

BACHELOR PAPER

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Anomaly detection in data for data cleansing

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Vienna, May 22, 2022

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Kurzfassung

Diese Bachelorarbeit befasst sich mit dem Thema Anomalie-Erkennung, mit einem Fokus auf Ausreißererkennung. Der Einstig bildet ein Überblick welche Merkmale Datenqualität ausmachen. Danach werden einige Methoden zur Erkennung von Ausreißern vorgestellt. Diese Methoden werden dann mit Daten aus der echten Welt getestet. Die Daten sind Wasserstandsdaten von Flüssen, welche verwendet werden, um Fluten rechtzeitig zu erkennen und betroffene Personen zu warnen. Bevor die Modelle mit den Daten getestet werden, wurde noch eine explorative Datenanalyse durchgeführt, um sich einen Überblick über die Daten zu verschaffen. Am Schluss werden die Ergebnisse der verschiedenen Ansätze Ausreißer zu erkennen verglichen und ausgewertet. Um die Ergebnisse verlgeichen zu können wurde eine passende Kennzahl definiert, welche auskunft über die Leistung des Modells gibt.

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Abstract

This bachelor thesis analyzes methods for anomaly detection, with a focus on outlier detection for time series data. In the beginning an overview of the characteristics that make up data quality are outlined. Afterwards some methods for outlier detection are presented. These Methods are then tested with real world data. The data used for testing consists of the water levels of different rivers, this data is originally used to warn people about upcoming floods in their area of interest. However before testing the models with the data, an explorative data analysis was conducted to provide an overview of the data. At the end, the results of the different approaches to detect outliers are compared and evaluated. In order to be able to compare the models, a suitable performance metric was defined.

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Contents

1	Ove	rview			ı
	1.1	Introdu	luction		1
	1.2	Resea	arch Question		1
	1.3	Resea	arch Method		1
2	Data	a Quali	ity	,	3
	2.1	Featur	res of Data Quality		3
	2.2	Improv	ving Data Quality		4
	2.3	Data C	Cleaning & Cleansing Approaches		5
	2.4	Data C	Cleaning		5
	2.5	Data C	Cleansing	!	5
3	Outl	lier Det	tection		7
	3.1	Outlier	er Types		7
	3.2	Outlier	er Detection Approaches	10	C
	3.3	Thresh	shold based Outlier Detection	1	1
	3.4	Outlier	er Detection using z-score	13	2
	3.5	Outlier	er Detection using modified z-score	1	3
4	Outl	lier Det	tection based on Water Level Data	1	4
	4.1	What i	is the Goal?	1	4
	4.2	How to	to retrieve the Data (Description of the API)	1	4
	4.3	Overvi	view of the Data	18	8
	4.4	Manua	al Classification of Outliers	18	8
	4.5	Explor	rative Data Analysis	19	9
		4.5.1	Aghacashlaun Station	19	9
	4.6	Outlier	er Detection performance Metrics	2	7
		4.6.1	Confusion Matrix	2	7
		4.6.2	Accuracy	2	7
		4.6.3	Precision and Recall	2	8
		4.6.4	F-score	2	9
	4.7	Impler	mentation of different Outlier Detection Approaches	2	9
		4.7.1	Mean Threshold	2	9
		4.7.2	Median Threshold	2	9
		473	MAD Threshold	3	2

		4.7.4	Z-Score	32	
		4.7.5	Modified z-score	32	
		4.7.6	Preprocessing the Data	35	
		4.7.7	Finding Parameters	35	
	4.8	Compa	are different Outlier Detection Approaches	36	
		4.8.1	Station Aghacashlaun, Aghacashlaun (36022-ie)	42	
		4.8.2	Station Murg, Frauenfeld (2386-ch)	42	
		4.8.3	Station Sieg, Betzdorf (2720050000-de)	45	
		4.8.4	Station Losse, Helsa (42960105-de)	45	
		4.8.5	Station Crana, Tullyarvan (39003-ie)	50	
5	Con	clusior	1	52	
6	Futu	ıre Wor	rk	52	
7	Арр	endix		54	
	7.1	Pythor	n Code	54	
		7.1.1	Manual outlier detection	54	
		7.1.2	Preprocessing	55	
	7.2	Outlier	Detection Methods Implementation	56	
	7.3	Param	eter Grid Search	60	
Bibliography 63					
Lis	st of	Figures	3	66	
Lis	List of Tables				
Lis	List of source codes				

1 Overview

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1.1 Introduction

With the growing popularity of Internet of Things (IoT) and digitizing business processes there is a growing amount of data available for analysis. In order to utilize the data from the IoT sensors it needs to be preprocessed. One step of preprocessing is data cleaning (also referred as data cleansing). The main goal of data cleansing is to increase the data quality and furthermore to detect and remove anomalies in the data. The quality requirements for the data can differ depending on the use case. Anomalies in sensor data are datapoints which do not picture the reality. For example an anomaly of a temperature sensor would be if the sensor reads 0 °C and the real temperature is 23 °C. This paper specifically focuses on the removal of outliers for water level sensors. The data is provided by FloodAlert [1], which provides a service to warn people about floods, for their area of interest.

1.2 Research Question

The research questions are:

- What are common methods to detect outliers for time series data?
- · How can outlier detection methods be compared, with a focus on water level data?
- Based on water levels from different rivers, which method is able to classify outliers most reliably?

1.3 Research Method

This thesis will provide an overview and comparison of different approaches to detect outliers. It will focus on time series data, especially water level measurements of rivers. To introduce the topic a general overview about data quality, data cleansing / cleaning and outlier types is provided. For the theoretical pars of the chapters literature research was conducted. After gathering knowledge on different outlier detection approaches they were implemented in Python. To test the performance a suitable performance metric needed to be chosen. To use real world

data to classify outliers, the water levels from different measurement stations were taken. In the end the performance of the different approaches to detect outliers are compared.

2 Data Quality

2.1 Features of Data Quality

This section will provide a few example key features of data quality.

