

- Models where either p or q vary ± 1 from the selected model, given that $p, q \geq 5$.
- Models where both p and q vary ± 1 from the selected model, given that $p, q \geq 5$.

From the selected model and all its variations, the model with the lowest AIC is chosen to be the new selected model, and step 3 is repeated. The algorithm stops when there are no variations of the selected model that have a lower AIC. In that case, the selected model is the optimal model, and forms the output of the Hyndman-Khandakar algorithm. The complete methodology of the algorithm as described above is summarized in Figure 2.2.

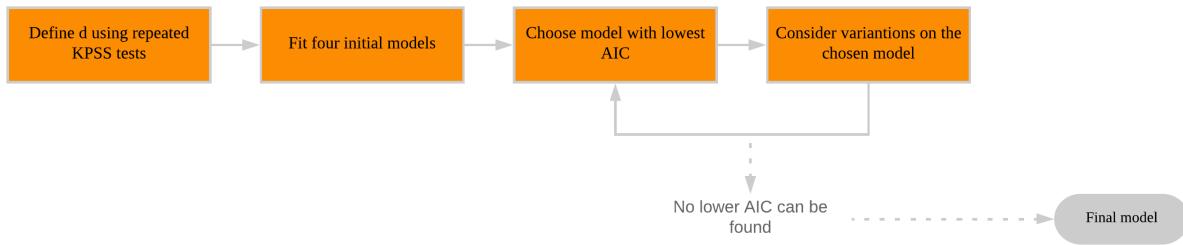


Figure 2.2: Summary of the Hyndman-Khandakar algorithm

2.4.2.3 Parameter estimation

When p , d and q are defined, the model parameters ϕ_1, \dots, ϕ_p and $\theta_1, \dots, \theta_q$ need to be estimated. Usually, this is done with *maximum likelihood estimation* (MLE). The likelihood is the probability of obtaining the observed data, given the model and specific parameter values. The parameter values that maximize the likelihood are called the maximum likelihood estimators of the true parameters, and will be used as the parameter estimates in the fitted ARIMA(p, d, q) model, which then is referred to as the maximum likelihood ARIMA(p, d, q) model. The detailed mathematical description of MLE for ARIMA models can be found in Brockwell & Davis (2002), section 5.2.

Note here that the Hyndman-Khandakar algorithm already produces a fitted model as output, and the parameter estimation as described in this section is done inside the algorithm, each time a model is fitted to the d -times differenced data.

2.4.2.4 Model checking

Model checking involves identifying if the fitted model is adequate. This is done by inspecting its residuals, which are defined as the difference between the actual observations and the corresponding fitted values, as shown in Equation (2.21).

$$\epsilon_t = y_t - \hat{y}_t \quad (2.21)$$

If the maximum likelihood ARIMA(p, d, q) model is the true process that generated the data, the residuals should be completely white noise. Recall, however, that the model is an estimation of the true process. Therefore, a good model that fits the data well, should have residuals with properties that *approximately* reflect those of white noise, i.e. a zero mean and no autocorrelation. If autocorrelation is present in the residuals, this means that there is still information left in the data, which could be used to create more accurate forecasts. A non-zero mean will lead to biased forecasts.

Autocorrelation in the residuals can be detected by a visual interpretation of the residual ACF plot, which will always show some autocorrelation, due to random variation. Therefore, given that n is the length of the modelled time series, and assuming a normal distribution, the residuals are considered to be uncorrelated when for at least 95% of the time lags, the residual ACF lies within the interval $[-1.96/\sqrt{n}, 1.96/\sqrt{n}]$.

Usually, several computations within the model fitting and forecasting process build on the assumption that the data come from a normally distributed population. For example, in MLE and the calculation of AIC, Gaussian likelihood is commonly used. Furthermore, prediction intervals of forecasts are in general derived by assuming a normal distribution. Normally distributed residuals indicate that these assumptions were valid, and are therefore a valuable property of a model. However, as stated by Brockwell & Davis (2002), using Gaussian likelihood is sensible even when the data are not normally distributed.

2.4.2.5 Forecasting

A fitted ARIMA(p, d, q) model can then be used to forecast the future values of a time series. To do so, Equation (2.19) is rewritten, such that the current value of the time series, y_t , is replaced by a future value of the time series, y_{t+h} , as showed in Equation (2.22).

$$\nabla^d y_{t+h} = \hat{\phi}_1 \nabla^d y_{t+h-1} + \dots + \hat{\phi}_p \nabla^d y_{t+h-p} + \hat{\theta}_1 \epsilon_{t+h-1} + \dots + \hat{\theta}_q \epsilon_{t+h-q} + \epsilon_{t+1} \quad (2.22)$$

Where h is the forecast horizon, i.e. the number of time lags ahead at which the forecast is made, p, d and q are known and constant, and $\hat{\phi}_1, \dots, \hat{\phi}_p$ and $\hat{\theta}_1, \dots, \hat{\theta}_q$ are the estimated parameter values, which are also constant.

When $h > 1$, more than one forecast has to be made. For example, the forecast of $\nabla^d y_{t+2}$, the value of the time series two time lags ahead, is based on $\nabla^d y_{t+2-1}$, the value of the time series one time lag ahead. Therefore, $\nabla^d y_{t+2-1}$ needs to be forecasted first, before $\nabla^d y_{t+2}$ can be forecasted. In general, this means that the uncertainty of the forecasts increases as h increases. This uncertainty is expressed by means of a prediction interval. Most often, the 95% prediction interval is used. Assuming normally distributed residuals, the lower and upper bound of the 95% prediction interval for the h -step forecast can be calculated with Equation (2.23) and Equation (2.24), respectively.

$$\ell = \hat{y}_{t+h} - 1.96 \hat{\sigma}_h \quad (2.23)$$

$$v = \hat{y}_{t+h} + 1.96 \hat{\sigma}_h \quad (2.24)$$

Where ℓ is the lower bound of the 95% prediction interval, v is the upper bound of the 95% prediction interval, \hat{y}_{t+h} is the forecasted value h time lags ahead. and $\hat{\sigma}_h$ is the estimated

standard deviation of the forecast distribution h time lags ahead, which is explained below. The 95% prediction interval can be interpreted as follows: there is a 95% probability that $\ell \leq y_{t+h} \leq v$.

Recall that in Definition 1, a time series was defined as a collection of random variables. In fact, to state it statistically correct, it is the distribution of the random variable h time lags ahead that is forecasted, rather than an individual value. This distribution is referred to as the forecast distribution, and the single forecasted value, also known as the *point forecast*, is then taken to be the mean of the forecast distribution. In Equation (2.23) and Equation (2.24), $\hat{\sigma}_h$ is the estimated standard deviation of the forecasted distribution, assuming it is a normal distribution with mean y_{t+h} and variance σ_h^2 . When $h = 1$, the residual standard deviation σ_ϵ is a good estimate for σ_h . However, for $h > 1$, computations get more complex. For a detailed description, see Shumway & Stoffer (2011), Section 3.5.

2.4.2.6 Accuracy evaluation

A good model fit, does not necessarily lead to accurate forecasts. Therefore, when evaluating its performance, the forecasting model should be used to forecast multiple values of new data that were not included in the model building process. The error of each individual forecast can be calculated with Equation (2.25).

$$e_{t+h} = y_{t+h} - \hat{y}_{t+h} \quad (2.25)$$

Where y_{t+h} is the observed data value h time lags into the future, and \hat{y}_{t+h} is the forecasted data value h time lags into the future. Obviously, future in this sense is relative to the model building period.

When making k different forecasts, the corresponding forecast errors e_1, e_2, \dots, e_k , can be summarized with an error metric. Several of those metrics exist. Some of them are only applicable to errors that all have the same units, while others may also be used when errors with different units are compared. Since all forecasts in this thesis are distances, the unit-dependent errors are adequate. Most commonly used are the Mean Absolute Error (MAE), which can be calculated with Equation (2.26), and the Root Mean Squared Error (RMSE), which can be calculated with Equation (2.27).

$$MAE = \frac{\sum_{i=1}^k |e_i|}{k} \quad (2.26)$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^k e_i^2}{k}} \quad (2.27)$$

Both the MAE and RMSE return values that are in the same scale as the original data. The MAE gives the same weight to all errors. The RMSE, however, gives large errors more weight than small errors, and therefore penalizes a large error variance. According to Chai & Draxler (2014), the RMSE usually is better at revealing differences in model performance.

In some of the works discussed in Section 1.3, such as Y. Li et al. (2015), Z. Yang et al. (2016) and Lozano et al. (2018), the Root Mean Squared Logarithmic Error (RMSLE) is

reported instead of the RMSE. Here, the natural logarithms of the observed and forecasted data values are used in the forecast error computation. The main reason for doing so, is that larger errors, usually occurring during peak hours or in areas/stations with a high usage intensity, do not dominate smaller errors.

2.4.2.7 Transformations

Often, forecasts can be improved by using mathematical transformations, such that the original data are adjusted for some known patterns causing non-stationary and/or non-linear behaviour. That is, the data are transformed in advance, and the modelling and forecasting procedures are applied to the transformed data. After forecasting the transformed data, forecasted values on the original scale are obtained based upon the inverse transformation, a process that is commonly called *back transforming*. A particularly useful transformation is the *log transformation*, which suppresses larger fluctuations that occur when the level of the time series increases. Furthermore, they guarantee strictly positive forecasted values. The log transformed data ω_t , is derived by taking the natural logarithm of the original data y_t , as showed in Equation (2.28).

$$\omega_t = \log y_t \quad (2.28)$$

However, care has to be taken when back transforming a log transformed forecast to the original scale. Intuitively, one would obtain the back transformed forecast \hat{y}_{t+h} by setting it equal to $e^{\hat{\omega}_{t+h}}$, where e is Euler's number. However, assuming that the forecast distribution of ω_{t+h} , Ω_{t+h} , is normal, with mean $\mu_{\Omega_{t+h}}$ and variance $\sigma_{\Omega_{t+h}}^2$, then the forecast distribution of y_{t+h} , Y_{t+h} , follows a log-normal distribution, with mean $\mu_{Y_{t+h}}$ as defined in Equation (2.29).

$$\mu_{Y_{t+h}} = e^{(\mu_{\Omega_{t+h}} + 0.5\sigma_{\Omega_{t+h}}^2)} \quad (2.29)$$

For the proof of this theorem, see Dambolena, Eriksen, & Kopcsó (2009). Hyndman & Athanasopoulos (2018) refer to $\mu_{Y_{t+h}}$ as the *bias-adjusted point forecast*.

2.4.3 Naïve forecasts

It is common practice to compare the errors of forecasts obtained with a fitted time series model to those of forecasts obtained with a very simple forecasting method. Such a simple method, is in that case referred to as a *baseline method*. If the more sophisticated model does not lead to considerably better forecast accuracies than the baseline, it can be dismissed (Hyndman & Athanasopoulos, 2018).

One of the simplest forecast methods around, often used as a baseline, is known as the *naïve method*. When forecasting with the naïve method, all forecasted values will be equal to the last observation, no matter how far the forecasting window h reaches, as shown in Equation (2.30).

$$\hat{y}_{t+h} = y_t \quad (2.30)$$

Where \hat{y}_{t+h} is the forecasted data value h time lags into the future, and y_t is the last observed data value.

2.4.4 Seasonal forecasts

ARIMA models as described in section 2.4.2 are designed for data without a seasonal component. With some modifications, they can be applied to seasonal data as well. That works as follows. Instead of an ARIMA(p, d, q) model, an ARIMA(p, d, q)(P, D, Q) model is fitted to the data. The (P, D, Q) part of the model works in a similar fashion as the (p, d, q) part, but relates to the seasonal component of the data. Hence, P is the number of seasonal autoregressive terms in the model, D is the order of seasonal differencing, and Q is the number of seasonal moving average terms. Where $p = 1$ means that the past observation y_{t-1} is used to model the current value y_t , setting $P = 1$ means that the past observation y_{t-m} is used to model the current value y_t , with m being the number of observations per seasonal cycle. The same holds for Q : setting $Q = 1$, means that the past error ϵ_{t-m} is used to model the current value y_t . Regarding the seasonal differencing parameter D , the first order seasonal difference of a time series is the series of changes from one seasonal period to the next (Shumway & Stoffer, 2011).

However, ARIMA(p, d, q)(P, D, Q), as well as several other commonly used seasonal models such as Holt Winters exponential smoothing, have two main limitations which make them unsuitable for some kind of data. Firstly, they were primarily designed to work with shorter seasonal periods, such as monthly data with patterns that repeat every year (i.e. $m = 12$). In the case of longer seasonal periods, which may occur for example in daily and sub-daily data, modelling becomes inefficient. In the R statistical software, for example, the `forecast` package (Hyndman & Khandakar, 2008) only allows seasonal periods up to $m = 350$ (Hyndman, 2010).

Secondly, these models can not handle more than one seasonal pattern at a time. Again, this can be problematic especially for daily data, in which both a weekly and yearly pattern may exist, and sub-daily data, in which even a daily, weekly and yearly pattern may exist. One of the alternative approaches proposed by Hyndman & Athanasopoulos (2018) works as follows. First, the data is decomposed into a trend, seasonal and remainder component. Then, the trend and remainder component are together modelled by a non-seasonal model, such as ARIMA(p, d, q), and forecasted accordingly. The seasonal component, in turn, can be forecasted with a seasonal naïve method, meaning that the forecasted value will be equal to the last observed value from the same season of the year. That is, the seasonal forecast for timestamp y_{t+h} will be equal to the last observed value in the sequence $\{y_{t+h-m \times 1}, y_{t+h-m \times 2}, \dots\}$. Then, the non-seasonal and seasonal forecasts are added back together, to obtain a single forecasted value.

2.5 Time series clustering

2.5.1 Dissimilarity measures

Time series clustering is a specific domain within the field of time series analysis. Given a set of individual time series, its objective is to group similar time series into the same cluster (Keogh & Lin, 2005). Logically, this involves the calculation of a measure that represents the similarity, or dissimilarity, between two time series. A wide range of such measures exist,

some of them based directly on the observations, others on specific features of the time series, and others on parameters or residual characteristics of models fitted to the time series.

Whenever the time series are of the same length, and observed at the same timestamps, a simple dissimilarity measure can be calculated by summing the ordered point-to-point distances between them. A well-known distance function is the Euclidean distance, as defined in Equation (2.31) (Cassisi, Montalto, Aliotta, Cannata, & Pulvirenti, 2012).

$$d(Y, X) = \sqrt{\sum_{t=1}^n (y_t - x_t)^2} \quad (2.31)$$

Where $d(X, Y)$ is the dissimilarity value between time series Y and X , y_t and x_t are the observations in respectively Y and X at time t , and n is the length of Y and X . A higher value of $d(X, Y)$ implies less similar time series. By definition, $d(X, Y) \geq 0$.

Using Euclidean distance as a dissimilarity measure is simple, but has drawbacks for certain applications. For example, it can not handle time series of different length, it is sensitive to outliers, and it can not capture out-of-phase similarities, which occur when two time series show similar patterns, but shifted over time. To deal with one or more of these drawbacks, several other dissimilarity measures for time series were developed, of which the *dynamic time warping distance* is best known. Dynamic time warping is based on classical algorithms for comparing discrete sequences with continuous sequences, and basically replaces the one-to-one comparison of Euclidean distances with a many-to-one comparison. However, despite its simplicity, the Euclidean distance approach still turns out to be very competitive with the more complex methods (Cassisi et al., 2012).

Once the dissimilarity values for all possible combinations between the analyzed time series are calculated, they are stored in an $n \times n$ matrix, where n is the number of analyzed time series, and the diagonal entries equal zero. Such a matrix is commonly referred to as a dissimilarity matrix, and can be used inside conventional clustering algorithms. In time series analysis, k-means clustering and hierarchical clustering are the most popular options for this task (X. C. Wang, Smith, & Hyndman, 2006). The latter is used in this thesis, and its theory is summarized briefly in the next section, based on G. Gan, Ma, & Wu (2007), Chapter 7 and Chapter 17.

2.5.2 Hierarchical clustering

Hierarchical clustering algorithms divide a set of data points into a sequence of nested partitions, where each partition consists of a different number of clusters. Two main types are distinguished: *agglomerative* hierarchical clustering, and *divisive* hierarchical clustering. In the first, the starting point is a partition in which all data points form a cluster on their own. Then, the two closest clusters, based on a pre-defined dissimilarity measure, are merged. This process is repeated until all data points are in one single cluster. The divisive method works the other way around: all data points start in the same cluster, which is split repeatedly, until the number of clusters equals the number of data points. Agglomerative hierarchical clustering is the most popular of the two types, and forms the focus of this section.

Again, defining a suitable dissimilarity measure is a core task in the process. A simple example is the *single link method*, where the dissimilarity between two clusters is defined as the shortest distance between a data point in the first cluster and a data point in the second cluster. In contradiction, the *complete link method* calculates the dissimilarity as being the longest possible distance between them. Other methods include the *group average method*, which calculates the average of the shortest distances between all pairs of data points, and the *centroid method*, which calculates the shortest distance between the cluster centroids. In all cases, the Euclidean distance is commonly used as the distance function.

A more general approach is known as the *Ward method*, developed by Ward Jr. (1963). In this method, the dissimilarity between two clusters is defined as the loss of information when the clusters are merged. The information loss of a merge between two clusters is quantified with Equation (2.32).

$$\Delta I = I(C_m) - I(C_1) - I(C_2) \quad (2.32)$$

Where ΔI is the information loss, C_m is the merge between clusters C_1 and C_2 , and $I(C_m)$, $I(C_1)$ and $I(C_2)$ are the information criteria of respectively C_m , C_1 and C_2 . Ward Jr. (1963) did not put a hard restriction on how such an information criterion should be quantified, but usually, it is set to be the *error sum of squares*, calculated with Equation (2.33).

$$I(C) = \sum_{i=1}^n (c_i - \mu(C))^2 \quad (2.33)$$

Where c_i are the data points in C , $\mu(C)$ is the center of mass of C , and n is the number of data points in C . In other words, $I(C)$ is the sum of the Euclidean distances from all data points in the cluster, to the center of mass of the cluster.

If one is interested in obtaining only one single partition, it is necessary to find a suitable value for the desired number of clusters k . It is common practice to do so by visually interpreting the dendrogram of the hierarchical clustering, which is a diagram representing the output in a tree structure, but automated approaches have been developed as well. Most of them are based on the idea that in an ideal situation, clusters are compact and clearly separated from each other. However, minimizing the variance within the clusters will always favor the situation where each data point forms a cluster on its own, while maximizing the variance between the clusters will always favor the situation where all data points are together in one cluster. Therefore, most approaches combine those two operations, in order to find the best possible partition.