Completeness

Data completeness describes the wholeness of data. If there are certain aspects of data missing the data is not complete. For example if each datapoint of a sensor includes the date, time and production speed, the data is not complete, if one of those features is missing or not entire, this datapoint is not complete. [2,3]

Accuracy

The accuracy of data describes the exactness. Example for possible data which decrease the accuracy are outliers or time shifts. Usually the accuracy of data is harder to measure than the completeness, consistency, structure or documentation. Due to the heterogeneity of sensor data (regarding numerical values like production speed or temperature, not categorical values like on/off) for each datapoint it is difficult to detect which values are genuine and which are sensor errors and therefore outliers. [2] Furthermore an obstacle to accurate data are calculation errors made by computers, because the datatype (e.g. float) is not always 100% exact. However there are methods to reduce these errors. Nevertheless this also needs to be considered when talking about accurate data. [4,5]

Consistency

One example for consistency would be, if the data interval is equal. For example there should be a datapoint every ten seconds. As soon as two datapoints are more than ten seconds apart from each other the data is not consistent anymore. [2]

Structure & Documentation

If the structure of the data is not homogeneous, it is very difficult to analyze in an automated way. As a result the data either needs to be structured from the beginning or a process needs to be fabricated to structure the data automatically. Furthermore documentation is required in order to structure and preprocess data. Documentation of data might include data format (Comma

Separated Values (CSV), parquet [6], Java Script Object Notation (JSON)), date format (e.g. ISO 8601 with UTC offset), valid value spans (e.g. temperature is only valid if it is between 100 and $400\,^{\circ}$ C) [2]

2.2 Improving Data Quality

This section will describe methods to improve data quality, based on the features elaborated in section 2.1.

Completeness

The most common methods to increase data completeness are statistical and deep learning based approaches. The goal of these methods are to fill in the missing values of a dataset. An example for a statistical method is DynaMMo [7]. For Artificial Neuronal Networks (ANNs) Long Short-Term Memory (LSTM) or Gated Recurrent Unit (GRU) can be used to predict missing data. [3]

Accuracy

One approach to increase the accuracy of data is to define constraints for each value. E.g. When a machine cannot produce more than ten pieces per second, because it is physically not possible, the value could be limited to less or equal than ten. However limiting the values to a specific range might hide the fact that the machine has an error and is producing faulty products at a rate of 15 pieces per second. This is one of the reasons why more sophisticated outlier detection methods are used. [3]

Consistency

To facilitate consistent data, statistical smoothing or forecasting methods can be used. Examples methods are: AutoRegressive Integrated Moving Average (ARIMA) or Gaussian Process (GP). ANNs can also be used to unify the time series interval between datapoints. [3]

Structure & Documentation

The process of structuring heterogeneous and messy data is called data wrangling. In order to unify the structure of the data at least some documentation is required. Therefore the documentation of the data is fundamental in order to analyse or further process it.

2.3 Data Cleaning & Cleansing Approaches

There are two main methods when it comes to data cleaning or data cleansing. Ignoring faulty data or replacing it with a representative value. This paper will use the term data cleaning to describe the process of ignoring or deleting incorrect data and the term data cleansing to portray the process of replacing invalid data with representative values. Faulty, incorrect, invalid or wrong data is data which is inaccurate, incomplete or inconsistent.

Example sensor data: (Valid values for $production_speed$ range from 0.00 to 2.00 meter(s) per minute)

ID	timestamp	production_speed (meter/minute)	machine_running
0	2021-12-01T12:00:00.000	1.56	True
1	2021-12-01T12:01:00.000	1.58	True
2	2021-12-01T12:02:00.000	3.50	True
3	2021-12-01T12:03:00.000	1.50	False
4	2021-12-01T12:04:00.000	1.50	True
5	2021-12-01T12:05:00.000	1.49	True

Table 1: Example of IoT sensor data

2.4 Data Cleaning

As already mentioned the approach for data cleaning is to ignore or delete faulty data. Depending on the use case either the entire datapoint needs to be ignored or just one value. The process of data cleaning will be shown with the example data pictured in Table 1. The first incorrect datapoint has the ID 2. This row is incorrect, because the production_speed exceeds the maximum value of 2.00. Depending on the use case (e.g. summary of how long the machine has been running) it can make sense to just ignore the row production_speed and keep the value for machine_running. The second appearance of a faulty datapoint has the ID 2. This datapoint is incorrect since machine_running is False but the value of production_speed is not 0.00. In this case it does not make sense to keep either of those values for further analysis, because it is impossible to determine which of the two columns are incorrect. A possible result after the data cleaning is shown in Table 2

2.5 Data Cleansing

Data cleansing pursues a different approach. Incorrect data is not ignored, but substituted by a representative value. This can only be done, when it is sure, that no future analysis steps

ID	timestamp	production_speed (meter/minute)	machine_running
0	2021-12-01T12:00:00.000	1.56	True
1	2021-12-01T12:01:00.000	1.58	True
2	2021-12-01T12:02:00.000		True
3	2021-12-01T12:03:00.000		
4	2021-12-01T12:04:00.000	1.50	True
5	2021-12-01T12:05:00.000	1.49	True

Table 2: Example of IoT sensor data after cleaning

depend on unaltered data. Since altering some datapoints is likely to change Key Performance Indicators (KPIs), which are calculated from the raw data. For example for the datapoint with the ID 2 there are several strategies that could be followed. For example the outlier value 3.50 could be replaced with the upper limit of the valid range, in this example 2.00, the value could also be replaced with the last valid value, in this example 1.58, or the value could be replaced with the average of the last n Values, for example with $\frac{1.56+1.58}{2}=1.57$. For the datapoint with the ID 3 there are also different approaches. Either the machine was indeed not running then it would make sense, to set the production_speed to 0.0, if short downtimes for this machine are very unlikely then the machine_running value could be set to True. A possible result after the data cleansing is shown in Table 3 [8]

ID	timestamp	production_speed (meter/minute)	machine_running
0	2021-12-01T12:00:00.000	1.56	True
1	2021-12-01T12:01:00.000	1.58	True
2	2021-12-01T12:02:00.000	2.00	True
3	2021-12-01T12:03:00.000	1.50	True
4	2021-12-01T12:04:00.000	1.50	True
5	2021-12-01T12:05:00.000	1.49	True

Table 3: Example of IoT sensor data after cleansing

3 Outlier Detection

3.1 Outlier Types

Outliers can be categorized as point outliers or subsequence outliers. Methods to detect outliers are described in section 3.2

Point Outliers

A point outlier is a single datapoint that strongly varies from the usual trend of the datapoints. [9] Examples of three point outliers are shown in Figure 1.

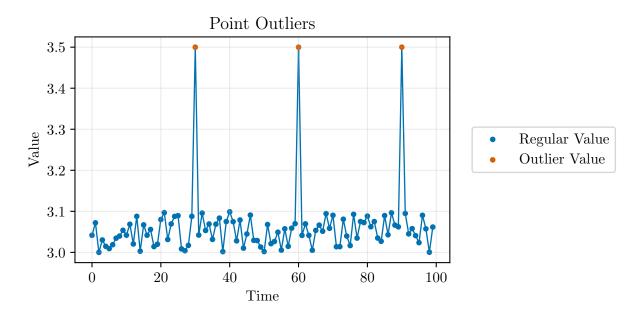


Figure 1: Examples of three point outliers

Subsequence outliers

Subsequence outliers are multiple consecutive datapoints that strongly vary from the usual trend of the datapoints. [9] In Figure 2 examples of subsequence outliers are shown.

Furthermore outliers can be divided into local and global outliers.

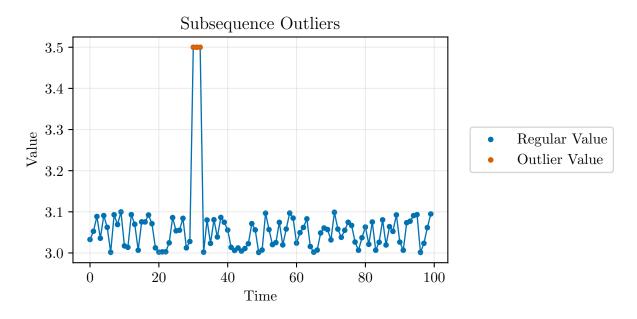


Figure 2: Examples of three subsequence outliers

Local Outliers

A local outlier has a greater variance to its direct neighbouring datapoints (previous and next one) [9] In Figure 3 and Figure 4 examples of local outliers are shown. The first two outliers in Figure 3 have a great variance towards it direct neighbours, however not to the values from Time 60 onwards.

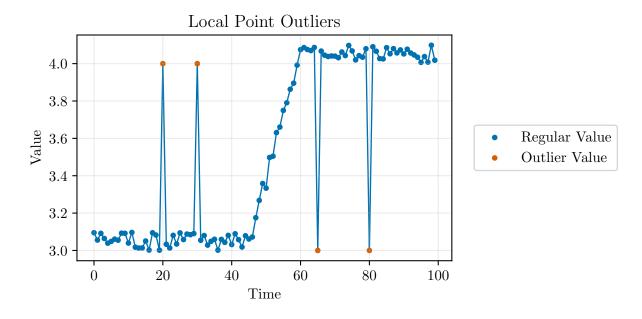


Figure 3: Examples of four local point outliers

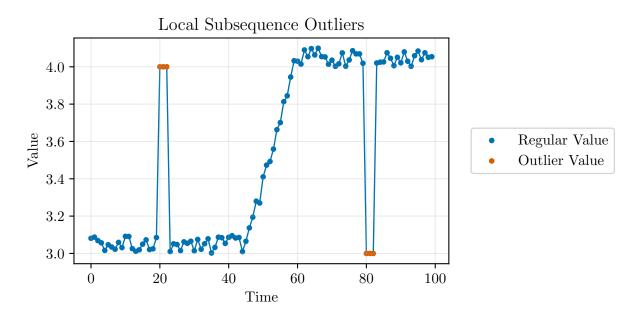


Figure 4: Examples of six local subsequence outliers

Global Outliers

Whereas a global outlier varies more in regard to all datapoints. Figure 1, 2 and 5 show picture examples of global outliers. [9]

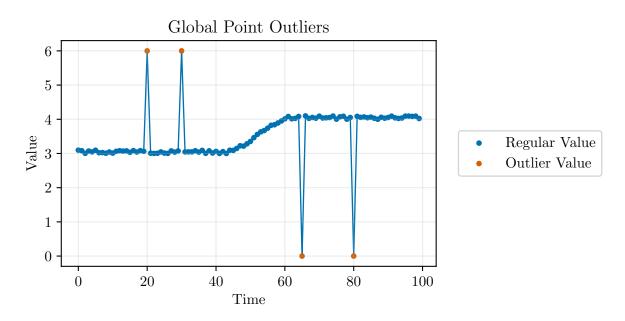


Figure 5: Examples of four global point outliers

3.2 Outlier Detection Approaches

Outlier detection methods can be divided into the following groups

Statistical

For statistical outlier detection, historical data is taken to develop a model that pictures the expected behavior of the data. An example of a statistical outlier detection is the threshold based method described in section 3.3 [10,11]

Distance based

For this approach a distance metric needs to be defined, (e.g. Euclidean distance). Then each datapoint is compared to the data preceding it. The greater the distance between the current and previous datapoints the greater the probability of an anomaly. [10–12]

Clustering

Clustering also requires a set of historical data in order to train the clustering model. Usually the data is clustered into two clusters: normal data and anomalous data. Depending on the distance of a new datapoint to the "normal" and the "anomalous" cluster it is classified. [10–12]

Predictive

In this approach a prediction model needs to be developed, based on previous data. The prediction of this model is then compared with the actual datapoint (new data, which was not used in training the model). If the actual datapoint differs too much from the prediction it is labelled as an anomaly. [10,11]

Ensemble

as the word ensemble suggests, this is a collection of outlier detection methods that use a specific vote mechanism to determine whether a datapoint is faulty or normal. For example using the majority vote system and a statistical, distance based and predictive method to detect outliers. If at least two methods flag a datapoint as an outlier the ensemble reports it as an outlier as well. If only one method reports it as an outlier the ensemble does not flag it as an anomaly. [10]

3.3 Threshold based Outlier Detection

Threshold based detection methods are able to identify outliers based on a given threshold τ . These Methods can be described with the following formula

$$|x_t - \hat{x}_t| > \tau$$
 [9]

Where x_t is the actual value and \hat{x}_t is the expected value and τ is a given threshold. Methods to calculate \hat{x}_t will be described in the following sections. Furthermore \hat{x}_t can be calculated using the entire data series or with subsets (of equal length) of the entire data series. This means \hat{x}_t can be either calculated for the whole data series or for just a segment. Depending on the sensitivity wanted for outlier detection an appropriate τ needs to be chosen. The greater τ is the fewer outliers will be detected. The smaller τ is the more outliers will be identified. [9]

Mean

$$\mathsf{mean} = \bar{x} = \frac{1}{n} \sum_{t=0}^{n} x_t \tag{2}$$

Where n is the total number of samples. Using the mean as an expected value is not robust to outliers, because the median is not as robust as the mean in hindsight to outliers. To calculate the mean all datapoints of a series must be summed up and then divided by the number of datapoints.

Median

If n is odd:

$$median(x) = x_{(n+1)/2} \tag{3}$$

If n is even:

$$median(x) = \frac{x_{n/2} + x_{(n+1)/2}}{2}$$
 (4)

Where x is a dataset of n elements ordered from smallest to largest

 $(x_1 \le x_2 \le x_3 \le \ldots \le x_{n-2} \le x_{n-1} \le x_n)$ [9] To calculate the median all values must be sorted from smallest to largest. If the number of datapoints is odd then the most center datapoint is the Median (e.g. if the series consist of 7 values the third value is the median). If the number of datapoints is even then the median is the mean of the two datapoints in the center.