An example of such an approach is the *Dunn Index*, developed by Dunn (1974). For a specific partition into k clusters, it calculates the ratio of the smallest distance between two data points that are not in the same cluster to the largest distance between two data points that are in the same cluster. This is shown in Equation (2.34).

$$V(\Lambda_k) = \min \left\{ \min \left(\frac{D(C_i, C_j)}{\max \text{diam}(C_l)} \right) \right\} \quad (2.34)$$

Where $V(\Lambda_k)$ is the Dunn Index of a partition Λ_k with k clusters, $1 \leq i, j, l \leq k$, $D(C_i, C_j)$ is the Euclidean distance between a data point in cluster $C_i \in \Lambda_k$ and a data point in cluster

$C_j \in \Lambda_k$, given that $C_i \neq C_j$, and $\text{diam}(C_l)$ is the largest Euclidean distance between two data points in cluster $C_l \in \Lambda_k$. To find the optimal partition Λ_k^* , the Dunn Index should be maximized.

2.5.3 Spatial time series clustering

Spatial time series are time series with a spatial reference, i.e. time series that are linked to geographical locations (Kamarianakis & Prastacos, 2005). With such series, similarity can not only be expressed in terms of similar data values, but also in terms of spatial proximity. These two, however, are likely to be related, given the concept of spatial dependence, which is similar to the temporal autocorrelation described in Section 2.2.1, in the sense that the structure of the correlation between random variables is derived from a specific ordering, determined by their relative position in geographic space (Anselin, 2010). Hence, time series linked to geographical locations that are close to each other, are likely to show similar temporal patterns.

When clustering a set of spatial time series, it may be desired that the clusters are not only similar in data values, but also form spatially connected sets. In that case, constraints need to be imposed on the possible outcomes of the clustering process. This can be done in a strict way, where the resulting partition is forced to consist of spatially contiguous clusters. When the spatial dependence between the series is really strong, this may be a sensible approach. In less coherent cases, however, this may group time series with different patterns into the same cluster, just because they are close to each other in space. Hence, an adequate balance between the data similarity and the spatial similarity, needs to be found, without artificially forcing a strong spatial dependence on the time series.

For this, Chavent, Kuentz-Simonet, Labenne, & Saracco (2018) developed a variation on the hierarchical clustering algorithm, called *spatially constrained hierarchical clustering*, which is summarized in this section. The algorithm takes two dissimilarity matrices as input. The first one gives the dissimilarity values in the *feature space*, i.e. the dissimilarities of the data values of the observations, while the latter gives the dissimilarity values in the *constraint space*, i.e. the dissimilarities of the geographical locations of the observations.

Spatially constrained hierarchical clustering uses a Ward-like method to define which clusters will be merged at each step, but with a different definition of the information criterion of a cluster, as shown in Equation (2.35).

$$I(C) = (1 - \alpha) \sum_{i=1}^n (c_i - \mu(C))^2 + \alpha \sum_{i=1}^n (c_i^* - \mu^*(C))^2 \quad (2.35)$$

Where c_i are the data points in C , with normalized values taken from the feature space dissimilarity matrix, and $\mu(C)$ is the center of mass of C , computed with those values. c_i^* are the same data points, but with normalized values taken from the constraint space dissimilarity matrix, and $\mu^*(C)$ is the center of mass of C , computed with those values. Furthermore, n is the number of data points in C and α is the mixing parameter, where $0 \leq \alpha \leq 1$. Chavent et al. (2018) also present more general approaches, in which the

calculated distances in Equation (2.35) are not necessarily Euclidean, and where observations can be weighted, but these are not covered in this thesis.

With the information criterion of a single cluster calculated as in Equation (2.35), the information loss of a merge between two clusters is calculated in the same way as in regular Ward hierarchical clustering (Equation (2.33)). Then, at each merging step, two clusters are merged such that the loss of information is minimized.

The mixing parameter α plays a key role in spatially constrained hierarchical clustering. It sets the importance that is given to the spatial constraint. The higher α , the more the result of the clustering procedure is influenced by the spatial locations of the data points. When $\alpha = 0$, the data are clustered without any spatial constraint, while $\alpha = 1$ leads to a clustering only based on the spatial location of the data points. Therefore, it is important to determine a suitable value for α . Chavent et al. (2018) propose the following approach. First, α is set to zero, and a hierarchical clustering without spatial constraint is performed. The resulting sequence of partitions is rendered as a dendrogram, and the optimal number of clusters k^* is defined visually. Then, several spatially constrained hierarchical clustering procedures are performed, each with a different value of α , and $k = k^*$. Since k is fixed, the outputs are always single partitions. For each cluster in such a partition the information criterion regarding the feature data (i.e. the first part of Equation (2.35)) and the information criterion regarding the constraint data (i.e. the second part of Equation (2.35)), are calculated separately, and also summed separately over all clusters in the partition. These two summed values are then plotted, with α on the x-axis. In the end, this lead to a plot that shows the loss of information in the feature space and the gain of information in the constraint space, as α gets larger. With such a plot, α can be chosen such that the trade-off between the loss and gain of information in the two spaces is considered acceptable.

Chapter 3

System architecture

This chapter describes the methodology of DBAFS. It builds on the theory discussed in Chapter 2, and is structured as follows. In the first section, a general overview of the complete forecasting system is given. Section two presents the software that underlies DBAFS. The third, fourth and fifth section discusses the inputs to the system, including the computations that are done on the database server of the dockless bike sharing system. Subsequently, section six, seven and eight cover the detailed methodologies of all the distinct components of the system architecture separately.

3.1 Overall design

The goal of DBAFS is to forecast the distance to the nearest available bike for a given location and a given timestamp in the future. It is meant to be used by both the operators and users of a dockless bike sharing system, which from now on are referred to as *users* of DBAFS. A forecast is made every time a user requests one. In intensively used bike sharing systems, this can mean that several hundreds of forecasts are required every day, all based on different historical datasets. All these datasets usually consist of a time series with a high temporal resolution. Although the data may be complex, it would be inconvenient for the users if forecasts take a lot of time or need manual interventions. Taking into consideration the above-mentioned challenges, DBAFS should be a *fast* and *automated* process that still produces as *accurate* forecasts as possible. Optimizing all of them, is a utopia. Faster forecasts, will probably have a negative affect on the accuracy, and aiming for an automated procedure, means that models can not be manually updated and fine-tuned. The goal, therefore, is to find an acceptable compromise between the three requirements.

The most time consuming part of the system is the selection of an appropriate model and the estimation of its parameters. If this had to be done at every forecast request separately, forecasts would take too much time. Therefore, in DBAFS, forecasting models are build only once in a while at a limited number of locations. Each individual forecast will inherit the structure and parameters of one of those pre-build models, rather than building a new model on its own.

The approach of building models only at a limited number of locations, involves the selection of those locations. In DBAFS, this is done by dividing the system area of the dockless bike sharing system into spatially contiguous clusters, where each cluster contains the areas that show similar weekly patterns in the historical data. Then, each cluster is represented by a single *model point*, which is a geographical location where a model is build. An individual forecast takes the model structure and parameters of the model point that is in the same cluster as the location of the forecast.

The architecture of DBAFS builds on two main assumptions, one regarding the spatial dependence in the data, and the other regarding the temporal dependence in the data. Firstly, it is assumed that the processes generating the historical data are spatially dependent, such that spatially contiguous clusters containing areas with similar temporal patterns can be constructed, and moreover, that they are similar enough at each location in a cluster to be described by the same model. Secondly, it is assumed that these processes do not change radically over a short time period, such that a model fitted to a set of historical data, can still adequately describe new data coming from a location in the same cluster. Of course, these assumptions will not always be completely valid, but are made to obtain a reasonable compromise between fast and accurate forecasts.

The clustering, model building and forecasting processes can be seen as three distinct processing loops, that together make up DBAFS. The forecast loop runs every time a user makes a forecast request. The model loop only runs every n_m weeks, and the cluster loop every n_c weeks. n_m should be chosen such that new models are build when the patterns in the historical data have changed considerably. n_c should be chosen such that new clusters are defined when the spatial distribution of the weekly patterns in the historical data has changed considerably, and will, in most cases, be much larger than n_m . The cluster, model and forecast loops are all completely automated and do not require any manual interventions. The overall design of DBAFS as described above is summarized in Figure 3.1. The inputs of the system, i.e. the system area, database and forecast request, are covered in Section 3.3, 3.4 and 3.5, respectively, while Section 3.6, 3.7 and 3.8 describe the detailed designs of the three processing loops.

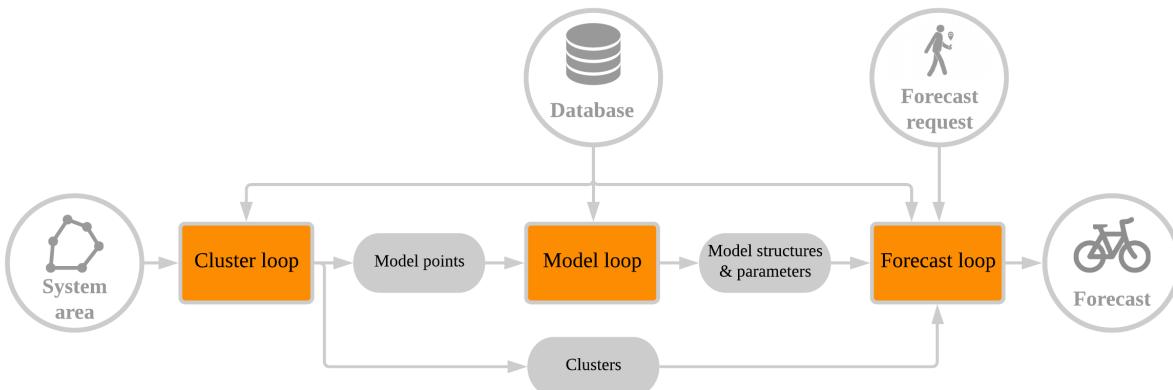


Figure 3.1: Overall design of DBAFS

3.2 Software

The underlying code of DBAFS (see Appendix A) is written in the R programming language (R Core Team, 2013). However, Structured Query Language (SQL) statements are nested within the R code to retrieve data from a PostgreSQL database (PostgreSQL, 2014), and to run some of the heavier data pre-processing computations on the database server. These computations are discussed in Section 3.4.

On top of functions that are included in R by default, DBAFS makes use of several extensions, listed below.

- The `ClustGeo` package, for spatially constrained clustering (Chavent et al., 2018).
- The `c1Valid` package, for calculating the Dunn Index (Brock, Pihur, Datta, & Datta, 2008).
- The `forecast` package, for building forecasting models, decomposing time series, and forecasting time series (Hyndman & Khandakar, 2008).
- The `lubridate` package, for processing dates and timestamps (Gromelund & Wickham, 2011).
- The `RPostgreSQL` package, for connecting to a PostgreSQL database and running SQL code on the database server (Conway, Eddelbuettel, Nishiyama, Prayaga, & Tiffin, 2017).
- The `sf` package, for processing spatial data (Pebesma, 2018).
- The `tsibble` package, for pre-processing time series datasets (E. Wang, Cook, & Hyndman, 2018).

3.3 System area

Each dockless bike sharing system has a system area, in which the bikes can be used. Usually, leaving a bike outside of the system area, will result in a fine. DBAFS produces forecasts only inside the system area, and therefore, the geographical outline of this area needs to be provided. DBAFS accepts all filetypes that can be read with a driver supported by the `st_read` function in the `sf` package, given that the included feature is either a polygon or multipolygon. The accepted filetypes include, among others, ESRI shapefiles, GeoPackage files and GeoJSON files. It is also possible to retrieve the feature from a PostgreSQL database.

3.4 Database

In a dockless bike sharing system, each bike is equipped with a Global Positioning System (GPS). Every i_d minutes, the geographical locations of all bikes are saved into a database, together with the corresponding timestamp. The locations of the bikes that are not in use at the current time, and thus available, are visible to the users of the system in a mobile application, and stored separately from the data regarding bikes that are in use.

The geographical location of a bike is spatial data, and should be stored as such. An advanced

and open source database management system for spatial data is PostgreSQL in combination with the PostGIS extension. DBAFS requires the data to be stored in such a database, and to have a sub-daily temporal resolution. Each feature represents the location of an available bike at a certain timestamp and should at least have the following fields.

- A timestamp of data type `timestamp with time zone`.
- A geographical location of data type `geometry(Point)`.
- A unique ID of the bike to which the feature belongs.

Data are pre-processed on the database server, and only the data that are needed, are loaded into memory. In DBAFS, this pre-processing step involves two different procedures. The first one leads to data that contain information about the distance to the nearest bike for several timestamps in the past, and is discussed in the next section, while the latter produces a dataset with all the bicycle pick-ups in the database, and is discussed in Section 3.4.2.

3.4.1 Distance data

For a given location, the distance from that location to the nearest available bike is calculated for each timestamp $t \in T$, where T is a regularly spaced time interval containing timestamps within the timespan of the historical data. The temporal resolution of T equals i_s minutes, where $i_s \geq i_d$. The nearest available bike is found by a nearest neighbour searching process that uses spatial indices on the geometries. In practice, this means that it is not needed to first compute the distances to all available bikes, which would slow down the process vastly. If no bike can be found, for example due to a server error at that timestamp, or the unlikely event that there are no bikes available anywhere in the system, the corresponding feature will be inserted in the data, with a non-available distance value, NA . That is, after pre-processing, the resulting time series will always be regular, with all timestamps $t \in T$ present. This also means that when data are queried for several locations at the same times, the resulting time series will always have the same length.

The calculated distances are great-circle distances assuming a spherical earth with a radius equal to the mean radius of the WGS84 ellipsoid, as showed in Equation (3.1).

$$L_{AB} = \frac{(2a + b)}{3} \times \frac{\pi}{180} \times \arccos(\sin\phi_A \sin\phi_B + \cos\phi_A \cos\phi_B \cos\Delta\lambda) \quad (3.1)$$

Where L_{AB} is the great-circle distance between point A and point B in meters, ϕ_A and ϕ_B are the latitudes of respectively point A and B in degrees on the WGS84 ellipsoid, and $\Delta\lambda$ is the difference in longitude between the two points, i.e. $\lambda_B - \lambda_A$, in degrees on the WGS84 ellipsoid. Furthermore, a is the equatorial radius of the WGS84 ellipsoid in meters, which is defined to be 6378137, and b is the polar radius of the WGS84 ellipsoid in meters, which is defined to be $6378137 \times (1 - 298.257223563^{-1}) = 6356752.3142$ (Iliffe & Lott, 2008).

The sphere is chosen since calculating distances on the ellipsoid itself slows down computations, and, on the geographical scale of a dockless bike sharing system, has an accuracy gain that can be neglected. Working with the shortest distance over the street network might in most cases be more appropriate, but at the same time involves much more complex

computations, especially when either the given location or the locations of the bikes are not exactly on the network lines.

The output of this pre-processing operation is a time series with T features and a temporal resolution of i_s , belonging to one single location in the system area of the dockless bike sharing system. Each feature contains a timestamp and the great-circle distance from the given location to the nearest available bike in meters. Such data are referred to in this thesis as *distance data*.

3.4.2 Usage data

A pick-up is the moment that a user of the dockless bike sharing system unlocks a bike to make a trip. For the historical database containing the locations of the available bikes, this means that the bike that is picked-up will be present in the data at the last timestamp before the pick-up, but missing at the first timestamp after the pick-up. In DBAFS, this is used to retrieve all the pick-ups from the database. Historical data with the highest possible temporal resolution, i.e. i_d minutes, are queried for one single bike ID. Then, all timestamps that are missing, are added to the data, but without an available location. If feature j has an available location, but feature $j + 1$ has not, j is considered a pick-up. This procedure is repeated for all individual bikes. If more than 20% of the features within the same minute are considered pick-ups, it is assumed that this was caused by a server error, and they are removed from the data.

The output of this pre-processing operation is a data frame with all the features in the database that are considered pick-ups. Each feature has at least a timestamp, a geographical location and a bike ID. The number of pick-ups in an area represents the usage intensity of the bike sharing system. Such data are therefore referred to in this thesis as *usage data*.

Obviously, the procedure described in this section has some deficiencies. The removal of a bike by the system operator, for redistribution or maintenance purposes, is falsely considered to be a pick-up. Specific information about redistribution patterns can be added, but will in many cases be unavailable, and even if available, those patterns may be too irregular to implement adequately in the workflow. However, in DBAFS, the usage data are only used to define the location of the model point in a cluster, and not to analyze usage patterns into detail. Therefore, fully accurate data are not indispensable for this purpose, and the current procedure forms a sufficient basis.

3.5 Forecast request

A forecast request is made by a user. DBAFS assumes such a request to be composed of the geographical coordinates of the location at which the forecast should be made. The coordinates can be expressed in any coordinate reference system that is included in the PROJ library (PROJ-contributors, 2018). The timestamp can be expressed in any time zone that is included in the Time Zone database (Eggert & Olson, 2018).

3.6 Cluster loop

The main purpose of the cluster loop is to find suitable locations for the model points. The loop starts by laying a grid with square cells of $p \times p$ meters over the system area of the dockless bike sharing system, such that each location in the system area is part of one of those grid cells. Then, the geographical coordinates of the centroids of the grid cells are calculated, and m_c weeks of distance data are queried for each of those centroids.

The result of this query operation is a set of n time series, where n is the number of cells in the overlaying grid. To reduce the dimensionality of the clustering task, each of those time series is simplified by averaging its values per hour of the week. This is followed by a min-max normalization, such that time series that show the same patterns over time, but with different means, will be considered similar. The normalized values are calculated with Equation (3.2).

$$\hat{y}_t = \frac{y_t - y_{min}}{y_{max} - y_{min}} \quad (3.2)$$

Where \hat{y}_t is the normalized value of y_t , y_{min} is the minimum value in the time series, and y_{max} is the maximum value in the time series. By definition, $0 \leq \hat{y}_t \leq 1$.

For all possible combinations of the n averaged, normalized time series, a dissimilarity value is calculated based on the Euclidean distance between the two series, as defined in Equation (2.31). Since all time series have the same length, and observations at the same timestamps, the Euclidean approach is appropriate, and for the sake of simplicity, chosen over dynamic time warping. Furthermore, since out-of-phase similarities are ignored, areas where similar peaks and valleys in the data occur at different times of the week, will be grouped into different clusters, which gives a better representation of the spatio-temporal dynamics of the bike sharing system.

All Euclidean dissimilarity values are stored together in a $n \times n$ matrix and form the time series dissimilarity matrix A . At the same time, a spatial dissimilarity matrix B is created. This matrix is equal to $1 - C$, where C is the adjacency matrix of the n grid cells. That is, B is a $n \times n$ matrix in which $b_{i,j} = 0$ when grid cells i and j are neighbours, and $b_{i,j} = 1$ otherwise.

A and B are used as the dissimilarity matrices of respectively the feature space and the constraint space in a spatially constrained hierarchical clustering procedure, which was introduced in Section 2.5.3. Before the final clustering procedure can start, the number of clusters k and the value of the mixing parameter α need to be set. DBAFS does this based on the approach proposed by Chavent et al. (2018), which was discussed in Section 2.5.3, but replaces the manual interpretation of plots by a fully automated method, as described below.

At first, only the dissimilarity values in the feature space are clustered, i.e. a spatially constrained hierarchical clustering with $\alpha = 0$ is performed, which results in a sequence of partitions $\{\Lambda_k\}$. For each $k \in K$, where K is a finite set of strictly positive integers, the Dunn Index $V(\Lambda_k)$ of a specific partition Λ_k is calculated with Equation (2.34). Then, the value of k that maximizes $V(\Lambda_k)$ is chosen as optimal value of k , and referred to as k^* .

Secondly, for each $\omega \in \Omega$, where $\Omega = \{0, 0.1, 0.2, \dots, 1\}$, a spatially constrained hierarchical clustering with $k = k^*$ and $\alpha = \omega$ is performed, which results in a set of partitions $\{\Lambda_\omega\}$, of the same length as Ω . For each partition Λ_ω , the sum $\sum I_f(C_i^\omega)$ and the sum $\sum I_c(C_i^\omega)$ are calculated, where C_i^ω are the clusters in Λ_ω , I_f is the information criterion regarding the feature data (i.e. the first part of Equation (2.35)) and I_c is the information criterion regarding the constraint data (i.e. the second part of Equation (2.35)). Then, the value of ω that maximizes $\sum I_c(C_i^\omega)$, given that $((\sum I_f(C_i^\omega)) / \sum I_f(C_i^0)) \geq 0.9$, is chosen as the optimal value of α , and referred to as α^* . That is, clusters are made as spatially contiguous as possible, with the restriction that this can never lead to an information loss in the feature space of more than 10%.

With A, B, k^* and α^* set, the final spatially constrained hierarchical clustering is performed. The output of this procedure is a single partition, in which all time series are grouped into a cluster. Some extra restrictions are imposed subsequently. Since the spatial constraint was not strict, it is not guaranteed that all the clusters in this partition are fully spatially contiguous. Clusters consisting of more than one set of spatially connected grid cells, can occur in situations where striving for full spatial contiguity would lead to a too large information loss in the feature space, and thus, clusters that would not truly represent areas with similar patterns in the distance data. In such cases, all distinct spatially contiguous areas in these clusters, will be treated as separate clusters, with their own model point. However, this may lead to a high number of model points that each represent a very small area. When this area has a high usage intensity, the described situation is acceptable. When this area has a very low usage intensity, on the other hand, it is unwanted to have a separate model point representing it. Therefore, whenever a cluster has a usage intensity of less than two bicycle pick-ups per day, it will be merged with the closest neighbouring cluster, which is found by minimizing the inter-centroid distance.

Now, each cluster is guaranteed to be spatially contiguous, and gets assigned one model point. Before the locations for the model points are chosen, usage data is queried from the database, and the total number of pick-ups is calculated for each grid cell. This number is assigned as a variable to the corresponding grid cell centroids. Then, for each cluster, the arithmetic means of the coordinates of all grid cell centroids in that cluster, are calculated, weighted by the number of pick-ups. Equation (3.3) shows the calculation of the weighted average latitude of a cluster, while Equation (3.4) shows the calculation of the weighted average longitude of a cluster.

$$\phi^* = \frac{\sum_{i=1}^m \phi_i \times p_i}{\sum_{i=1}^m p_i} \quad (3.3)$$

$$\lambda^* = \frac{\sum_{i=1}^m \lambda_i \times p_i}{\sum_{i=1}^m p_i} \quad (3.4)$$

Where ϕ^* and λ^* are respectively the weighted average latitude and the weighted average longitude of the cluster, ϕ_i and λ_i are respectively the latitude and longitude of the i^{th} grid cell centroid in the cluster, p_i is the number of pick-ups in the i^{th} grid cell in the cluster, and m is the total number of grid cells in the cluster.

The combination $\{\phi^*, \lambda^*\}$ forms the coordinate pair of the weighted centroid of the cluster. This weighted centroid is then chosen to be the model point of that cluster. In this way, a

model point is a cluster centroid which is dragged towards the areas where the usage intensity of the bike sharing system is higher, and where accurate forecasts are thus more important. The model points of all clusters are send to the model loop. Finally, for each cluster, grid cells are first dissolved, and then clipped by the system area, to form one geographic outline of that cluster. The geographic outlines of all clusters, stored as polygons, are send to the forecast loop. The complete methodology of the cluster loop as described above is summarized in Figure 3.2.

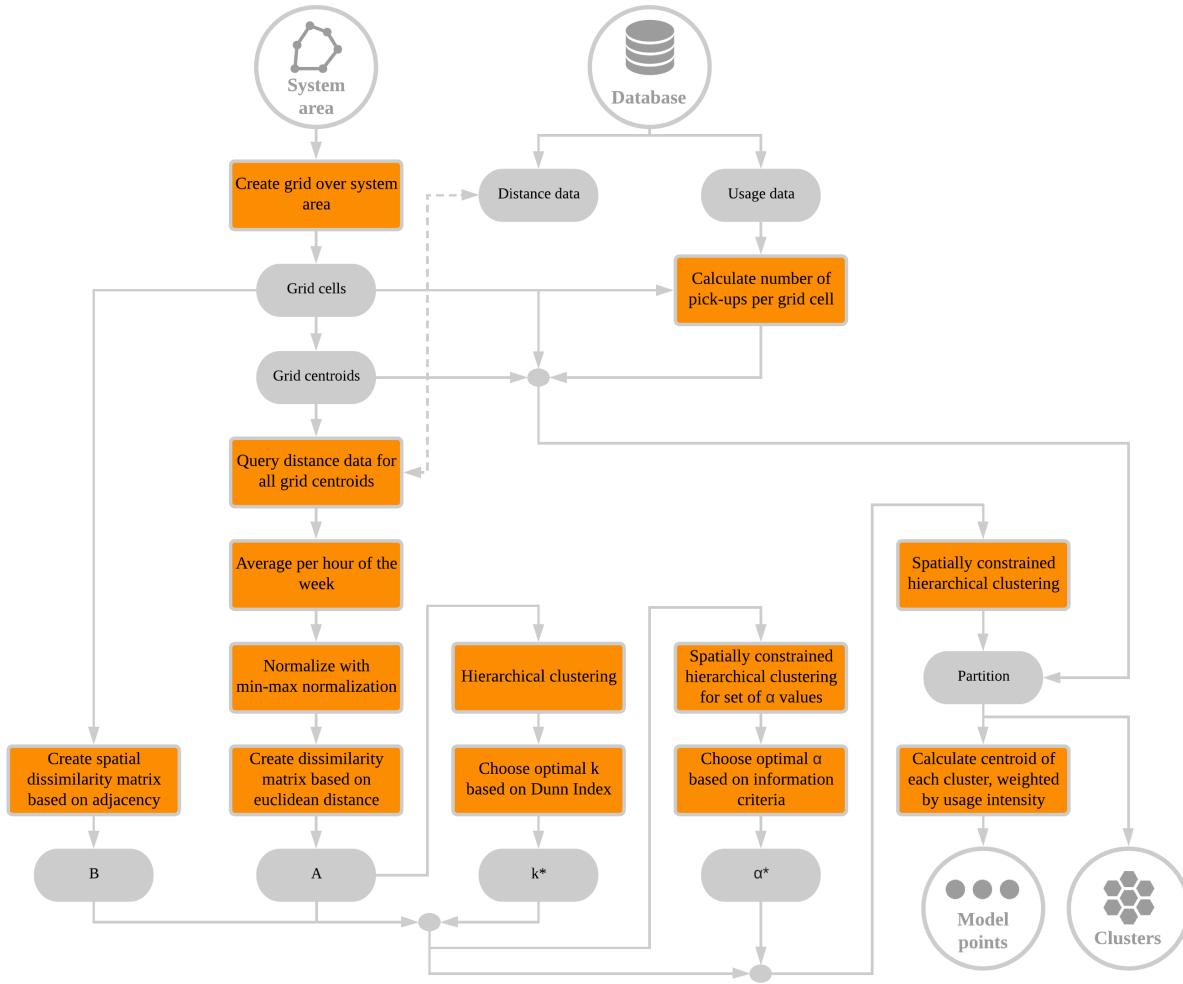


Figure 3.2: Methodology of the cluster loop

3.7 Model loop

The main purpose of the model loop is to fit time series models to the historical data of a limited set of geographical locations. These locations are called the *model points*, and result from a previous pass through the cluster loop. For each model point, m_m weeks of distance data are queried. All data are log-transformed, to stabilize the variance, and to make sure

that, when using the models for forecasting, the forecasted distances will always be larger than zero.

If the data are seasonal, they will pass through the decomposition process sequence. There, they will be decomposed into a trend, seasonal and remainder component with STL, as introduced in Section 2.3.3. Single seasonal data, with either a daily or a weekly seasonal pattern, will be decomposed once. Multiple seasonal data, that show both a daily and a weekly seasonal pattern, will first be decomposed assuming that only daily seasonality is present, after which the trend and remainder component are added together, and decomposed again, now assuming weekly seasonality. Hence, such data are eventually decomposed in a trend, remainder and two seasonal components. Since STL is performed on the log transformation of the original data, this indirectly implies that the original data are decomposed in a multiplicative way.

STL requires a set of parameters to be defined in advance. For most of them, there exist clear guidelines for the choice of their values, indited by R. B. Cleveland et al. (1990). Below, all STL parameters are listed, including their quantification as used in DBAFS.

- n_p , the number of observations per seasonal cycle. When decomposing assuming daily seasonality, $n_p = 60 \times 24/i_s$, and when assuming weekly seasonality, $n_p = 60 \times 24 \times 7/i_s$.
- n_i , the number of passes through the inner loop within one pass through the outer loop. It should be chosen large enough such that the updating of the seasonal and trend components converges. R. B. Cleveland et al. (1990) show that this convergence happens very fast, and that, inside a pass through the outer loop, only one pass through the inner loop is already sufficient. Hence, in DBAFS, $n_i = 1$.
- n_o , the number of passes through the outer loop. To have near certainty of convergence, R. B. Cleveland et al. (1990) recommend ten passes through the outer loop. In R, to be extra safe, the default is set to fifteen passes. This will not be changed in DBAFS, hence $n_o = 15$.
- n_s , the seasonal smoothing parameter. It should be chosen large enough to avoid overfitting, but small enough to allow slight variations over time. The choice of n_s is the only one where R. B. Cleveland et al. (1990) propose a manual approach, that involves a visual interpretation of the time series plot. For an automated process that decomposes several time series, this is problematic. Hyndman & Athanasopoulos (2018), however, argue that a value of thirteen usually gives a good balance between overfitting and allowing slight variations. In DBAFS, their recommendation is used. Hence, $n_s = 13$.
- n_l , the low-pass filter smoothing parameter. R. B. Cleveland et al. (1990) show that n_l always can be set equal to the least odd integer greater than or equal to n_p , which is done in DBAFS as well.
- n_t , the trend smoothing parameter. It should be chosen large enough such that seasonal variation does not end up in the trend component, but small enough such that low-frequency effects do not end up in the remainder component. To achieve this goals, R. B. Cleveland et al. (1990) show that n_t should be chosen to be the smallest odd integer that satisfies the inequality $n_t \geq 1.5n_p/(1 - 1.5n_s^{-1})$. In DBAFS, this is done as well.

Once the data are decomposed in a trend component, a remainder component and one or two seasonal components, the trend and remainder are added together, and send to the ARIMA process sequence. This part of the data can be seen as the log-transformed, deseasonalized original data, and should not contain seasonal patterns anymore. Data that were originally already non-seasonal, skip the decomposition process sequence completely, and are send to the ARIMA process sequence directly after the log transformation. Both types are from now on referred to as the *non-seasonal data*.

In the ARIMA process sequence, an ARIMA(p, d, q) model is fitted to the non-seasonal data, by applying the Hyndman-Khandakar algorithm, as described in Section 2.4.2.2. In R, the Hyndman-Khandakar algorithm is implemented in the `auto.arima` function from the `forecast` package, with the extra restriction that the order of differencing d is not allowed to be larger than two. It also allows missing values, by handling them exactly. This is an important characteristic, since it means that models will be fitted even if some observations are missing due to server errors.

To determine if the data of a model point should pass through the decomposition process sequence, and if yes, how many seasonal components should be subtracted, it is necessary to first identify the seasonal patterns in the data. This is done with a variation on what Hyndman & Athanasopoulos (2018) refer to as *time series cross-validation*, and works as follows. Four different seasonality options are considered:

- no seasonality
- only daily seasonality
- only weekly seasonality
- both daily and weekly seasonality.

Then, the first two of the n_w weeks of data are selected and log-transformed. Four different models are fitted to these data, each assuming a different seasonality option. That is, when the option of no seasonality is considered, the data are directly inputted into the ARIMA process sequence. When one of the other options is considered, the data first pass through the decomposition process sequence, and then, the deseasonalized data are inputted into the ARIMA process sequence. Subsequently, each day in the first week following the ‘model building weeks’, is forecasted separately. For the first day, this simply means that the non-seasonal data on which the ARIMA(p, d, q) model is build, are forecasted $60 \times 24/i_s$ time lags ahead. If present, the seasonal component is forecasted in a naïve way, and added to each result. For the second day, however, one extra day of data is added, and the same ARIMA(p, d, q) model is used to forecast the non-seasonal part of this extended data $60 \times 24/i_s$ time lags ahead, and if present, the naïve seasonal forecasts are added to the results. This process repeats for all seven days, each time using one extra day of data.

Once all days in this ‘forecasting week’ are forecasted, the two weeks of data on which the models were build, are now extended by one week of new data. On this three-week dataset, new models are build for each of the four seasonality options, and again, each day in the next week is forecasted separately. This shifting of the model building period keeps repeating, until there are no more weeks left to forecast. Then, for each of the seasonality options, the total RMSE of all forecasts is calculated. The option with the lowest RMSE, is the identified

seasonal pattern of the data.

After the log-transformation, seasonality detection, possible decomposition, and model building, the following output is obtained. All model points have an ARIMA(p, d, q) model that describes the non-seasonal part of their data. Additionally, the length of the seasonal period in their data is known. This can either be a single non-zero integer, in the case of only a daily or weekly seasonality, a vector of two non-zero integers, in the case of both a daily and a weekly seasonality, or zero, in the case of no seasonality. The chosen values p, d and q of the ARIMA model, the estimated parameter values $\hat{\phi}_1, \dots, \hat{\phi}_p$ and $\hat{\theta}_1, \dots, \hat{\theta}_q$ of the ARIMA model, and the identified length of the seasonal period, L_s , are send to the forecast loop. The complete methodology of the model loop as described above is summarized in Figure 3.3.

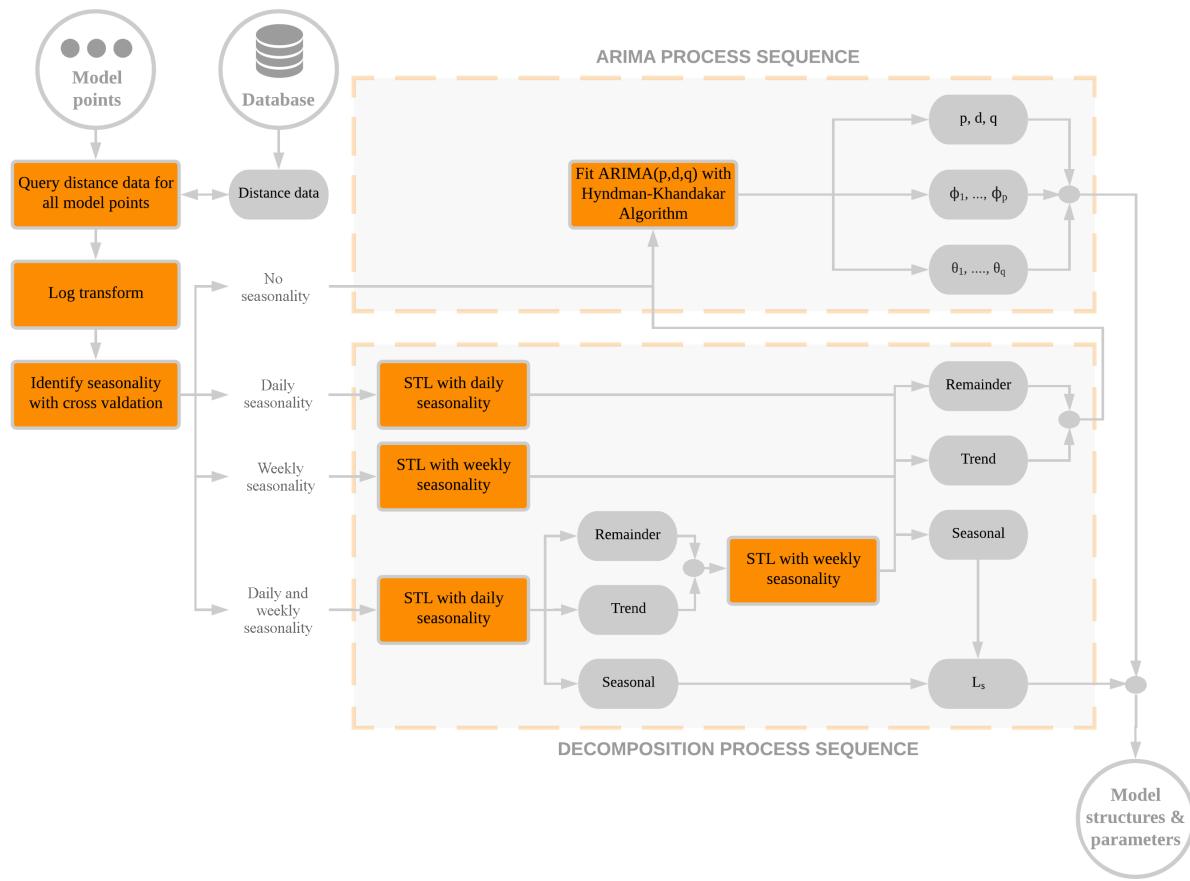


Figure 3.3: Methodology of the model loop

3.8 Forecast loop

The main purpose of the forecast loop is to produce a forecast whenever it is requested by a user. The forecasting task is split in two: seasonal forecasts capture the seasonal patterns in the data, while an ARIMA(p, d, q) model takes care of the short-term dynamics.

The geographical location that comes with such a forecast request, is intersected with the clusters that resulted from a previous pass through the cluster loop. This process returns the cluster in which the requested forecast location lies. Subsequently, the model structure and parameters from the model that belongs to this specific cluster, are taken from a previous pass through the model loop.

Since the clusters represent areas with similar patterns in the data, but not necessarily with similar means, the inherited model structure only provides the length of the seasonal patterns, and not the values corresponding to each season. Therefore, for the location of the forecast request, m_f weeks of distance data are queried, which will be used for seasonal decomposition, whenever the inherited model structure has an identified seasonality. The length of these data should be at least twice the length of the longest seasonal pattern, plus one observation. For example, when a weekly seasonality is present in hourly data, the data needed for forecasting should at least contain $24 \times 7 \times 2 + 1 = 337$ observations.

The queried distance data are log-transformed. Then, they are decomposed by STL, using the identified seasonal period length(s) L_s , which is stored in the provided model structure. When $L_s = 0$, this decomposition step is skipped, and the data are treated in the same way as the combination of trend and remainder that outputs from STL. Both types are referred to as the *non-seasonal data*.