Median Absolute Deviation (MAD)

The Median Absolute Deviation

$$MAD = median(|x_t - median(x)|)$$
(5)

MAD is a more robust (regarding outliers) way to calculate the deviation of a dataset. To calculate the MAD firstly the median of the dataset must be calculated. Then the absolute difference between x_t and the median of the dataset is calculated. The Median of all differences results in the MAD [13,14]

3.4 Outlier Detection using z-score

The z-score, also known as the standard score, is the factor of how many standard deviations a datapoint differs from the mean. Using standard score to detect outliers works best, when the data is distributed normally. Because then it can be assumed, that e.g. the top and bottom 0.5% are outliers and therefore every value with $|z| > \approx 2.576$ can be classified as an outlier. A visual representation of the z-score in a normal distribution is shown in Figure 6

$$z_t = \frac{x_t - \mu}{\sigma} \tag{6}$$

Where μ is the mean of the dataset and σ is the standard deviation. When the mean and the standard deviation of the entire dataset is now known the mean and the standard deviation of a known sample can be used. [15–17]

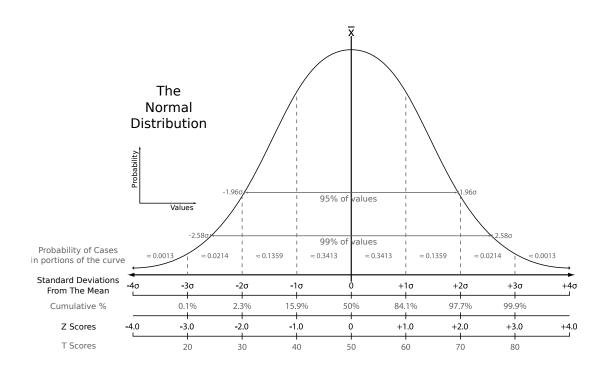


Figure 6: Standard Score in a normal distribution [18]

$$\sigma = s = \sqrt{\frac{1}{n-1} \sum_{i=1}^{n} (x_i - \bar{x})^2}$$
 (7)

[16, 17]

To check whether the value x_t is an outlier the absolute of its z-score is compared against a threshold (τ) and if the absolute value of the z-score exceeds the threshold x_t is classified as an outlier.

$$|z_t| > \tau \tag{8}$$

3.5 Outlier Detection using modified z-score

Because the mean and standard deviation are not robust towards outliers the z-score can be modified to use more robust metrics for the expected value and the variation of the values. To make the outlier detection with the z-score more robust the mean can be replaced with the median and the standard deviation with the MAD or the Normalized Median Absolute Deviation (MADN). A possible formula for a modified z-score, as described in [19], could be:

$$m_t = \frac{|x_t - median(X)|}{MADN(X)} \tag{9}$$

Where the formula for the MADN is:

$$MADN(X) = \frac{MAD(X)}{0.6745} \tag{10}$$

The constant value 0.6745 is the 75th percentile of a standard normal distribution, which is equal to the MAD of a standard normal distribution with $\sigma = 1$. [19]

The classification of outliers using the modified z-score (m_t) is the same for the regular standard score described in section 3.4:

$$|m_t| > \tau \tag{11}$$

4 Outlier Detection based on Water Level Data

FloodAlert (or "Pegelalarm" in German) is a service that provides water levels from about 30,000 measurement stations. It provides notifications to registered individuals, when a certain water level threshold is reached. Thus warning people about possible floods in their area. [1]

Unfortunately sometimes an incorrect water level is reported by the sensors, which are not maintained by the team of FloodAlert. FloodAlert just fetches the data from different maintainers of sensors. To reduce the frequency of false alarms, outliers should be identified and flagged. The theoretical parts of the previous sections are applied and tested on real-word data.

4.1 What is the Goal?

The ideal goal of FloodAlert would be to have a general model, that works on a variety of rivers. The model should be able to predict the probability of being an outlier for each water level value, without knowing future values. Thereby making it possible to classify incoming datapoints in real time, without needing future datapoints to make a prediction. Furthermore it would be ideal if the outlier detection method is able to adjust its parameters automatically for each river / water level measurement location. Because different rivers have different fluctuations in water level. Therefore each water level measurement station needs individual parameters. For example one river regularly has an increase and decrease of 10 centimeters whereas for another river 10 cm of water level variance from one datapoint to the next is definitely an outlier.

Another approach would be to also take future values into consideration when predicting the probability of a value being an outlier. This method is probably easier and likely leads to better results. However a method which does not take future values into consideration would be more useful for FloodAlert, since the values could be classified immediately.

4.2 How to retrieve the Data (Description of the API)

To make the access to the API easier SOBOS GmbH developed a Python wrapper which returns the requested data as a Pandas dataframe. [20] The code for the Python wrapper is available on GitHub [21]: https://github.com/SOBOS-GmbH/pegelalarm_public_pas_doc [22]

In order to request data, an API key needs to be requested using credentials. To request the API key a POST request needs to be sent to this endpoint https://api.pegelalarm.at/api/login, where the request body contains the users' credentials as shown in Listing 1. To generate

Listing 1 Request body to get API key

the actual API key the key from the response needs to be hashed using the Keyed-Hashing for Message Authentication (HMAC) Algorithm. This is done using Python's built in "hmac" module. [23]. Afterwards the HMAC is byte64 encoded, so it can be sent in the "X-AUTH-TOKEN" header field.

To get the unique identifier for a specific measurement station the list endpoint can be used. Which accepts three optional query parameters (qStationName - station name, qWater - water name and commonid - the unique identifier of a station) and returns a list of matching stations with metadata like coordinates, country or last water level. E.g. to retrieve the identifier of the Danube station located in Linz the URL is the following: https://api.pegelalarm.at/api/station/1.1/list?qStationName=Linz&qWater=Donau. Keep in mind in order to retrieve any data the header value "X-AUTH-TOKEN" must be set. An example response of this request is shown in Listing 2. Where the unique identifier is the "commonid" in line 9.

To retrieve historical data, the history endpoint can be used. The request URL has the following structure: https://api.pegelalarm.at/api/station/1.1/<unit>/<commonid>/history? <parameters>. The unit can either be "height" or "flow". For this thesis only height data was used. The following parameters can be set:

- loadStartDate: The start timestamp of the queried data.
- loadEndDate: The end timestamp of the gueried data.
- granularity: The granularity of the response.

Possible values for the granularity are: "raw" (for the last 3 months of data), "hour", "day", "month", "year" or "era" (era returns one value for a given time) When requesting aggregated data (anything other than "raw"), the maximum value of the timespan is used. The timestamps are in the following format: "<DD>.<MM>.<YYYY>T<HH>:<MM>:<SS><+-UTCOFFSET>", where the '+' is URL encoded to "%2B". E.g.: "31.03.2022T13:35:40%2B0200". If no parameters are provided the API returns the last few datapoints.

An example request would be: https://api.pegelalarm.at/api/station/1.1/height/207068-at/history?loadStartDate=01.03.2022T13:35:40%2B0200&loadEndDate=01.03.2022T18:00: 00%2B0200&granularity=hour The result of this request is shown in Listing 3.

Listing 2 Example response of the list endpoint

```
1
       "status": {
2
            "code": 200
3
       },
       "payload": {
            "stations": [
                     "name": "Donau / Linz / at",
                     "commonid": "207068-at",
                     "country": "Österreich",
10
                     "stationName": "Linz",
                     "water": "Donau",
12
                     "region": "Oberösterreich",
13
                     "latitude": 48.306915712282,
14
                     "longitude": 14.284689597541,
15
                     "positionKm": 2135.17,
16
                     "altitudeM": 247.74,
17
                     "defaultWarnValueCm": 550.0,
                     "defaultAlarmValueCm": 630.0,
19
                     "data": [
20
                         {
21
                              "type": "height in cm",
22
                              "value": 358.0,
23
                              "requestDate": "19.04.2022T14:59:51+0200",
24
                              "sourceDate": "19.04.2022T14:45:00+0200"
25
                         }
26
                     1,
27
                     "trend": 10,
28
                     "situation": 10,
                     "visibility": "PUBLIC",
                     "stationType": "surfacewater"
31
32
           ]
33
34
35
```

Listing 3 Example response of historical water level data for one station

```
1
        "status": {
2
            "code": 200
3
        },
4
        "payload": {
5
            "history": [
6
                 {
                     "value": 360.0,
                     "sourceDate": "01.03.2022T13:00:00+0100"
9
                 },
10
                 {
11
                     "value": 360.0,
12
                     "sourceDate": "01.03.2022T14:00:00+0100"
13
                 },
14
                 {
15
                     "value": 359.0,
16
                     "sourceDate": "01.03.2022T15:00:00+0100"
17
                 },
18
19
                     "value": 361.0,
20
                     "sourceDate": "01.03.2022T16:00:00+0100"
21
                 },
22
                 {
23
                     "value": 362.0,
24
                     "sourceDate": "01.03.2022T17:00:00+0100"
25
26
            ]
       }
28
   }
29
```

4.3 Overview of the Data

To test and tune the outlier detection methods the entire history of data was used. The granularity of the data usually is hourly up to the last three months of data. There are a few exceptions, where the granularity is not hourly, because either one or a few datapoints are missing. For the last three months the granularity is "raw", which is different for each station. Additionally the base (where the sensor reports water level equals zero) also differs per station. Some station have an arbitrary zero level whereas some stations have the sea level as a base. Thus the water level does not actually reflect the actual height, or depth, of the water. Instead it represents the relative water level to a specific height.

The following water level measurement stations were used to test the outlier detection methods:

Station Aghacashlaun, Aghacashlaun (36022-ie)

This station, on the river Aghacashlaun and in the area of Aghacashlaun, is located in northern Ireland. The coordinates of this station are: 54.03647, -7.94672 (Latitude (Lat), Longitude (Long)). [24]

Station Murg, Frauenfeld (2386-ch)

The station, on the river Murg and in the area of Frauenfeld, is located in northern Switzerland. The coordinates of this station are: 47.56852, 8.89432 (Lat, Long). [25]

Station Sieg, Betzdorf (2720050000-de)

The station, on the river Sieg and in the area of Betzdorf, is located in western Germany. The coordinates of this station are: 50.79332, 7.86390 (Lat, Long). [26]

• Station Losse, Helsa (42960105-de)

The station, on the river Losse and in the area of Helsa, is located in central Germany. The coordinates of this station are: 51.25574, 9.68537 (Lat, Long). [27]

• Station Crana, Tullyarvan (39003-ie)

The station, on the river Crana and in the area of Tullyarvan, is located in northern Ireland. The coordinates of this station are: 55.14356, -7.45239 (Lat, Long). [28]

4.4 Manual Classification of Outliers

In order to speed up the manual labeling of outliers a program was written. The program is a Plotly Dash [29] web application which displays the water level data as a scatter chart. By clicking the datapoints in the chart the user is able to toggle the datapoint as an outlier or back to a regular value. In Listing 9 the source code of the Dash application is shown. In Figure 7 the Website of the Python app is shown, the red dots between 25 and October 28 are already classified outliers. Below the chart a rangeslider is located, to move the zoomed

in view horizontally. The refresh button on the left side refreshes the graph, thus updating the color and label of previously selected outliers. Furthermore it saves the data to a parquet file. The upper and lower limit of the y-axis also gets updated, when pressing the refresh button. The limits are automatically set to the lowest and highest regular value. This was implemented, because some datasets had outliers with a huge difference towards the regular data. Without the automatic scaling of the y-axis, detecting other outliers with a smaller difference was not possible.

Manual Outlier Selection

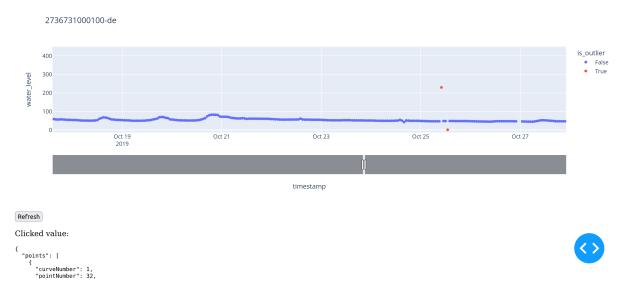


Figure 7: Dash Webapp to classify outliers

Manual Outlier Detection Webapp using Dash

The Python code for the webapp can be found in the appendix (Listing 9)

4.5 Explorative Data Analysis

add another sta-

4.5.1 Aghacashlaun Station

Table 4 shows seven number summary for all datapoints (outliers and regular values). The column "water_level_diff" is the difference in water level between two consecutive datapoints. The column "timedelta" is the time difference between two consecutive datapoints in hours. Table 5 and Table 6 picture seven number summaries for regular and only outlier values. The standard deviation is clearly higher for outlier values when compared to the standard deviation of regular values.

	water_level	water_level_diff	timedelta
count	27189.000000	27188.000000	27188.000000
mean	36.009754	-0.000077	0.809990
std	14.716286	7.220175	1.256409
min	0.000000	-107.500000	0.000000
25%	26.400000	-0.300000	1.000000
50%	31.700000	-0.100000	1.000000
75%	40.300000	0.000000	1.000000
max	190.000000	94.800000	178.000000

Table 4: Seven number summary of Aghacashlaun - Aghacashlaun (all values)

	water_level	water_level_diff	timedelta
count	26544.000000	26543.000000	26543.000000
mean	35.381205	-0.411276	0.808311
std	13.763332	5.165770	1.268532
min	20.000000	-107.500000	0.000000
25%	26.400000	-0.300000	1.000000
50%	31.400000	-0.100000	1.000000
75%	39.800000	0.000000	1.000000
max	151.600000	51.900000	178.000000

Table 5: Seven number summary of Aghacashlaun - Aghacashlaun (regular values)

	water_level	water_level_diff	timedelta
count	645.000000	645.000000	645.000000
mean	61.876744	16.921550	0.879070
std	25.476859	28.411003	0.560844
min	0.000000	-90.000000	0.000000
25%	40.000000	-10.000000	1.000000
50%	60.000000	12.500000	1.000000
75%	80.000000	39.400000	1.000000
max	190.000000	94.800000	9.000000

Table 6: Seven number summary of Aghacashlaun - Aghacashlaun (outlier values)

In figure Figure 8 the class distribution is shown. The classes are not balanced, there are far more regular values than outliers. This needs to be kept in mind when choosing a performance metric.