With the ARIMA(p, d, q) model that was taken from the model loop, the non-seasonal data are forecasted h time lags ahead. $h = (T_f - T_c)/i_s$, where i_s is the temporal resolution of the pre-processed distance data, T_c is the timestamp in the distance data that is closest to the time at which the forecast request was send and T_f is the last timestamp in the interval $\{T_c, T_c + i_s, T_c + 2i_s, T_c + 3i_s, \dots, T_c + ki_s | T_c + ki_s \leq T_r\}$, where T_r , in turn, is the time for which the forecast is requested. For example, imagine a situation in which the distance data contain values for each quarter of an hour, the forecast request was send at 15:48, and the forecast is requested for 16:40. Then, T_c will be 15:45, the last timestamp in the queried distance data, and T_f will be 16:30, the last quarterly hour timestamp before the requested forecast time. Hence, $h = 3$. That is, a forecast meant for 16:40, will in that case effectively be a forecast for 16:30. The values of p , d , and q in the ARIMA model are inherited from the model structure provided by the model loop, just as the estimated parameter values $\hat{\phi}_1, \dots, \hat{\phi}_p$ and $\hat{\theta}_1, \dots, \hat{\theta}_q$.

For the data that were decomposed, the seasonal component is forecasted separately. This is done with a seasonal naïve forecasting method, as described in Section 2.4.4. Then, the point forecast of the seasonal component is added to the point forecast of the non-seasonal data, to construct a reseasonalized point forecast. This point forecast is backtransformed with bias-adjustment, to the original scale of the data, as explained in Section 2.4.2.7. The seasonal point forecast is also added to the upper and lower bounds of the prediction intervals, to construct reseasonalized prediction intervals, which are backtransformed with bias-adjustment as well. That is, the prediction intervals of the non-seasonal data are shifted in line with the point forecast, but do not get wider. Hence, the uncertainty of the seasonal forecasts is not included in the final prediction intervals. This keeps calculations simple, and is a reasonable approach, according to Hyndman & Athanasopoulos (2018).

The forecasted distance to the nearest available bike, for the requested time and location, together with the corresponding 95% prediction interval, forms the output of DBAFS, and is send back to the user. The complete methodology of the forecast loop as described above is summarized in Figure 3.4.

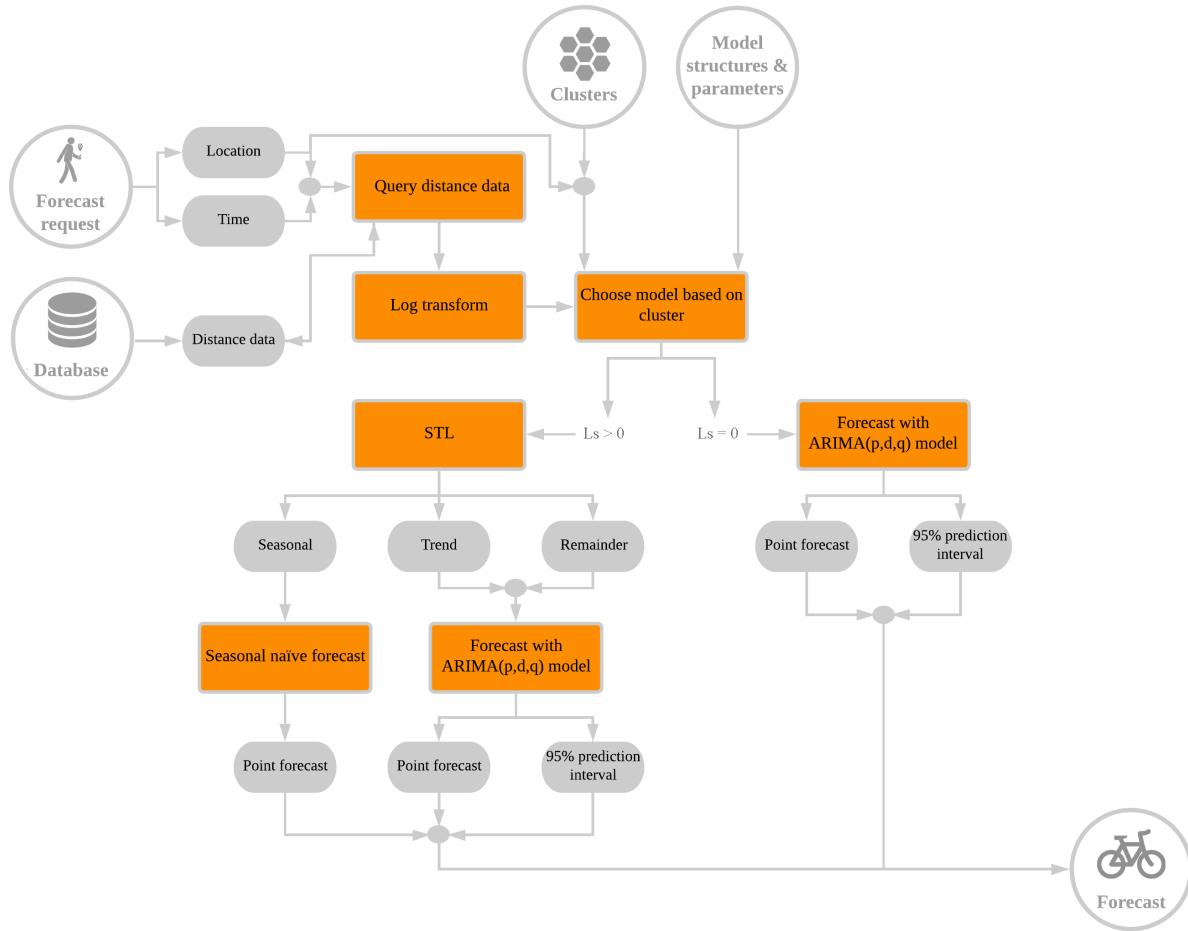


Figure 3.4: Methodology of the forecast loop

Chapter 4

Data and experimental design

This chapter describes the case study that was done to test the performance of DBAFS. It is structured as follows. First, the characteristics of the bike sharing system that served as a data source for the experiment, are presented. The data retrieval process is described in section two. The third section explains into detail the methodology of the experiment itself. Finally, in the fourth section, the additional software packages used in the experiment are listed.

4.1 Data source

DBAFS' forecasting power was evaluated with data from the dockless PBSS of San Francisco, California. The system there is exploited by JUMP Bikes (<https://jump.com/>), an American company founded in 2010, that went through a rapid development after being acquired by ride hailing giant Uber in April 2018 (Khosrowshahi, 2018). In February 2019, JUMP was active in 16 cities in the United States, as well as in Berlin, Germany. All provided bicycles have electric pedal assistance, up to a maximum speed of 32 km per hour.

In January 2018, the San Francisco Municipal Transportation Agency (SFMTA) offered JUMP Bikes the city's first official, exclusive permit to operate a dockless PBSS, for an 18 month trial period, in order to "evaluate, collect data, and assess whether further increases would serve the public interest" (Jose, 2018a). SFMTA allowed up to 250 bikes in a system area of approximately 47 km², which is shown in Figure 4.1. After nine months, a mid-point evaluation lead to the allowance of expanding the fleet to 500 bikes (Jose, 2018b).

The JUMP Bikes system in San Francisco, works as follows. A user needs to download the JUMP mobile application and create an account. The app shows the real-time locations of all available bikes. An available bike can be unlocked with a unique code that is send to the user account. A single trip costs \$2 for a total time of 30 minutes. For every minute that exceeds the 30 minute timeframe, \$0.07 will be charged. Options for subscription pricing, with a fixed amount per month or year, are not available.

It is possible to reserve a bike up to 30 minutes before unlocking it. In that case, the bike

will not be labeled as available anymore, and can not be taken by another user. However, the trip clock starts ticking from the moment of reservation. When a user wants to stop somewhere during a ride, the bike can be put ‘on-hold’ for maximum an hour, meaning that the bike stays unavailable during the stop. Also in this case, the regular fee will be charged. When ending the ride, the bike needs to be locked legally to a fixed object. Not doing so, will result in a fee of \$25. Additionally, leaving the bike outside of the system area, results in a \$25 fee as well (Harris, 2018).

Since all JUMP bikes are electric, battery life forms an important issue. A fully charged bike can travel 48 to 64 kilometers with the pedal assist. Bikes with a battery level of less than 25% are collected, and charged. Furthermore, other bikes are regularly charged during nighttime. Charging takes in most cases about four to six hours, and is done in a JUMP Bikes depot. Some of the charged bikes are placed outside of the depot, where they can be picked up, while others are redistributed over the system area. In the near future, this process will change considerably, since the newly produced bikes, which will be introduced in the first months of this year, have swappable batteries, such that there is no need anymore to bring low-battery bikes to the depot (Foley, 2018).

In the first year of the trial period, 63000 users took over 625000 trips. On average, trips were 4.2 kilometers long, while around 1% of the trips, exceeded 24 kilometers. Each individual bike, was on average used seven times per day. In September 2018, this was over eight times per day. Even when the size of the fleet doubled in October 2018, the utilization remained consistent until the first half of November, when it started to decrease slightly, due to cold weather (Rzepecki, 2019). While the demand is high, the supply is still restricted by SFTMA, putting extra emphasis on the need for efficient rebalancing, and accurate bike availability forecasts.

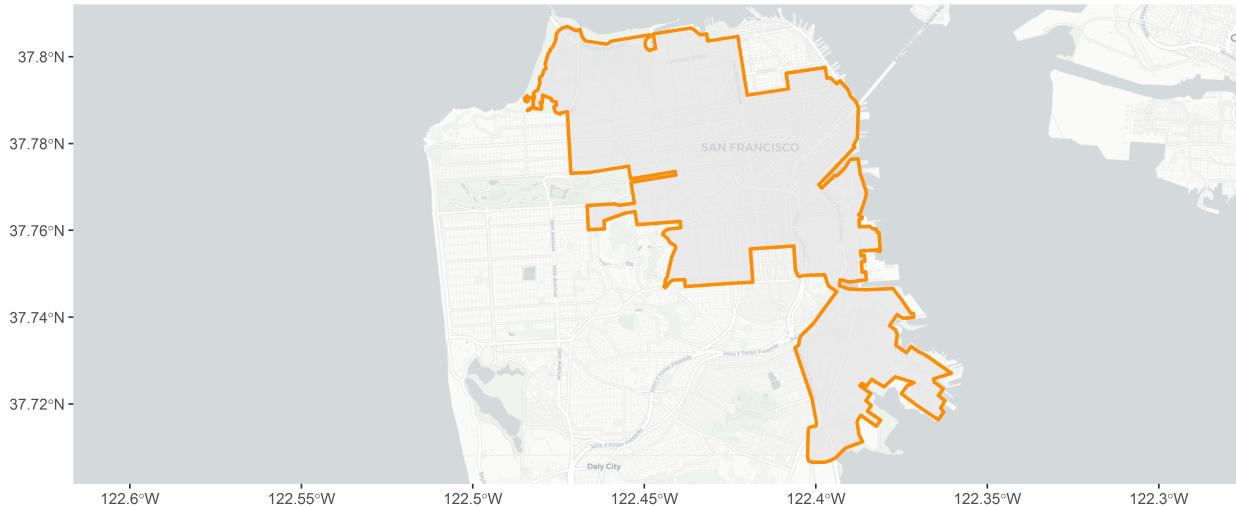


Figure 4.1: System area of JUMP Bikes in San Francisco

4.2 Data retrieval

JUMP Bikes provided access to a database containing the geographical locations of their available bikes in San Francisco. The database fulfilled all DBAFS requirements described in Section 3.4. Data collection started at September 9th, 2018, 15:41:08, Pacific Daylight Saving Time (PDT). The data had a temporal resolution of one minute, meaning that every minute, the location of each available bike in the system was recorded. Timestamps were stored with six-digit precision. Because of that, the time of recording was not exactly the same for each available bike, but could vary up to a few seconds. Therefore, before using the data in DBAFS, all timestamps were truncated to minute precision.

4.2.1 Distance data

When calculating distances, only the historical data at every quarter of an hour were used in the experiment. Hence, i_s was set equal to 15 minutes. There were several reasons for this choice. Firstly, it is not expected that the data change drastically from minute to minute. That is, using data with a temporal resolution of one minute will probably not contain a lot more information than using data with a temporal resolution of 15 minutes. Consequently, if a forecast for a specific timestamp is in practice a forecast for a few minutes earlier, this will not be problematic. On the other hand, using only data every 15 minutes will decrease the size of the data with a factor 15, and speed up computations considerably. Furthermore, a lower order ARIMA(p, d, q) model can be used to capture the same patterns in the data. This is important, since lower order models will result in lower errors arising from parameter estimation (Brockwell & Davis, 2002). After defining i_s , distance data pre-processing steps on the JUMP Bikes database server were taken as described in Section 3.4.1.

4.2.2 Usage data

Based on the specific knowledge of the JUMP Bikes system presented in Section 4.1, an extra restriction was added to the in Section 3.4.2 described process of retrieving pick-ups from the original data. If a feature that was initially considered to be a pick-up, was not followed by a drop-off within a two hour timeframe, the feature was removed from the usage data. Taking into account the average trip length of only 4.6 kilometers, the fact that trips become more expensive after half an hour, the maximum allowed reservation time of 30 minutes, and the maximum allowed ‘on-hold’-time of one hour, the threshold of two hours was considered to be a safe border. In this way, pick-ups that occur because the system operator is collecting bikes to be charged (i.e. pick-ups that do not reflect the usage intensity of the system), were taken out.

Of course, there may have been some real trips that were longer than two hours. However, given that during the first year of the trial period only 1% of the trips exceeded a distance of 24 kilometers, and the electric pedal assistance allows a speed of more than 30 kilometers per hours, this was assumed to be a negligible share of the total number of trips.

4.3 Experimental design

4.3.1 Training and test periods

As mentioned in Section 4.1, usage of the JUMP Bikes system in San Francisco remained rather constant in September, October, and the start of November. An exploratory analysis on the distance data at several locations in the system area enabled to draw similar conclusions, with a sudden change in temporal patterns after mid-November. Recall that in DBAFS, parameter n_w , the number of weeks between two passes through the model loop, should be chosen such that an ‘old’ model is not used anymore when the patterns in the historical data have changed considerably. Therefore, to test the performance of DBAFS in an adequate way, both the period used for model building, called the *training period*, and the period used for forecasting, called the *test period*, should preferably fall within a timeframe where no large changes in the data patterns occur. However, they should not overlap each other either, since the forecasting performance of a model can only be truly evaluated when forecasts are made for data that the model has not seen yet.

The training period, used to query data for both the cluster and model loop, spanned the first four full weeks plus one observation (i.e. 2689 observations) in the data collection period, from Sunday September 16th, 2018, 23:45:00 PDT, up to and including Sunday October 13th, 2018, 23:45:00 PDT, as shown in Figure 4.2. Hence, a situation was simulated in which the weeks of data used for clustering, i.e. m_c , and the weeks of data used for model building, i.e. m_m , were both set to be four weeks. p , the side length of the square grid cells, was set to 500 meters. Taking into account the size and shape of the system area, along with some exploratory research on the demographic characteristics of San Francisco, K , the set of integers containing all values considered as the number of desired clusters k , was chosen to be $\{3, 4, 5, \dots, 10\}$.

The obtained model structures and parameters resulting from the model loop, were used to make several forecasts during a test period of one week. For each forecast, two weeks of distance data, plus one observation, were retrieved from the database, such that in the case of a weekly seasonality, a sufficient amount of data would be present for decomposition. Hence, $m_f = 2$. To make sure that in no case the data used for forecasting would overlap with the data used for model building, a two week period separated the training and test period. That is, the test week ranged from Monday October 29th, 00:00:00 PDT, up to and including Sunday November 4th, 2018, 23:45:00 PST, as shown in Figure 4.2.

Defining where and when to forecasts, was done by simulating real-world forecast requests, and sending them to the forecast loop. To do this in a realistic way, the following requirements had to be fulfilled.

- More forecast requests should occur at locations where the usage intensity of the system is higher.
- More forecast requests should occur at times when the usage intensity of the system is higher.
- It should be accounted for, that the times when the usage intensity is higher, can vary per location, and vice versa.

Bearing these requirements in mind, the following approach was developed. All pick-ups during the test week were retrieved from the database. Ten pick-ups per cluster where randomly sampled, guaranteeing that each cluster was represented in the sample. Subsequently, $500 - 10 \times k$ pick-ups were randomly sampled from the remaining ones, regardless to which cluster they belonged. This lead to a dataset of 500 pick-ups in total, from which the location-timestamp combinations were retrieved. Pick-ups reflect the usage of the bike sharing system. That is, a random sample of them will contain more locations in areas where the usage intensity is high, and more timestamps at times when the usage intensity is high. Furthermore, the location and timestamp come as a combination, rather than as separate entities. In this way, the approach fulfills all three requirements mentioned above. The location-timestamp combinations in the sample will from now on be referred to as the *test points*.

Starting from the timestamp of the test point, all time lags up to one day ahead, i.e. 96 time lags in total, were forecasted. Having 500 test points, in total, 48000 forecasts were made. To evaluate their performance, historical distance data for all forecasted time lags were retrieved from the database, and the forecast RMSE (see Section 2.4.2.6) was calculated for each test point separately.

By using the approach described above, the reported overall forecast errors will be dominated by those made during peak hours, when obtaining accurate forecasts is generally harder, and in crowded areas, where obtaining accurate forecasts is generally harder. However, this is intended, because reporting a large amount of forecast errors made during off-peak hours, and in non-crowded areas, or, alternatively, using adjusted error metrics such as the RMSLE, may give results that look nicer, but do not reflect the real usefulness of the forecasting system.

To examine the forecasting power of DBAFS in a relative manner, all test points were also forecasted 96 time lags ahead with a simple baseline method. The naïve method, as described in Section 2.4.3, was chosen for this task. Therefore, the baseline forecasting system will from now on be referred to as the Naïve Forecasting System (NFS). For each test point, the RMSE's of the forecasts of NFS were calculated, and compared to those of DBAFS.

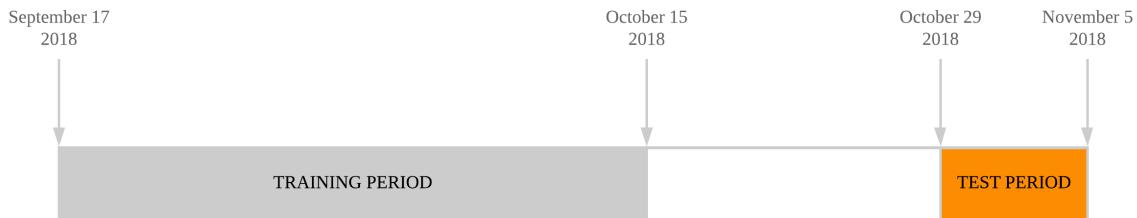


Figure 4.2: Training and test period

4.3.2 Additional software

On top of those mentioned in Section 3.2, some additional R packages were used for reporting the results of the experiment, as listed below.

- The **feasts** package (Hyndman, O'Hara-Wild, & Wang, 2019) was used to estimate the ACF (see Section 2.2.1) of time series.
- The **tsfeatures** package (Hyndman, Kang, Talagala, Wang, & Yang, 2019) was used to calculate the spectral entropy (see Section 2.2.3) of time series.
- Data and results were visualized graphically with the **ggplot2** package (Wickham, 2016). Additionally, the packages **tidyverse** (Wickham & Henry, 2018), **dplyr** (Wickham, François, Henry, & Müller, 2019) and **tibble** (Müller & Wickham, 2019) were used to transform some data into formats that are compatible with **ggplot2**.
- Maps were created with the **ggspatial** package (Dunnington, 2018). Besides, with the **rosm** package (Dunnington, 2017), all basemap tiles were retrieved from CARTO (CARTO, 2018).
- For maps with a continuous color scheme, the **orange_material** color scheme from the **ggsci** package (Xiao, 2018) was used.

For the R code used in the experiment, see Appendix A.

Chapter 5

Results and discussion

This chapter presents and discusses the results of the experiment described in Chapter 4. It is structured as follows. The first section shows the clusters that resulted from the cluster loop, along with their main characteristics, and the chosen locations of the model points. Section two presents the structures of the models that were build in the model loop, and the residual diagnostics for each them. Then, the third section focuses on the accuracies of the forecasts, and their patterns in both space and time. Finally, in the fourth section, the limitations of DBAFS are discussed, and recommendations for possible improvements are given.

5.1 Clustering

Figure 5.1a shows the grid overlaying the JUMP Bikes system area in San Francisco, including the centroid of each grid cell. In total, the grid contains 249 cells, each 500 meter high and 500 meter wide.

Figure 5.1b shows the calculated number of pick-ups per grid cell, during the training period. In total, 54365 pick-ups were calculated within the extent of the grid. That is, on average, there were approximately 218 pick-ups per grid cell, which corresponds to approximately eight pick-ups per day. The maximum number of pick-ups in a grid cell was 1985 (i.e. 71 per day on average), while in 25 of the 249 grid cells, there were no pick-ups at all. It can be seen that high counts of pick-ups occurred in the grid cells along the diagonal axis from south-west to north-east. Mainly in the south-eastern corner of the system area, the usage intensity was very low.

Figure 5.2 shows the temporal patterns of the usage data, with the pick-ups per day of the week, and per hour of the day. Friday was the day with on average the most pick-ups, while Saturday and Sunday had the least. The busiest hours of the day, where 8:00 and 9:00, during morning rush hours, and 16:00 and 17:00, during afternoon rush hours. The lowest numbers of hourly pick-ups, as expected, occurred during the night.

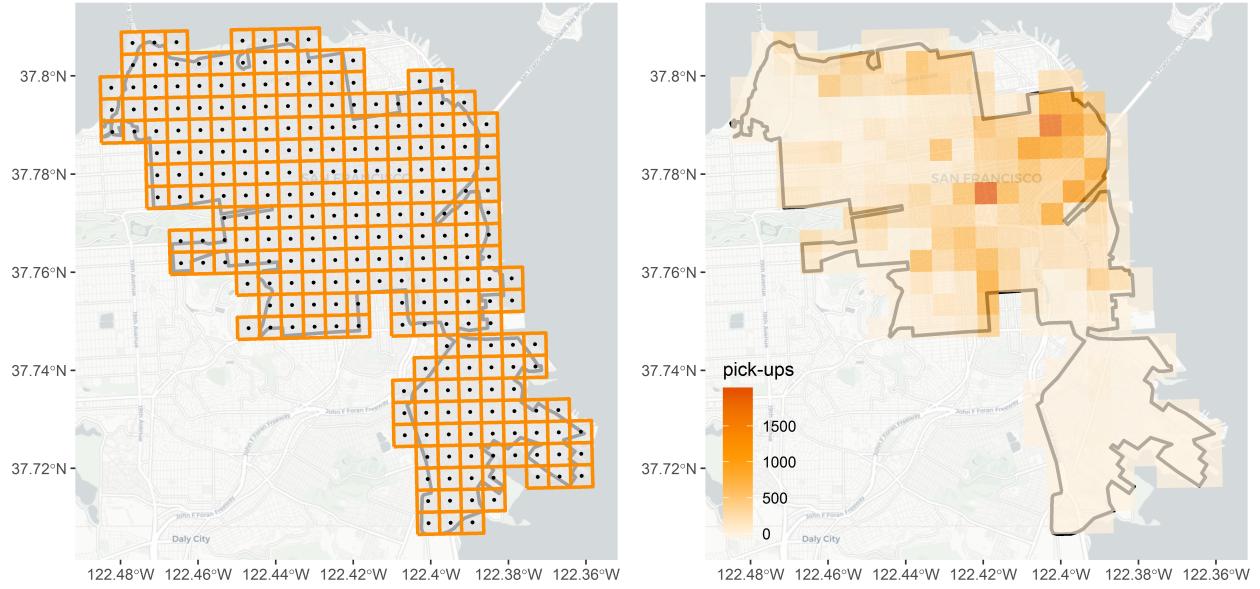


Figure 5.1: a) grid overlaying the system area; b) number of pick-ups per grid cell

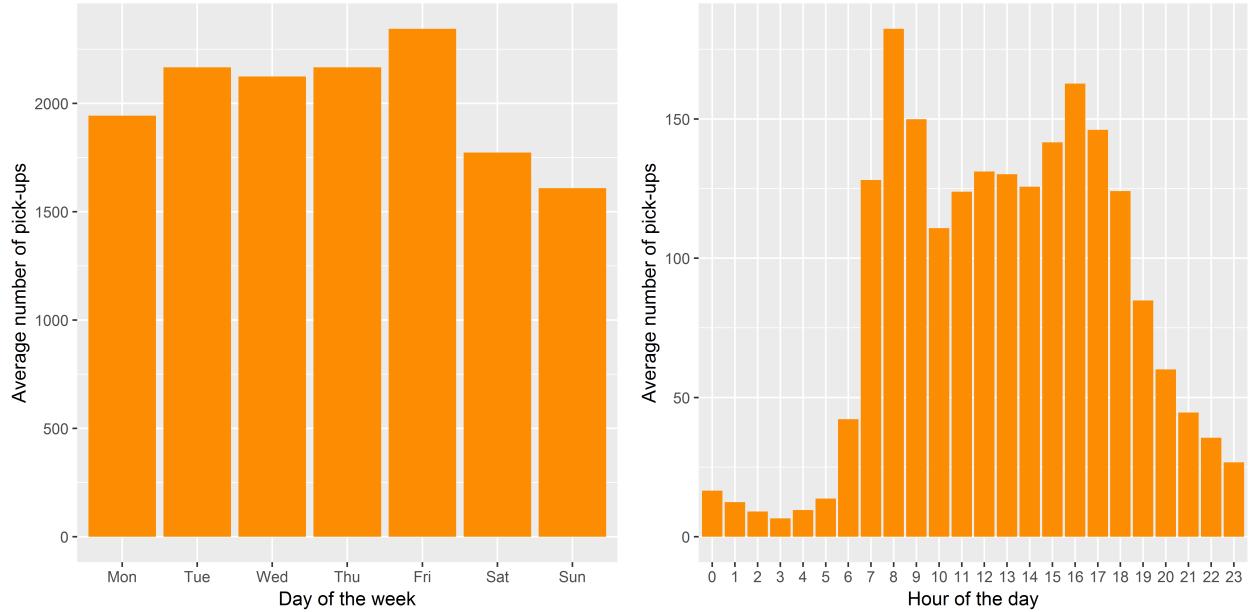


Figure 5.2: a) pick-ups per day of the week; b) pick-ups per hour of the day

Recall that for each grid cell centroid, a time series of historical distance data was queried, and that the normalized, average weekly patterns in these data were clustered using spatially constrained hierarchical clustering. The automatic procedure of defining the number of clusters k and the mixing parameter α , lead to a definition of $k = 4$ and $\alpha = 0.6$. This resulted in a partition containing four fully spatial contiguous clusters. The geographical outlines of these clusters are shown in Figure 5.3a. The centroid of each cluster, weighted

by the number of pick-ups in the corresponding grid cells, are shown in Figure 5.3b. These weighted centroids serve as the model points in DBAFS.

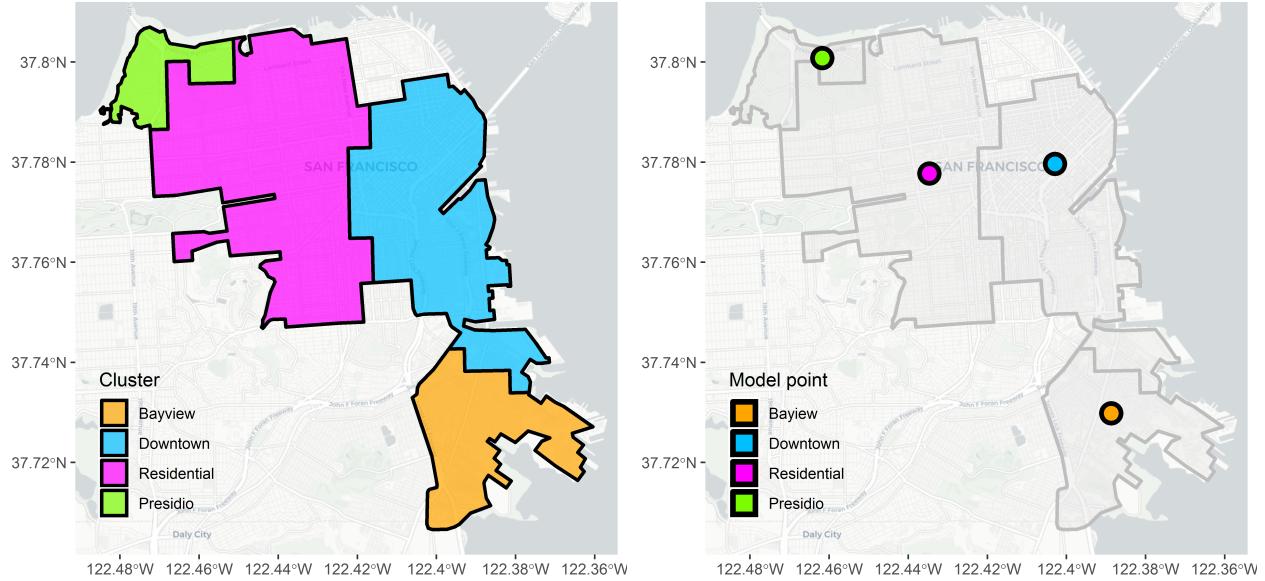


Figure 5.3: a) cluster outlines; b) model point locations

Roughly speaking, and based on a large study of neighbourhood indicators in San Francisco (San Francisco Department of Public Health, 2014), the four clusters can be characterized as follows. The orange cluster covers the Bayview/Hunters Point neighbourhood, which is a rather isolated area, with a high percentage of low-income households and relatively high crime rates. The blue cluster forms the city center of San Francisco, containing the neighbourhoods with the highest population densities, but also with a relatively high job density compared to the residential density, and large areas zoned for commercial usage. The purple cluster mainly contains neighbourhoods where the residential density is high compared to the job density, and the area zoned for commercial usage is relatively small. Finally, the green cluster covers the Presidio Park, a recreational area with few inhabitants, and a relatively high number of bike lanes. For the sake of clarity, the orange, blue, purple and green clusters are from now on referred to as the *Bayview*, *Downtown*, *Residential* and *Presidio* clusters, respectively. Consistently, the four corresponding model points will be called the *Bayview*, *Downtown*, *Residential* and *Presidio* model points, respectively.

Table 5.1 presents some descriptive statistics of the time series, averaged per cluster, and averaged over the whole system area. From the 249 grid cells, more than a hundred are located within the Residential cluster, while the Presidio cluster is by far the smallest of the four. During the training period, the nearest available bike was on average located 619 meters from the grid cell centroids. In the Bayview cluster, however, this was more than one kilometer, a difference of almost a factor two compared to the Downtown cluster, and even more compared to the Residential and Presidio clusters. The Bayview cluster also showed the largest variation in the data, with a high average standard deviation compared to the

other clusters, and an average range that spanned more than four kilometers. This can possibly be explained by the low usage intensity of the bike sharing system in this part of the system area. When the number of bikes in an area is low, the nearest available bike and the second nearest available bike are more likely to be far away from each other. In that case, when the closest of them gets picked-up, the distance to the nearest available bike will suddenly increase substantially. The other way around, when all available bikes are far away, and one bike gets dropped-off inside the area, the distance to the nearest available bike will suddenly decrease substantially.

Although not as extreme as the Bayview cluster, also the other clusters had on average high ranges when compared to the mean and standard deviation. However, the standard deviation itself turned out to be rather small relative to the mean. This implies either the presence of outliers, or population distributions with thin, but wide tails.

The first order autocorrelation measures the average dependency between data values at time t and corresponding data values at time $t - 1$. In the whole system area, this dependency was strong, especially in the Bayview and Presidio clusters. These high autocorrelation values are important, since they imply that it is reasonable to use past observations when forecasting future ones. However, the calculated spectral entropy values show that in general, the data are also very complex, and the forecastability is low. This mainly concerns the Downtown and Residential clusters, which contain, as could be seen in Figure 5.1b, the areas where the pick-up density is high. In such areas, the data are more dynamic, since bikes get picked-up and dropped off constantly, and the location of the nearest available bike will change often. In most cases, the more dynamic the data, the harder to forecast.

Table 5.1: Descriptive statistics of the grid cell centroids distance data

	N	μ	$range$	σ	$\rho(1)$	H
Total	249	619	2726	422	0.82	0.77
Bayview	46	1080	4021	631	0.95	0.67
Downtown	81	557	2551	352	0.77	0.81
Residential	103	490	2410	371	0.79	0.81
Presido	19	462	2057	310	0.92	0.68

Except N , all metrics are calculated for each time series separately, and averaged afterwards.

¹ N is the total number of grid cell centroids

² μ is the mean of the data, in meters

³ $range$ is the difference between the maximum and minimum data value, in meters

⁴ σ is the standard deviation of the data, in meters

⁵ $\rho(1)$ is the first order autocorrelation, see section 2.2.1

⁶ H is the normalized spectral entropy, see section 2.2.3

Figure 5.4 shows the normalized, average weekly patterns of the time series, averaged once again per cluster. The patterns can be explained intuitively. The Bayview cluster has a low usage intensity, and although there are peaks in the data every day, a clear and consistent pattern is absent. The Downtown cluster has a high density of jobs and commercial activities.

During working hours, the demand for bikes is low, which leads to a high number of available bikes, and consequently, short distances to the nearest available bike. In the afternoon, just after working hours, the demand starts increasing, and it gets harder to find an available bike nearby. This peak in the data continues during the evening, when the activity in the commercial zones is high. Later in the evening, the demand decreases again. However, the data lacks a clear peak during morning peak hours, as well as a clear difference between weekdays and weekends, indicating that there is a substantial share of non-commute related usage.

The Residential cluster shows the exact opposite pattern. In the morning rush hours, commuters use the bike to get to work, and not many available bikes are left in the residential areas. Hence, in those areas, the distance to the nearest available bike is higher during working hours. In the afternoon, commuters come back from work, and leave the bikes in the residential areas, causing a decrease in distance to the nearest available bike. Hence, the distance data peaks during working hours. In the weekends, the peaks seem to be slightly lower, but this difference is not as large as might have been expected. They do happen later on the day, corresponding to the same periods as the Downtown cluster.

Finally, the Presidio cluster is mainly a recreational area. There are a lot of bikes, but during weekdays, they are used less, leading to small and relatively constant distances to the nearest available bike. In weekends, and mainly on Sunday afternoon, the usage intensity is high, and it takes longer to find an available bike.

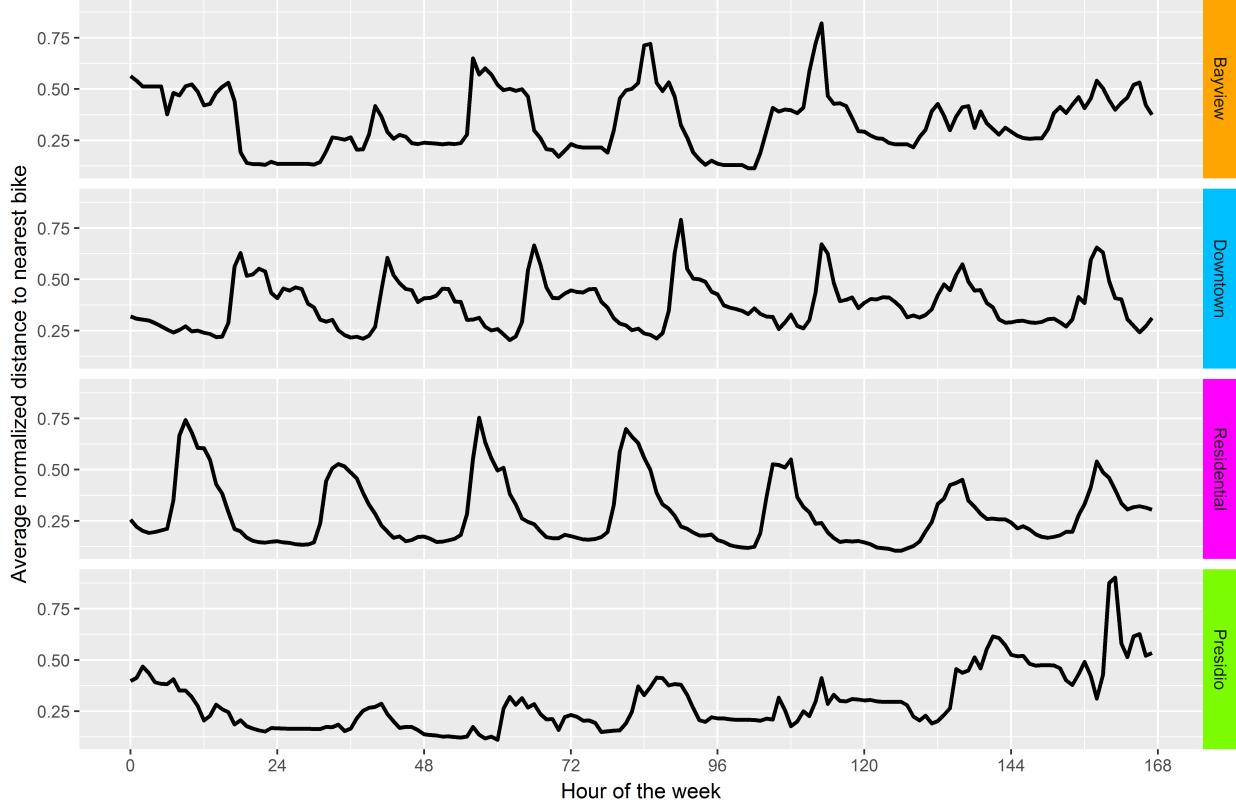


Figure 5.4: Patterns of the distance data for the grid centroids, per cluster

5.2 Model building

Figure 5.5 shows the time plots of the distance data that were queried for each of the model points in Figure 5.3b, with the dark grey shaded areas representing weekends. The plots endorse the findings in the previous sections. The data corresponding to the Bayview model point show large variation, interspersed with flat sections, and lack a clear repeating pattern. The data corresponding to the Downtown and Residential model points are most dynamic. A daily pattern shows for both of them. However, in both datasets, this pattern is far from smooth, and the daily peaks vary considerably in height from day to day. This underlines the high spectral entropies that were found for these clusters. A clear difference between weekdays and weekends, can not be seen. The Presidio model point shows the most constant data, with a low mean and long flat sections. Sunday afternoons stand out clearly in most of the weeks, but not in all of them. The last Sunday, for example, shows only a minor peak in the data. In less extent, this also applies to the other clusters, with lower peaks than normal, in the last weekend. Finally, none of the datasets contain missing values, and clear evidence for non-constant variances is not present.