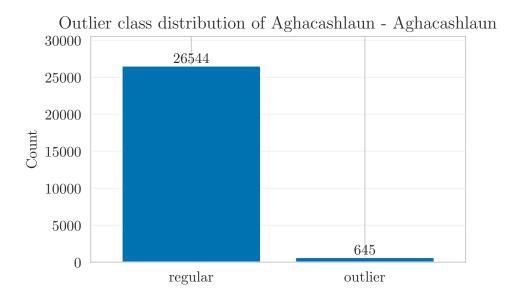


Figure 8: Class distribution of Aghacashlaun - Aghacashlaun

Figure 9 shows boxplots for all values, regular values and outlier values. The boxplots show, that the upper and lower whisker boundaries cannot be used to classify outliers reliably. Since there are many regular values that exceed the upper limit of the whisker, which is 1.5 times the InterQuartile Range (IQR).

In Figure 10 histograms of the different water levels are shown. The y-axis is scaled logarithmically, so less common values are also visible. The histogram shows, that values between 20 and 40 are most common and the higher the water level is the less common it becomes. Figure 11 is quite similar, but instead of the water level the difference in water level between two consecutive datapoints is used.

Figure 12 Shows the histogram of the time difference, in hours, between each datapoint. The largest gap of data is 178 hours, which is about one week.

In Figure 13 the water level over the time is shown. This chart shows, that the water level usually oscillates between 20 and 100. Figure 14 displays an example of subsequence outliers. Within one hour the water level rises by double the previous value. This is very unlikely, thus these values were classified as outliers. The reason, for multiple consecutive outliers, with decreasing water level over time could be, that the station does not report the actual water level but a moving average over the last few recorded values. This would at least explain the pattern of outliers shown in Figure 14.

Code: [30] _

Add Code in ap pendix

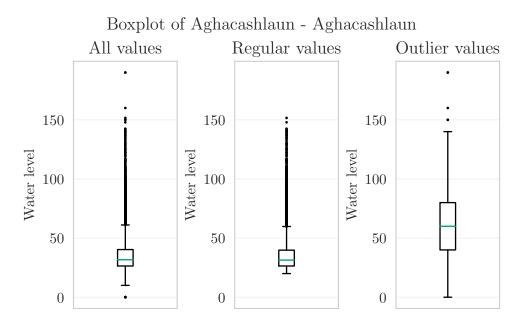


Figure 9: Boxplot of Aghacashlaun - Aghacashlaun

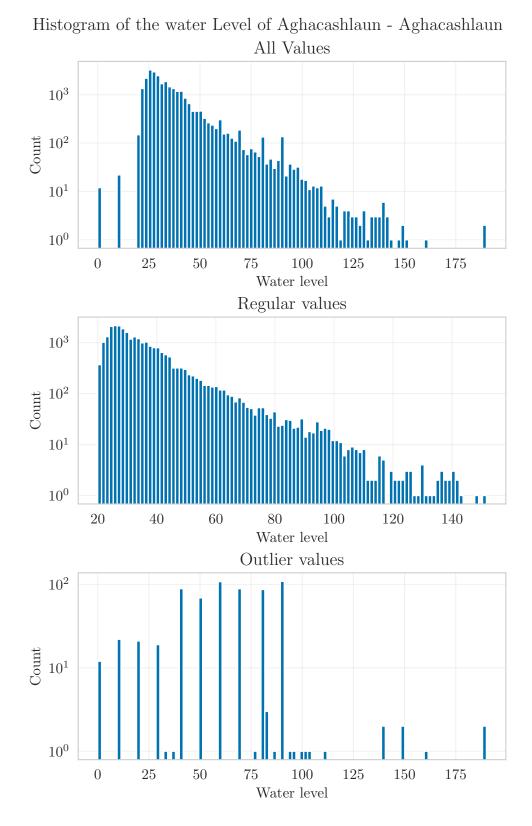


Figure 10: Histogram of the water level of Aghacashlaun - Aghacashlaun

 $\operatorname{Histogram}$ of the water level delta of Aghacashlaun - Aghacashlaun

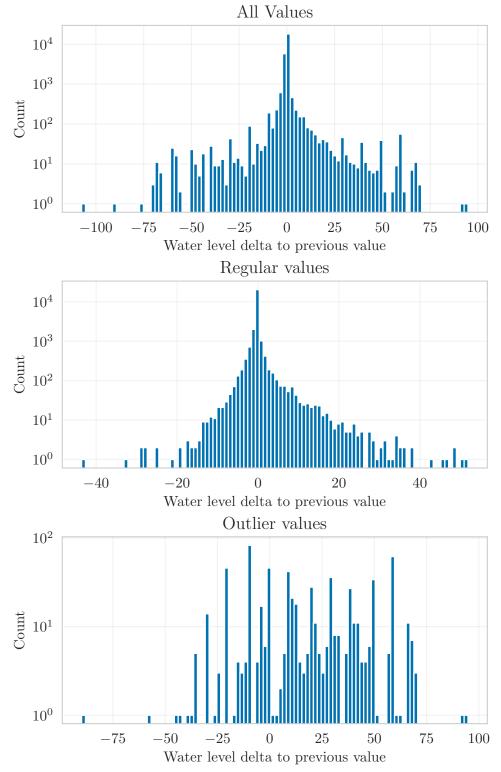


Figure 11: Histogram of the water level delta of Aghacashlaun - Aghacashlaun

 $\operatorname{Histogram}$ of the time delta between values of Aghacashlaun - Aghacashlaun



Figure 12: Histogram of the time delta (in hours) of Aghacashlaun - Aghacashlaun

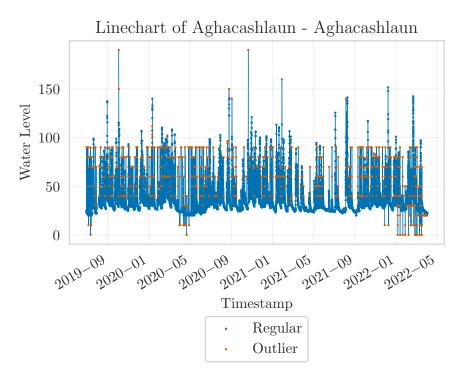


Figure 13: Line chart of Aghacashlaun - Aghacashlaun (whole data)