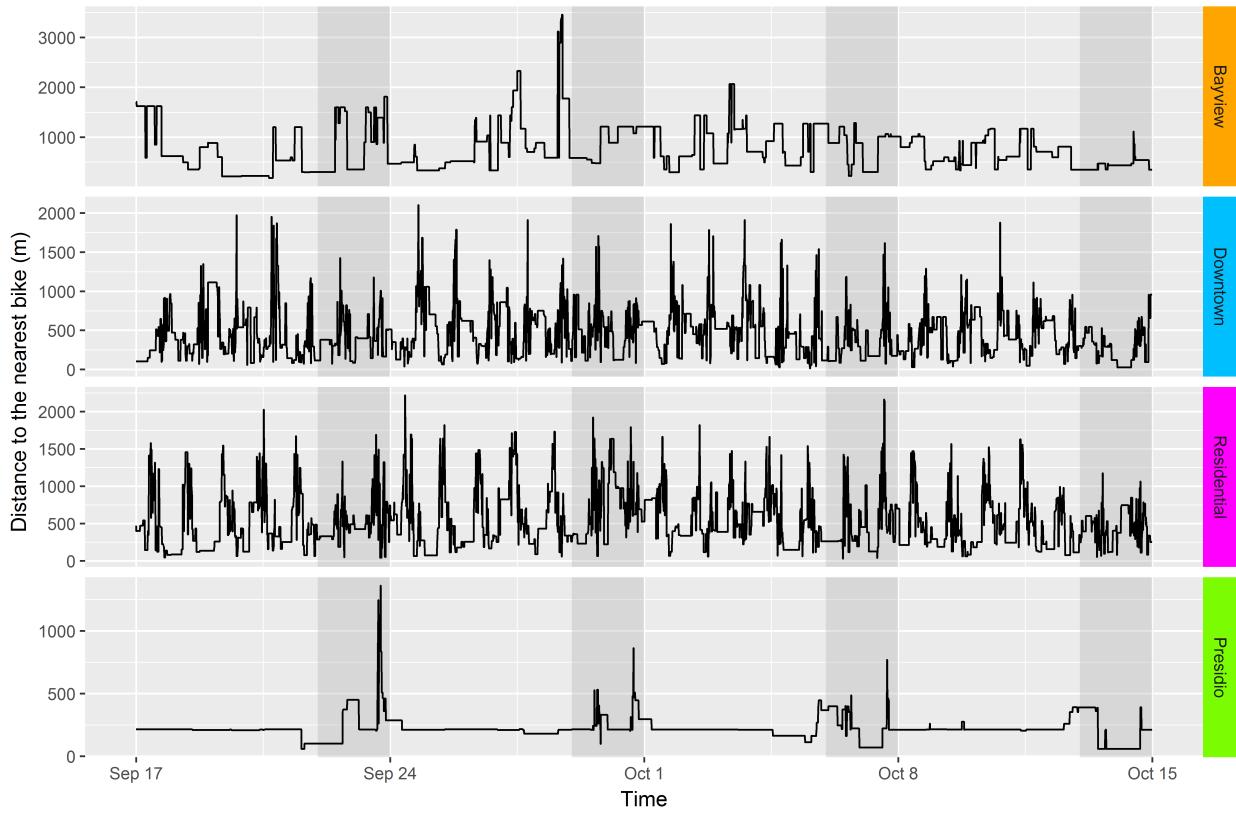


Figure 5.5: Time plots of the distance data for the model points

The structures of the fitted models are shown in Table 5.2. The automatic seasonality detection resulted in a daily seasonal pattern for both the Downtown and the Residential model point. As expected, a weekly seasonal pattern was found for the Presidio model point, and no seasonality for the Bayview model point. The ARIMA(p, d, q) models for

the Bayview and Downtown model points, have a relatively high number of autoregressive terms, while for the Presidio model point, the number of moving average terms is high. For the Residential model point, the best fit was obtained by only including one autoregressive and one moving average term. All datasets passed the KPSS test for stationarity after one differencing operation. The full details of the components and fitted models, including parameter estimates and decomposition plots, can be found in Appendix B.

Table 5.2: Model structures

	seasonality	p	d	q
Bayview	none	3	1	1
Downtown	daily	3	1	2
Residential	daily	1	1	1
Presidio	weekly	1	1	4

Figure 5.6 shows the residuals of each model, plotted over time. All models have residuals with an approximately zero mean, and the variances look approximately constant. Comparing Figure 5.6 with Figure 5.5, it can be seen that for the less dynamic data in Bayview and Presidio, the models struggle to find a good fit for the peaks and valleys in the data, while the flat sections are explained accurately.

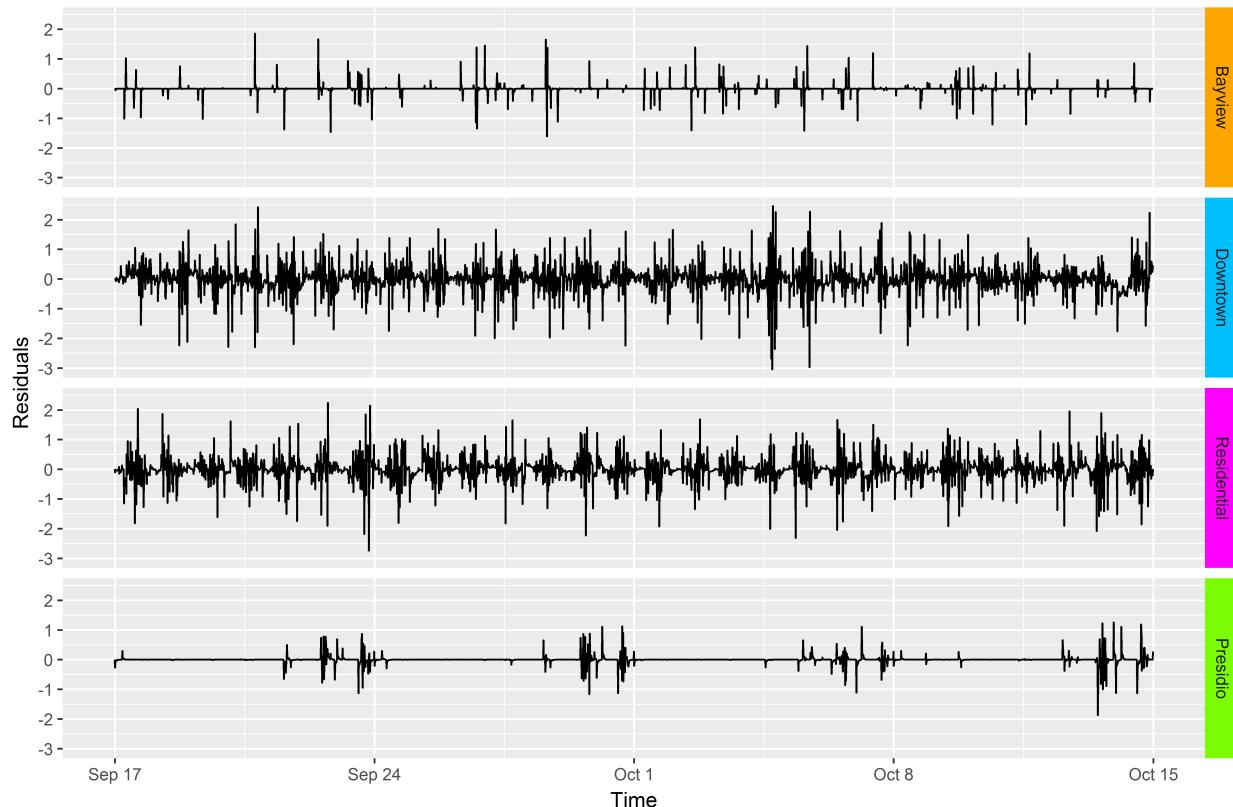


Figure 5.6: Time plots of the model residuals

The autocorrelations at several time lags in the residuals are shown in Figure 5.7. Since the data have a temporal resolution of 15 minutes, 96 time lags correspond to one day, and 672 time lags, the total span of the x-axis in the figure, to one week. The dotted orange lines form the lower and upper 95% confidence bounds, assuming a normal distribution. This means that the residuals are considered to be a realization of a white noise process when at least 95% of the autocorrelation values fall within these bounds. It is important to note here that when working with real-world data, finding perfectly random model residuals is an exception, especially when the data have a high entropy. Taking that into account, the autocorrelation plot of the Bayview, Downtown and Residential models look good, and their residuals seem to approximate white noise.

However, for the Presidio cluster, the residual autocorrelation has a strong peak at lag 672, corresponding to one week. Recall that the data of the Presidio model point was relatively flat during the weekdays, and spiky in the weekends. These spikes, however, varied considerably in amplitude from week to week. The weekly seasonal component that was subtracted from the data, accounts for the recurring patterns, but can not completely capture the differences from week to week. Therefore, errors during the ‘spiky’ weekends, will still be higher than during the ‘flat’ weekdays, causing autocorrelation in the residuals. With just a stochastic time series model, it is hard to solve this. Including exogenous variables that explain the variation, could be an option, and will be discussed in section 5.4.2.

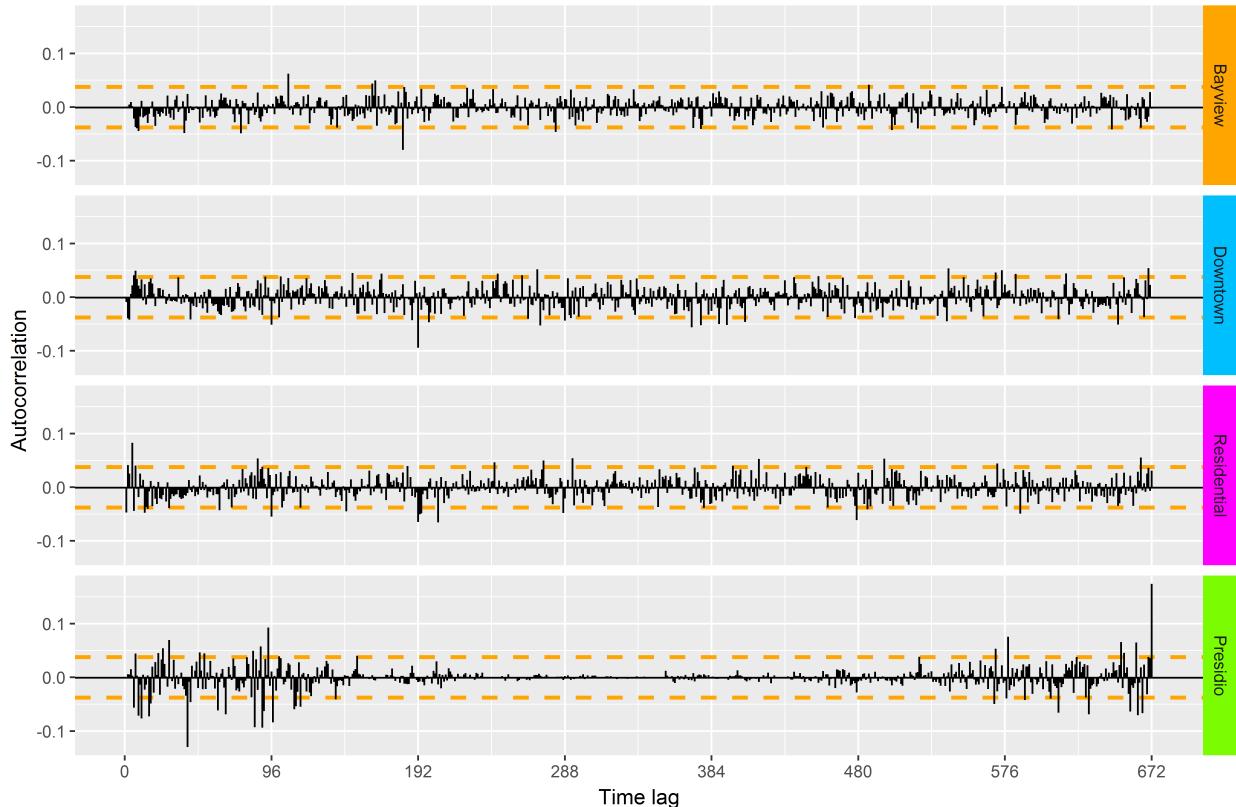


Figure 5.7: ACF plot of the model residuals

Finally, Figure 5.8 shows the histograms of the model residual distributions. As expected, for the Bayview and Presidio models, most values are clustered closely around the zero mean, with the tails being extremely thin and long, especially for the Bayview model. The residuals of the Downtown and Residential models follow a distribution that comes closer to a normal one, but also here, the tails are wide.

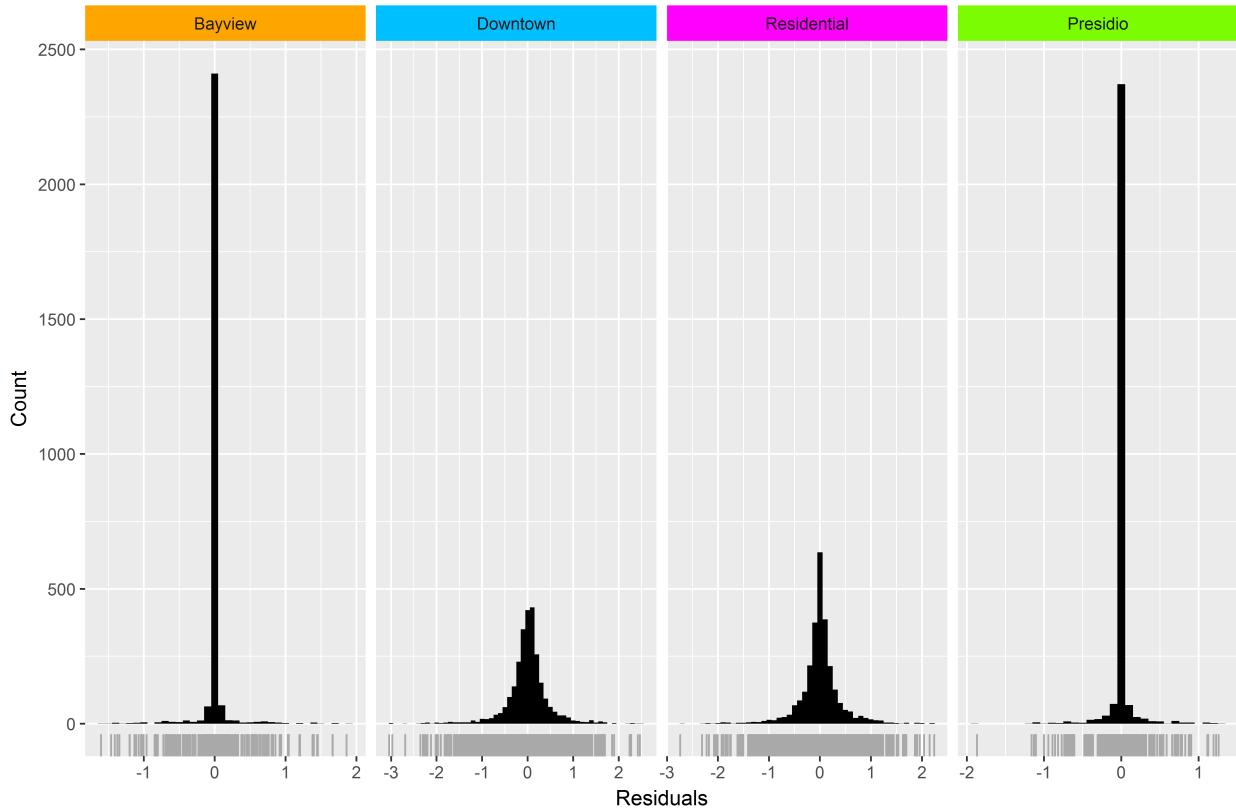


Figure 5.8: Histograms of the model residuals

5.3 Forecasting

Figure 5.9a shows the spatial distribution of the 500 test points. As planned, areas with high usage intensity have more test points, with 94% located in the Downtown and Residential clusters, and only the minimum of ten test points in the Bayview cluster. Figure 5.9b shows the temporal distribution test points. All days in the test week are well covered, with less test points during working times and in the night, and more during the morning rush hours and in the evening. On weekend days, there is only one strong peak, around noon. Furthermore, it can be seen that the morning peak on November 1st is somewhat lower compared to the other weekdays. This may be, because it is the morning of All Saint's Day, following the Halloween night. For the full information on the test points, with all unique location-time combinations, see Appendix A.

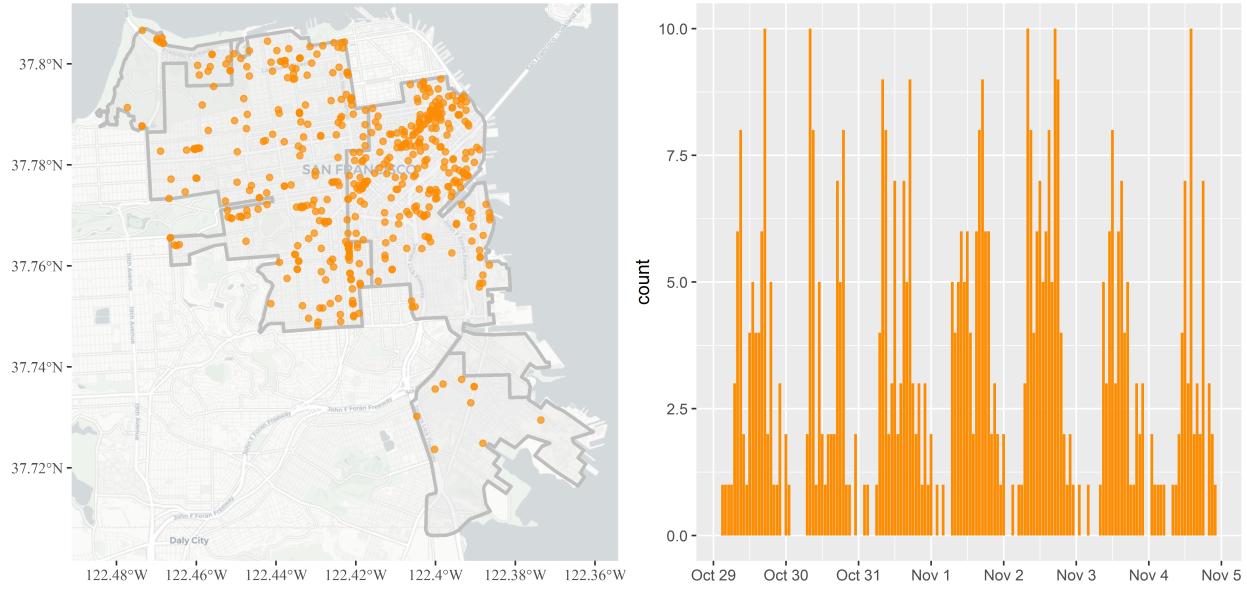


Figure 5.9: a) test points locations; b) test point timestamps, counted per hour

The first row of Table 5.3 lists the RMSE's, averaged over the whole system area, of the forecasts produced by DBAFS, and of the forecasts produced by the baseline system, NFS. DBAFS clearly outperforms NFS, by producing forecasts with errors that are on average 31% lower. Furthermore, the range of error values is much lower for DBAFS, than for NFS. The minima are comparable, but NFS produces forecasts with error values up to 1644 meters, while DBAFS never exceeds 1004 meters.

Table 5.3: Forecast RMSE's, in meters

	DBAFS				NFS		
	n	mean	min	max	mean	min	max
Total	500	282	38	1004	408	37	1644
Bayview	10	389	38	1004	389	38	1004
Downtown	259	248	122	523	414	116	927
Residential	211	317	97	705	411	37	1644
Presidio	20	299	80	577	320	175	699

Regarding the spatial patterns of the forecast errors, the remaining rows of Table 5.3 show the RMSE's averaged per spatial cluster. With NFS, the lowest errors are obtained in the Bayview and Presidio clusters, where the data are less dynamic. In the Bayview cluster, NFS gives the same results as DBAFS, and in the Presidio cluster, DBAFS performs only slightly better than NFS. For DBAFS, however, the lowest errors are not found in those clusters, but in the highly dynamic Downtown cluster. Here, DBAFS gives errors that are 40% lower than those of NFS. In the Residential cluster, there are larger errors than in the

Downtown cluster, but also here, DBAFS outperforms NFS with errors that are 23% lower. It shows the strength of DBAFS in forecasting dynamic data, when compared to NFS.

Regarding the temporal patterns of the forecast errors, Figure 5.10 shows the RMSE's averaged per hour of the day, and per forecast lag. The lowest forecast errors occur during the night, when the usage intensity of the system is low. During the day, higher errors occur, with peaks at the morning rush hour, around noon (i.e. the peak hour in the weekend) and after working hours. This patterns are similar for NFS, but with higher RMSE's at each hour. The forecast errors of both methods rise steeply directly after the first forecast lag, but for NFS, this increase is much larger than for DBAFS.

What strikes, is that the RMSE does not increase constantly when the forecast horizon gets larger. From the forecasting lag of 12 hours, the errors for both DBAFS and NFS decrease again. Moreover, at a forecasting lag of approximately 18 hours, the RMSE of the DBAFS forecasts is, on average, back at almost the same level as the one at a forecasting lag of just 15 minutes. This conspicuousness can be explained as follows. Most of the simulated forecast requests are made at times with a high usage intensity, that are hard to forecast. The first forecast lags, will still correspond to high usage times, but after a while, forecasts will be made during night time. As could be seen in Figure 5.10a, these night time forecasts have much lower errors. Therefore, it can happen that, despite the length of the forecasting window, ‘far-ahead’ forecasts have lower errors than ‘close-by’ forecasts.

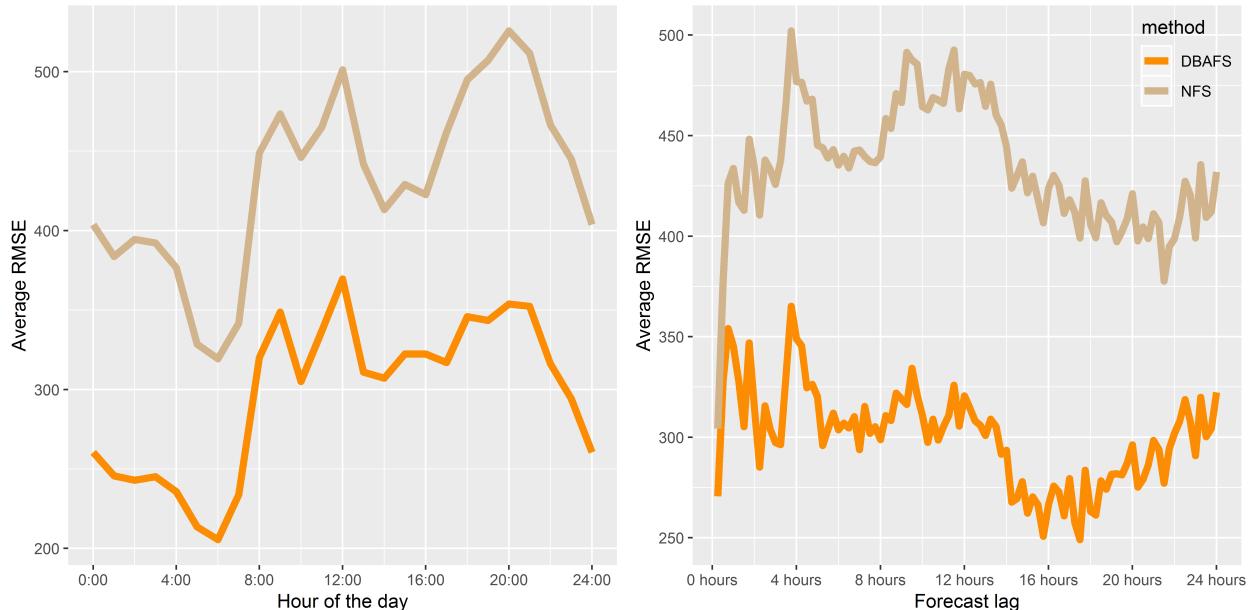


Figure 5.10: a) RMSE averaged per hour of the day; b) RMSE averaged per forecast lag

5.4 Limitations and recommendations

5.4.1 Limits of forecastability

Although DBAFS outperforms the baseline, the average forecast RMSE of almost 300 meters can be considered high when looking at it from an absolute perspective. To get a more detailed understanding of the performance of DBAFS, it may be beneficial to look at some individual forecast results, rather than at general, averaged metrics. Therefore, Figure 5.11 shows the forecasts at the four model point locations, for the whole test period. Each day is forecasted separately, with two weeks of historical data.

As already pointed out earlier in this chapter, the forecasts in the Bayview cluster act in a similar way as naïve forecasts, with approximately straight lines every day. Peaks in the true data occur randomly, and can not be captured well by the fitted model. In the Downtown and Residential clusters, the ones of primary interest, DBAFS performs very well in forecasting when peaks are going to occur, but fails to accurately capture the variation in the height of those peaks from day to day. Equivalently, in the Presidio cluster, the varying amplitude of the Sunday afternoon peak, is problematic for the forecasts. When this peak has been relatively low in the two weeks before, DBAFS will expect it to stay low, and never forecast the reoccurrence of a higher peak.

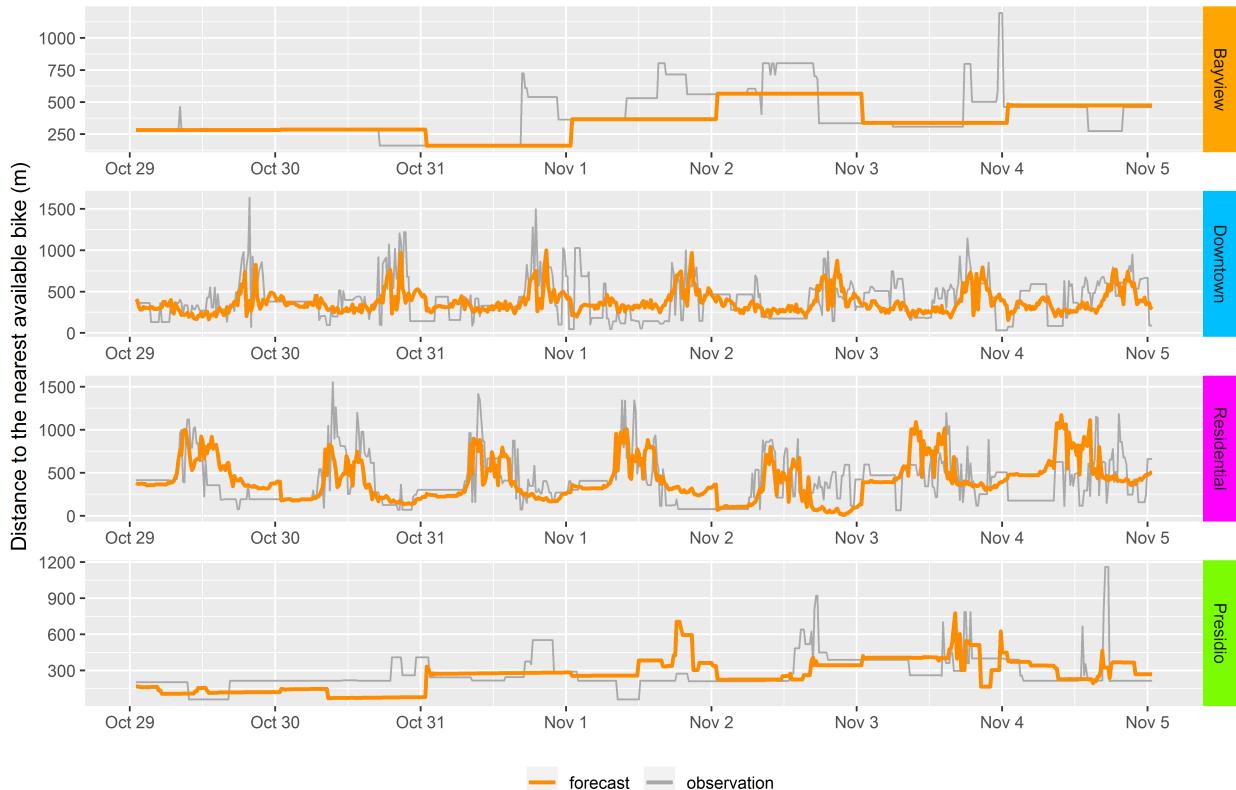


Figure 5.11: Detailed forecasts for the model point locations

The irregularity of the patterns in the data, and consequently, their high entropy, can be linked to the flexible and dynamic nature of dockless PBSS. Users can pick up bikes spontaneously, whenever they see one around. This in contradiction to station-based PBSS, which have a more organized structure, where trips are usually planned in advance, at regular moments in time. Some studies in the United States already explored these differences between dockless and station-based systems. A report of the National Association of City Transportation Officials showed that the usage in station-based systems follows typical commuting patterns, while in dockless systems, it is more dispersed (NACTO, 2018). This is in line with the conclusions drawn from Figure 5.4, earlier in this chapter. Moreover, Mckenzie (2018) found similar results in Washington D.C.

In San Francisco, the differences between station-based and dockless systems may even be stronger, for the following reason. For single-trips, JUMP Bikes is cheaper than the station-based Ford GoBike system. However, in contradiction to GoBike, JUMP Bikes has no subscription pricing. That is, for irregular usage, JUMP Bikes is the better option, but when using a JUMP Bike every working day for two trips of half an hour (\$2 each), this will cost around \$1040 per year, compared to only \$149 for a yearly subscription on GoBike (Harris, 2018).

To strengthen the findings discussed above, Figure 5.12 is adapted from the mid-point evaluation of JUMP Bikes in San Francisco, performed by SFMTA, and shows the number of trips per bike per day, for both JUMP Bikes and GoBike, during five months in 2018 (SFMTA Board of Directors, 2018). It clearly confirms the expected differences between the two. The course of the GoBike line is very regular, with peaks during weekdays, and valleys during weekends. JUMP Bikes, in contradiction, follows a highly irregular pattern. Such irregularity, obviously, sets limits on the ability of models to forecast the data accurately.

5.4.2 Exogenous variables

That the forecastability of dockless bike sharing data is limited, does not mean that the forecasts produced by DBAfs can not be improved in any way. There may be exogenous variables that can explain at least a part of the variation in peak height from day to day. The most relevant of those, probably relate to weather conditions. Several studies addressed the relationship between cycling activity in PBSS and weather conditions already (Campbell, Cherry, Ryerson, & Yang, 2016; Corcoran, Li, Rohde, Charles-Edwards, & Mateo-Babiano, 2014; Faghih-Imani, Eluru, El-Geneidy, Rabbat, & Haq, 2014; Shen et al., 2018). Most notably, heavy rain or snowfall, high humidity, strong winds, extremely low temperatures, and extremely high temperatures, all have a negative impact on PBSS usage, both for recreational and commuting trips. It must be noted, that DBAfs already deals with long-term weather variations, since models are updated regularly, and moreover, STL allows the seasonal pattern to change slightly over time. The short-term weather variation, however, may be an important factor influencing the variability in the data, which DBAfs is not able to account for. Therefore, including weather condition variables in the forecasting system, can possibly decrease the forecast errors substantially.

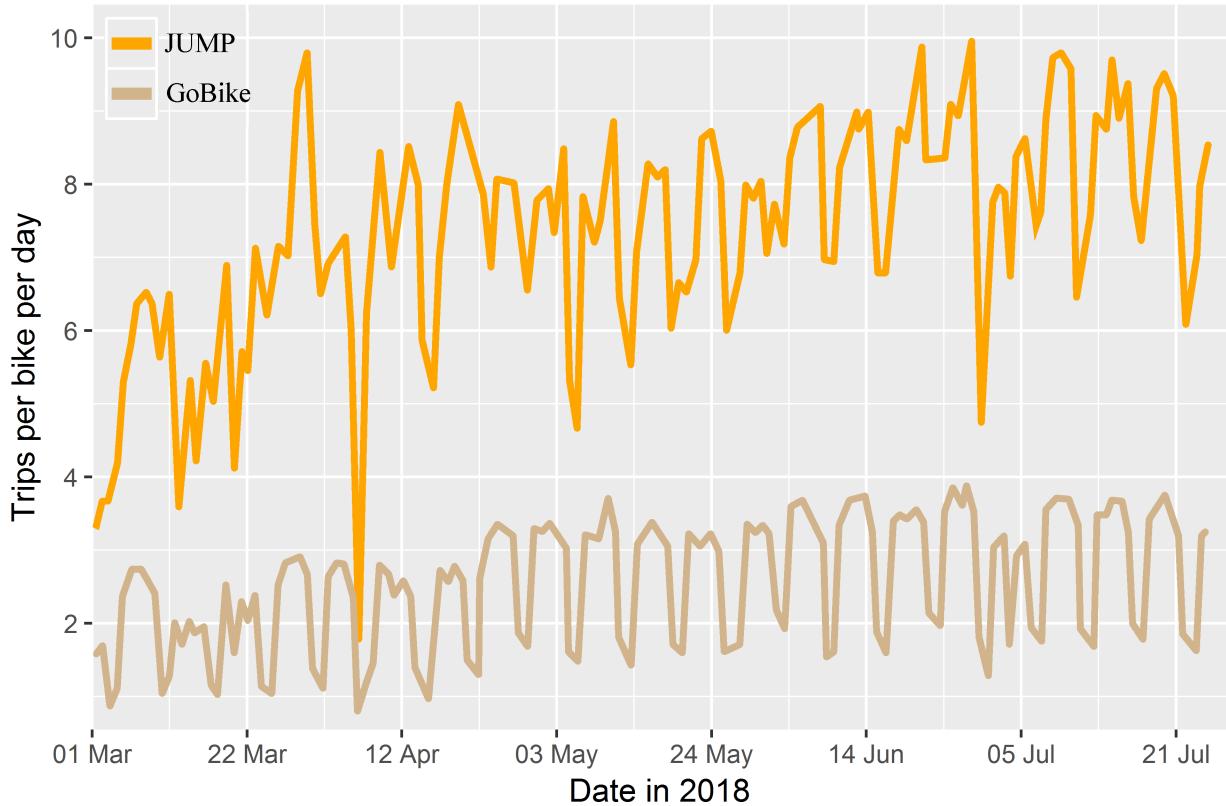


Figure 5.12: Dockless versus station-based, adapted from SFMTA

Above average peaks in the data may occur when special events, such as sport matches, concerts or conferences, take place. Furthermore, public holidays may cause abnormal data patterns (Corcoran et al., 2014). These are also factors that are not considered by DBAFS. Modelling their relationship with PBSS usage is complicated, especially for the events, since the influence will not be the same at all locations within each cluster. However, they will contain information that can explain a part of the variability in the data, as well.

As explained in Section 2.4.1, time series forecasting models relate future patterns to past patterns in the same data. That is, in essence, they do not allow for exogenous variables. However, several methods have been developed to overcome this issue. For example, Hyndman & Athanasopoulos (2018) recommend dynamic regression models, in which the exogenous variables are included in a linear regression, with an ARIMA(p, d, q) model fitted to the autocorrelated errors. Optionally, seasonal patterns can be captured by including Fourier terms in the regression as well. Another option is the `fasster` package in R (O'Hara-Wild, 2018), which is, at the time of writing, still under development. Fasster stands for ‘Forecasting with Additive Switching of Seasonality, Trend and Exogenous Regressors’, and is a model designed to capture both the influence of exogenous regressors as multiple seasonal patterns in a state space framework, by using state switching. Finally, machine learning regression methods are widely used in forecasting, and allow the use of exogenous variables as well. It is recommended to test these approaches with the exogenous variables described

above, and examine the accuracy gain compared to the current approach of DBAFS.

5.4.3 Residual distributions and prediction intervals

Another point of concern regards the non-normality of the models' residual distributions, which showed clearly in Figure 5.8. Both in the calculation of the AIC, for model selection, and in the estimation of the model parameters, Gaussian likelihood is used, assuming a normal distribution. In the literature, approaches have been developed to use different likelihood functions, such as the Laplace Likelihood and Student's t likelihood, that may be more appropriate to use for models with widely tailed residual distributions such as those identified in Figure 5.8 (Huang & Pawitan, 2000; Lehr & Lii, 1998; W. K. Li & McLeod, 1988). However, such approaches will increase the complexity of the system. Moreover, the accuracy gain will probably be of minor extent, since, as discussed in section 2.4.2.4, using Gaussian likelihood is sensible even for models with non-normally distributed residuals, especially when sample sizes are large. It should also be noted that in the `forecast` package, Gaussian likelihood is the only available option.

The non-normality of the residuals does have an important effect on the validity of the prediction intervals, however. When 95% prediction intervals are calculated, assuming normality of the forecast distribution, they can not be interpreted as such. To emphasize this, Table 5.4 shows the percentage of true observations that fall within the calculated 95% prediction interval of the forecasts. As can be seen, for all clusters, and especially those where seasonality was detected, this percentage is extremely low. That is, the calculated prediction intervals are far to narrow, making them not useful in any sense.