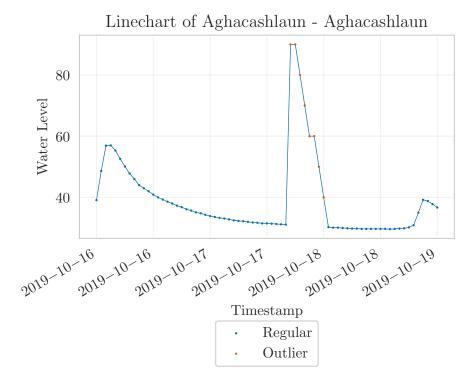


Figure 14: Line chart of Aghacashlaun - Aghacashlaun (2019-10-16 - 2019-10-19)

4.6 Outlier Detection performance Metrics

4.6.1 Confusion Matrix

To compare the performance of two classification methods a confusion matrix, shown in Table 7, can be used to provide an overview. A confusion matrix consists of the following elements (explained on the basis of outlier detection):

- True Positive (TP): actual class: outlier, predicted class: outlier
- False Negative (FN): actual class: outlier, predicted class: regular
- True Negative (TN): actual class: regular, predicted class: regular
- False Positive (FP): actual class: regular, predicted class: outlier

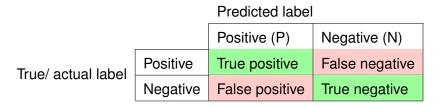


Table 7: Example of binary confusion matrix

The green cells represent the correctly classified values (TP & TN) and the red cells represent the incorrectly classified values (FN & FP). The confusion matrix is the basis of many more performance metrics.

4.6.2 Accuracy

To make the comparison easier, the confusion matrix can be aggregated into one single value as a metric. There are numerous ways how this single metric can be calculated. One of the Most common and basic methods is the Accuracy:

$$Accuracy = \frac{Number\ of\ correct\ predictions}{Total\ number\ of\ predictions} = \frac{TP + TN}{TP + FN + TP + FP} = \frac{TP + TN}{P + N} \tag{12}$$

The accuracy provides information what percentage of values are correctly classified. However if the classes are not equally distributed, the accuracy is a bad metric. This is especially true for heavily imbalanced classes. For example if the dataset has $1\,000\,000$ positive values and 10 negative, when optimizing for a high accuracy it can happen that the classifier predicts every value as positive and still achieves a very high accuracy:

$$Accuracy = \frac{1\,000\,000 + 0}{1\,000\,000 + 10} = 0.99999 \tag{13}$$

Thus for measuring the performance of outliers, the accuracy is not a suitable metric.

4.6.3 Precision and Recall

Figure 15 shows a visual comparison between precision and recall. The precision provides information about what percentage of positive predictions were actually correct. Whereas the recall provides information about what percentage of all positive values were actually predicted as such. Precision and Recall are used to calculate the F-Score described in subsection 4.6.4.

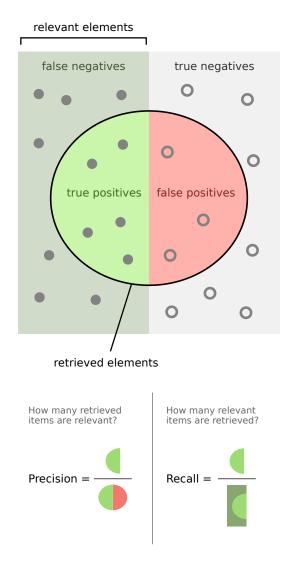


Figure 15: Precision vs Recall [31]

Precision

$$Precision = \frac{TP}{TP + FP} \tag{14}$$

Recall

$$Recall = \frac{TP}{TP + FN} \tag{15}$$

4.6.4 F-score

The $F_1-score$ is the harmonic mean of the precision and recall.

$$F_1 - score = \frac{2}{\frac{1}{Precision} + \frac{1}{Recall}} = \frac{2}{\frac{Precision + Recall}{Precision \cdot Recall}} = \frac{2 \cdot Precision \cdot Recall}{Precision + Recall}$$
(16)

[32, 33]

The $F_{\beta}-score$ is more sophisticated compared to the $F_1-score$ where an additional parameter (β) needs to be chosen, which is used to weight the precision.

$$F_{\beta} - score = \frac{(\beta^2 + 1) \cdot Precision \cdot Recall}{\beta^2 \cdot Precsion + Recall}$$
(17)

[33, 34]

The $F_1 - score$ uses 1 for β so the precision and the recall are equally weighted.

4.7 Implementation of different Outlier Detection Approaches

The input data structure for the different approaches is a pandas DataFrame. [20] The structure of the DataFrame is equal for all measurement stations. It contains the following columns:

- water_level: the water level of the river in cm (datatype: float64)
- timestamp: the date and time of the datapoint in UTC (datatype: datetime64[ns, UTC])
- is_outlier: true or false depending if the value is an outlier (datatype: bool)

To test the performance of the models the column is_outlier contains the ground truth, which was manually labeled. An example of the input data can be seen in Table 8.

To speed up the process of calculating the result of the outlier detection method ($|x_t - \hat{x}_t|$, the z-score or the modified z-score) is all done in one step and in the second step the result of this calculation is compared against a range of thresholds.

4.7.1 Mean Threshold

Calculating \hat{x}_t using the mean for a pandas DataFrame [20] is quite straightforward and is shown in Listing 4. To reduce the amount of duplicate code, the imports are only included in Listing 4.

4.7.2 Median Threshold

The calculation of the median is guite similar to the mean. It is shown in Listing 5.