Table 5.4: Interpretation of the calculated prediction intervals

	Percentage of observations within 95% prediction interval
Total	0.9
Bayview	17.5
Downtown	0.5
Residential	0.6
Presidio	0.1

As proposed by Hyndman & Athanasopoulos (2018), in the case of non-normally distributed model residuals, a technique called bootstrapping is a useful alternative for calculating prediction intervals. It does not make assumptions about the distribution of the residuals, and only requires them to be uncorrelated. Many possible futures for each forecasted time lag are obtained by repeatedly sampling from the model residuals, and replacing the error terms of the forecasts by these sampled values. Then, the 95% prediction interval for each forecast is equal to the interval that contains 95% of the calculated 'possible futures'. A detailed description of this technique is given by McCullough (1994).

Another important reason for the extremely narrow prediction intervals, is that not all sources of uncertainty are included in its calculation. In DBAFS, there are at least six

different sources of uncertainty.

- The random error component of the ARIMA(p, d, q) model.
- The parameter estimates of the ARIMA(p, d, q) model.
- The choice of the model.
- The continuation of the data generating process into the future.
- The continuation of the seasonal patterns into future.
- The use of a model fitted on the model point's data, for other locations within the same cluster.

In the `forecast` package, only the first of these sources is taken into account when calculating prediction intervals (Hyndman & Athanasopoulos, 2018). In most cases, this leads to acceptable estimates. Even when an ARIMA forecast is combined with a seasonal naïve forecast, this is often true, since seasonal patterns are expected to be constant. However, as already noticed earlier in this chapter, in dockless bike sharing data, there may be a large variation from season to season, and simply ignoring the seasonal uncertainty, is not valid anymore. Bootstrapping can help to partly overcome this issue as well. However, that is a time consuming process, and therefore not suitable to perform at every individual forecast. That is, it still does not account for the last source of uncertainty, which influence is expected to be large. Hence, to provide sensible prediction intervals, an adequate methodology that captures all sources of uncertainty to an acceptable extent, should be developed.

5.4.4 GPS accuracy

One special type of uncertainty does not relate directly to the forecasting process, but to the location provided by the bicycle's GPS instead. In highly built-up urban areas, this GPS location may differ considerably from the true location of the bicycle. According to Uber's research team, such an inaccuracy can have a margin of error of 50 meters or more (Iland, Irish, Madhow, & Sandler, 2018). Since DBAFS essentially forecasts the GPS location, this has an influence on the reliability of the forecasts as well. Including these inaccuracies in the prediction interval, may be a complex challenge, but focused research could take a first step in quantifying the influence of GPS errors on the forecast uncertainty.

Chapter 6

Conclusion

This thesis presented a fully automated forecasting system for bike availability in dockless bike sharing systems. To balance speed and accuracy, the system took advantage of the spatio-temporal nature of the data, and used an approach in which the structures of forecasting models build at specific locations and specific timestamps, were inherited by forecast requests for nearby locations, and future timestamps.

The proposed system was tested through a case study in San Francisco, California. The results showed that time series forecasting models, nested inside the proposed structure of model inheritance, can produce forecasts that outperform simple baseline methods. However, they also highlighted the limited forecastability of dockless bike sharing data, especially when compared to conventional station-based systems.

In future studies that address the same problem, the forecast accuracy may be improved by including exogenous variables, related to weather conditions and special events, which can explain some of the uncaptured variation. Furthermore, methodologies to provide sensible prediction intervals, need to be developed.

Results are believed to be of direct, practical interest for operators of dockless bike sharing systems. In the broader picture, the most important contribution of this thesis is that it is one of the first works that aimed to get a deeper, scientific understanding of the spatio-temporal dynamics of dockless bike sharing systems, and the forecastability of their data. As such, it took a new step on the way to reliable, convenient bike sharing systems, that can provide a serious alternative to motorized transport, and increase the liveability in urban environments.

Appendix A

Code

All the R code used in this thesis, as well as the nested SQL code, is bundled in the `dockless` package (Van der Meer, 2019). Its source code, including documentation for each function, can be found on GitHub, through the following link: <https://github.com/luukvdmeer/dockless>. An R version of at least 2.10 is required. The package is optimized for the case study in San Francisco, but can easily be adapted to other systems.

The JUMP Bikes database is not openly accessible. Therefore, to query the data, and pre-process them on the database server, database credentials are needed. Please contact the author for more information. However, to enable reproducibility, all necessary pre-processed datasets have been included in the package. These are the following:

- `distancedata_centroids`: an object of class `dockless_dfc` containing the distance data for all 249 grid cell centroids, during the training period.
- `distancedata_modelpoints`: an object of class `dockless_dfc` containing the distance data for all 4 model points, during the training period.
- `distancedata_testpoints`: an object of class `dockless_dfc` containing the distance data for all 500 test points, during the test period, and the two weeks before.
- `usagedata_train`: an object of class `sf` with POINT geometry, containing all calculated pick-ups during the training period.
- `usagedata_test`: an object of class `sf` with POINT geometry, containing all calculated pick-ups during the test period.
- `testpoints`: an object of class `sf` with POINT geometry, containing all location-timestamp combinations of the 500 test points.
- `systemarea`: an object of class `sf` with POLYGON geometry, containing the geographical outline of the JUMP Bikes system area in San Francisco.



The `dockless` package can be downloaded from github with the following code. Please make sure that the `devtools` package is installed in advance.

```
devtools::install_github('luukvdmeer/dockless')
```

Then, the complete analysis can be reproduced as follows. Furthermore, reproducible scripts for all tables and figures in chapter 5 can be found through the following link: <https://github.com/luukvdmeer/dockless/tree/master/scripts>

```
require(dockless)
require(sf)

## ----- CLUSTER LOOP -----
# Create grid
gridcells = dockless::create_grid(
  area = systemarea,
  cellsize = c(500, 500)
)

# Calculate grid cell centroids
gridcentroids = gridcells %>%
  dockless::project_sf() %>%
  sf::st_centroid() %>%
  sf::st_transform(crs = 4326)

# Usage intensity per grid cell
gridcells$intensity = dockless::usage_intensity(
  usage = usagedata_train,
  grid = gridcells
)

# Add intensity information to grid cell centroids
gridcentroids$intensity = gridcells$intensity

# Cluster
clusters = dockless::spatial_cluster(
  data = distancedata_centroids,
  grid = gridcells,
  area = systemarea,
  K = c(3:10),
  omega = seq(0, 1, 0.1)
)
```

```
# Add cluster information to grid cells and grid cell centroids
gridcells$cluster      = clusters$indices
gridcentroids$cluster = clusters$indices

# Create model points
modelpoints = dockless::create_modelpoints(
  centroids = gridcentroids
)

## ----- MODEL LOOP -----
# Build models
models = dockless::build_models(
  data = distancedata_modelpoints,
  auto_seasonality = TRUE,
  seasons = list(NULL, 96, 672, c(96, 672))
)

## ----- FORECAST LOOP -----
# Forecast test points with DBAFS and NFS
forecasts_dbafs = dockless::forecast_multiple(
  data = distancedata_testpoints,
  method = 'DBAFS',
  points = testpoints,
  models = models
)

forecasts_nfs = dockless::forecast_multiple(
  data = distancedata_testpoints,
  method = 'NFS',
  points = testpoints
)

# Calculate RMSE's
errors_dbafs = dockless::evaluate(
  forecasts_dbafs,
  type = 'RMSE',
  clusters = testpoints$cluster
)

errors_nfs   = dockless::evaluate(
  forecasts_nfs,
  type = 'RMSE',
  clusters = testpoints$cluster
)
```

Appendix B

Models

This appendix provides more detailed information about the models that were fitted to the non-seasonal historical data of each model point. This information includes parameter estimates, error variance, Gaussian log-likelihood, and information criteria such as AIC. For those model points where seasonality was detected, the decomposition plots are provided as well.

B.1 Bayview model point

Model

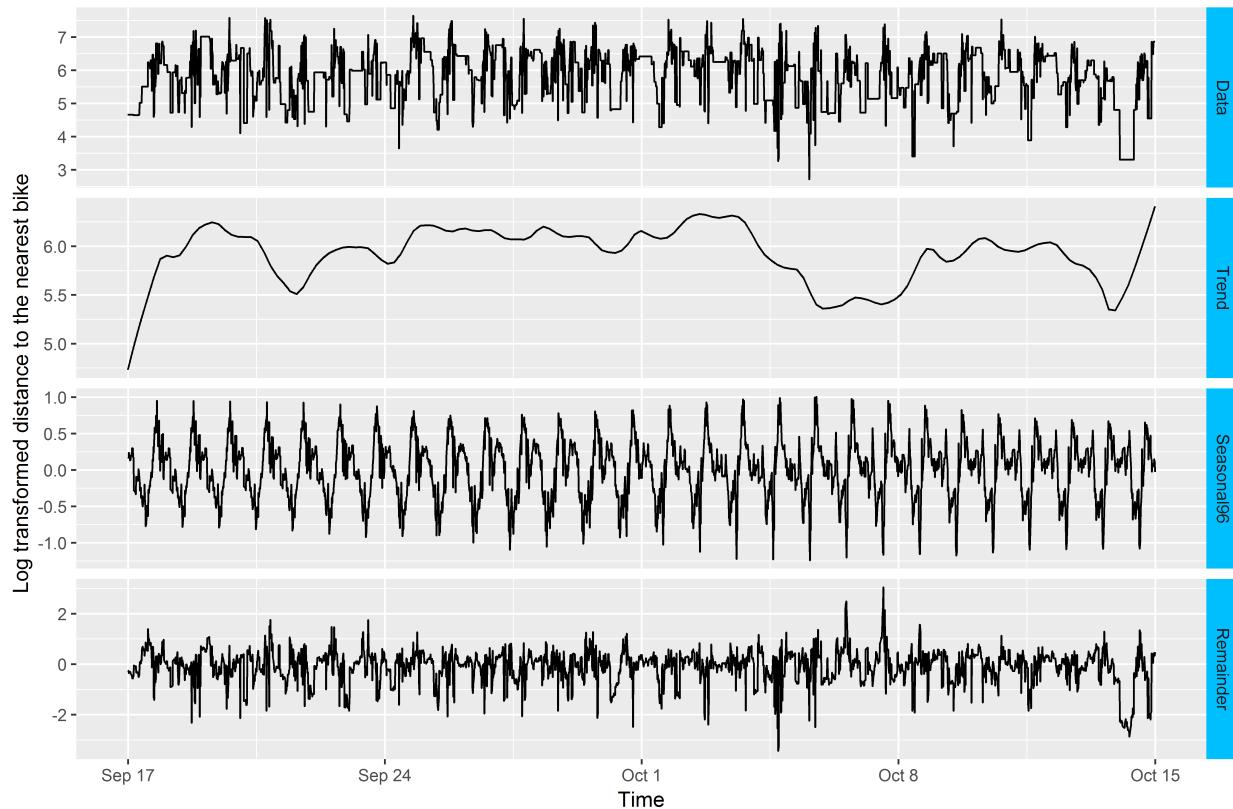
```
Series: x
ARIMA(3,1,1)
Box Cox transformation: lambda= 0

Coefficients:
      ar1      ar2      ar3      ma1
    -0.7636  -0.1269  -0.0724  0.6610
  s.e.   0.2148   0.0320   0.0195  0.2148

sigma^2 estimated as 0.03032:  log likelihood=886.22
AIC=-1762.45  AICc=-1762.42  BIC=-1732.96
```

B.2 Downtown model point

Decomposition plot



Model

Series: x
ARIMA(3,1,2)

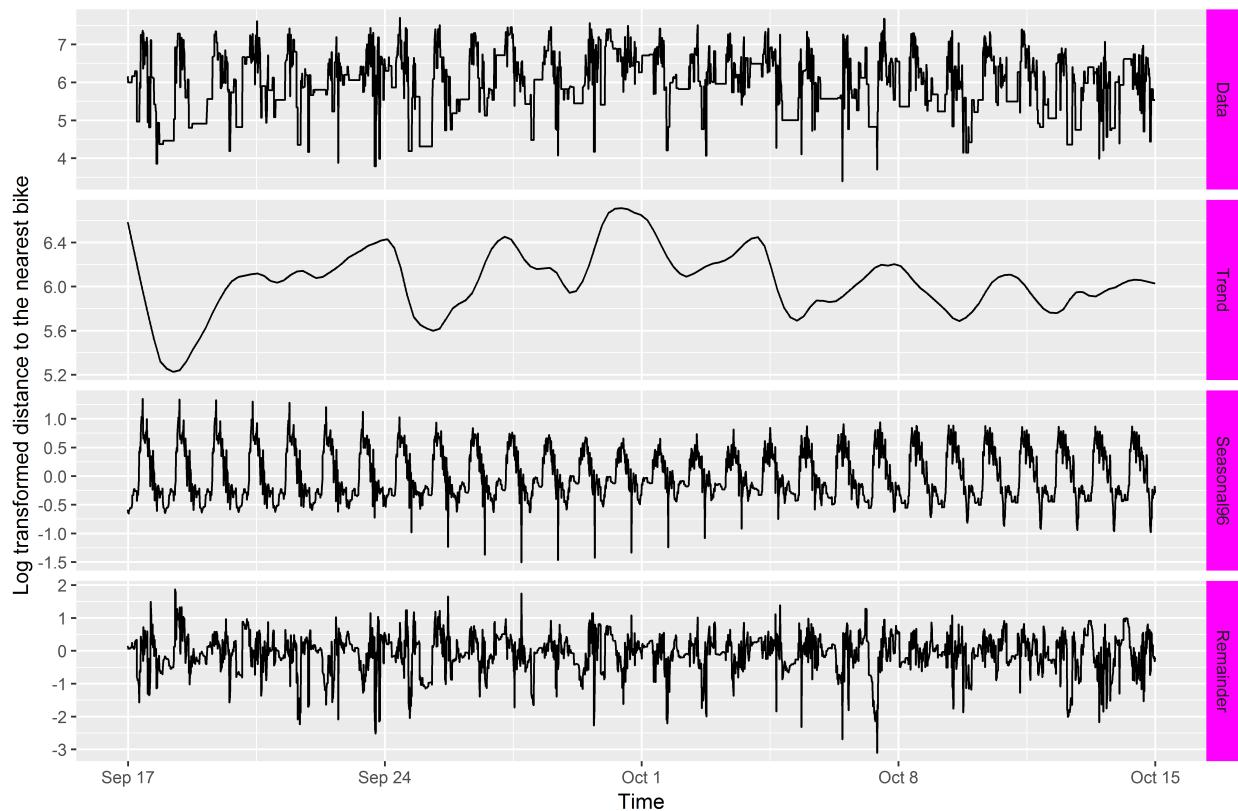
Coefficients:

	ar1	ar2	ar3	ma1	ma2
	-0.1423	0.5707	0.1873	-0.2605	-0.719
s.e.	0.3526	0.2258	0.0351	0.3600	0.352

sigma^2 estimated as 0.2219: log likelihood=-1788.92
AIC=3589.84 AICc=3589.87 BIC=3625.22

B.3 Residential model point

Decomposition plot



Model

Series: x
ARIMA(1,1,1)

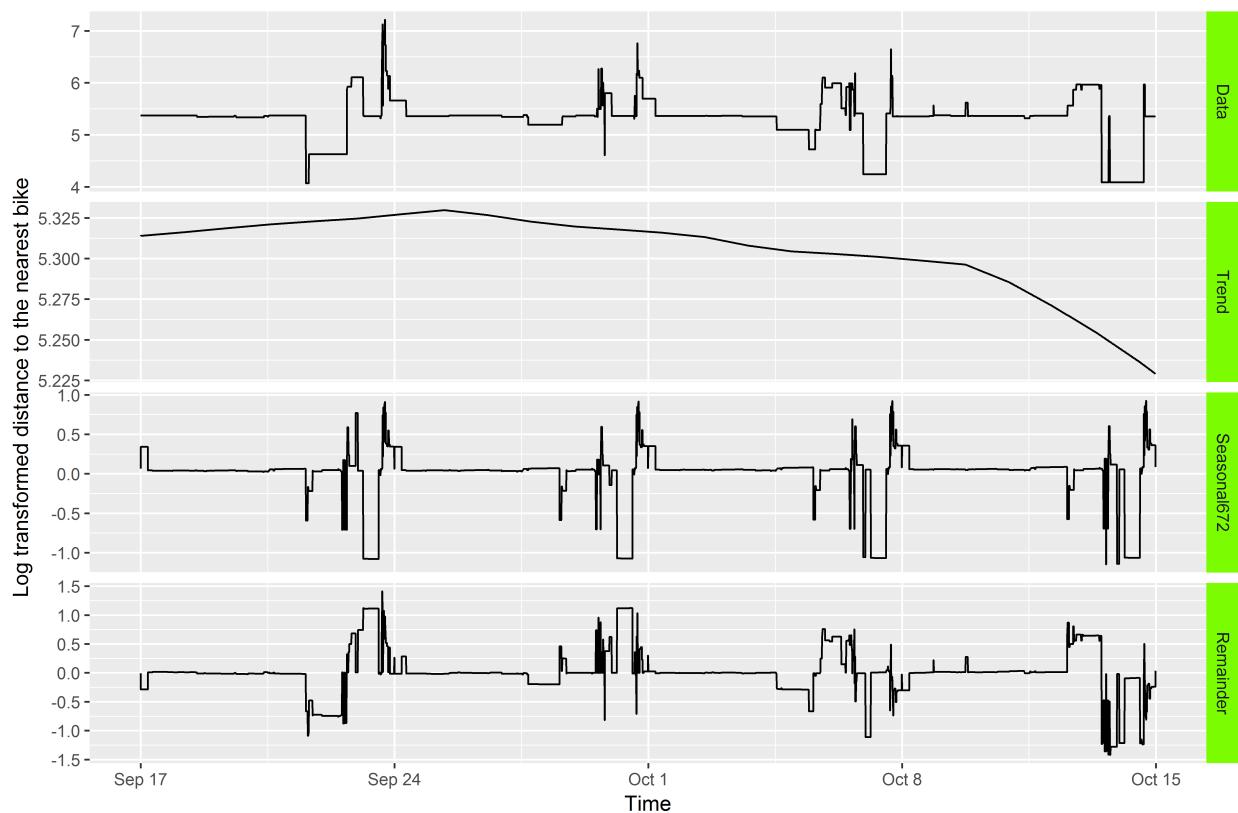
Coefficients:

	ar1	ma1
0.6263	-0.9128	
s.e.	0.0394	0.0257

sigma^2 estimated as 0.1714: log likelihood=-1442.62
AIC=2891.25 AICc=2891.26 BIC=2908.94

B.4 Presidio model point

Decomposition plot



Model

Series: x
ARIMA(1,1,4)

Coefficients:

	ar1	ma1	ma2	ma3	ma4
	-0.6904	0.4389	-0.2201	-0.1439	-0.1430
s.e.	0.0781	0.0790	0.0275	0.0232	0.0192

sigma^2 estimated as 0.02021: log likelihood=1431.7
AIC=-2851.41 AICc=-2851.37 BIC=-2816.03

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