Listing 4 First step of classifying outliers using the mean

```
from typing import Union
2
  import numpy as np
  import pandas as pd
5
  def mean_outlier_detection(input_df: pd.DataFrame,
                               window: Union[int, None],
                               center_window: bool):
       . . . .
10
       Detects outliers in a dataframe using a (moving) average.
11
       :param input_df: the input dataframe where the values are stored
12
                         in the column water_level
13
       :param window: the size of the window, None if no window should
14
                       be used
       :param center window: whether the window should be centered or not
16
       :return: a copy of the input dataframe where the column result
17
                should be compared to a threshold to detect outliers
18
       . . . .
19
       od_df = input_df.copy()
20
       if window is None:
           od_df['x_hat'] = od_df['water_level'].mean()
22
       else:
23
           od df['x hat'] = \
24
               od_df['water_level'].rolling(window=window,
25
                                              center=center window,
26
                                              min_periods=1).mean()
       od_df['result'] = np.abs(od_df['water_level'] - od_df['x_hat'])
28
       return od_df
29
```

water_level	timestamp	is_outlier
24.9	2019-06-30 15:00:00+00:00	False
24.9	2019-06-30 16:00:00+00:00	False
24.8	2019-06-30 17:00:00+00:00	False
24.4	2019-06-30 18:00:00+00:00	False
24.4	2019-06-30 19:00:00+00:00	False
24.3	2019-06-30 20:00:00+00:00	False
24.1	2019-06-30 21:00:00+00:00	False
24.0	2019-06-30 22:00:00+00:00	False
90.0	2019-06-30 23:00:00+00:00	True

Table 8: First 9 values of Aghacashlaun - Aghacashlaun

Listing 5 First step of classifying outliers using the median

```
def median_outlier_detection(input_df: pd.DataFrame,
                                 window: Union[int, None],
                                 center_window: bool):
       . . . .
4
       Detects outliers in a dataframe using a (moving) average.
       :param input_df: the input dataframe where the values are stored
                         in the column water_level
       :param window: the size of the window, None if no window should
                       be used
       :param center_window: whether the window should be centered or not
10
       :return: a copy of the input dataframe where the column result
                should be compared to a threshold to detect outliers
12
       . . . .
13
       od df = input df.copy()
14
       if window is None:
15
           od_df['x_hat'] = od_df['water_level'].median()
       else:
17
           od_df['x_hat'] = \
18
               od_df['water_level'].rolling(window=window,
19
                                              center=center_window,
20
                                              min_periods=1).median()
       od_df['result'] = np.abs(od_df['water_level'] - od_df['x_hat'])
22
       return od_df
23
```

Listing 6 First step of classifying outliers using the MAD

```
def mad_outlier_detection(input_df: pd.DataFrame,
                              window: Union[int, None],
                              center window: bool):
       11 11 11
       Detects outliers in a dataframe using a (moving) average.
       :param input_df: the input dataframe where the values are stored
                         in the column water level
       :param window: the size of the window, None if no window should
                       be used
       :param center_window: whether the window should be centered or not
10
       :return: a copy of the input dataframe where the column result
11
                should be compared to a threshold to detect outliers
12
       . . . .
13
       od_df = input_df.copy()
14
       if window is None:
           od_df['x_hat'] = np.median(
               np.abs(od_df['water_level'] - np.median(
                    od_df['water_level'])))
18
       else:
19
           od_df['x_hat'] = \
20
               od_df['water_level'].rolling(window=window,
21
                                              center=center_window,
                                              min_periods=1).apply(
23
                    lambda x: np.median(np.abs(x - np.median(x))))
24
       od_df['result'] = np.abs(od_df['water_level'] - od_df['x_hat'])
25
       return od_df
26
```

4.7.3 MAD Threshold

In Listing 6 an example for an implementation for calculating the MAD is provided.

4.7.4 Z-Score

Listing 7 shows how to calculate th z-score in Python.

4.7.5 Modified z-score

The code for calculating the result of the modified z-score (using the MADN) is shown in Listing 8.

Listing 7 First step of classifying outliers using the z-score

```
def z_score_outlier_detection(input_df: pd.DataFrame,
                                  window: Union[int, None],
2
                                  center_window: bool):
3
       . . . .
       Detects outliers in a dataframe using a (moving) average.
       :param input_df: the input dataframe where the values are stored
                         in the column water_level
       :param window: the size of the window, None if no window should
                       be used
       :param center_window: whether the window should be centered or not
10
       :return: a copy of the input dataframe where the column result
11
                should be compared to a threshold to detect outliers
12
13
       od_df = input_df.copy()
14
       if window is None:
15
           od_df['mean'] = od_df['water_level'].mean()
16
           od_df['std'] = od_df['water_level'].std()
17
18
           od_df['mean'] = \
               od_df['water_level'].rolling(window=window,
20
                                              center=center_window,
                                              min_periods=1).mean()
22
           od_df['std'] = \
23
               od_df['water_level'].rolling(window=window,
24
                                              center=center_window,
25
                                              min_periods=1).std()
26
       od_df['result'] = \
           (od_df['water_level'] - od_df['mean']).divide(od_df['std'])
28
       return od_df
29
```

Listing 8 First step of classifying outliers using the modified z-score (MADN-z-score)

```
def madn_z_score_outlier_detection(input_df: pd.DataFrame,
                                        window: Union[int, None],
                                        center_window: bool):
       . . . .
       Detects outliers in a dataframe using a (moving) average.
       :param input_df: the input dataframe where the values are stored
                         in the column water_level
       :param window: the size of the window, None if no window should
                       be used
       :param center_window: whether the window should be centered or not
10
       :return: a copy of the input dataframe where the column result
11
                should be compared to a threshold to detect outliers
12
       . . . .
13
       od_df = input_df.copy()
14
       if window is None:
15
           od_df['median'] = od_df['water_level'].median()
16
           od_df['mad'] = np.median(
               np.abs(od_df['water_level'] - od_df['median']))
18
           od_df['madn'] = od_df['mad'] / 0.6745
19
       else:
20
           od_df['median'] = \
21
               od_df['water_level'].rolling(window=window,
                                              min_periods=1,
                                              center=center_window) .median()
           od_df['mad'] = \
25
               od_df['water_level'].rolling(window=window,
26
                                              min_periods=1,
27
                                              center=center_window).apply(
28
                    lambda x: np.median(np.abs(x - np.median(x))))
           od_df['madn'] = od_df['mad'] / 0.6745
       od_df['result'] = \
31
           (od_df['water_level'] - od_df['median']).abs() \
32
                .divide(od_df['madn'])
33
       return od df
34
```

4.7.6 Preprocessing the Data

In the preprocessing step outliers which extremely vary from the usual trend of the other values were removed. This was done by defining and upper and lower limit for the data. If a value is not inside this limit it is removed from the dataset. The thought behind preprocessing the data was to increase the model performance by removing extreme outlier values from the beginning. The disadvantage of the preprocessing step is, that two limits need to be defined for each measurement station. The limits need to be chosen carefully. On the one hand, if the valid value range is too large, no extreme outliers are removed and the preprocessing is useless, on the other hand if the valid value range is too small the preprocessing might remove valid values, which would indicate a possible flood. Thus it is also a good idea to regularly check and maybe update those limits.

The Python code for preprocessing the data can be found in the appendix in Listing 10.

4.7.7 Finding Parameters

To find the best parameters a grid search was used. The first step was to calculate the results for different methods, window sizes and types (centered an non centered). For each unique parameter combination the result dataframe was stored as a file, where the filename provided information about the parameters. An example for a filename would be "12_cw_median.parquet", where "12" is the window size, "cw" stands for center window ("nocw" is for no center window) and "median" is the method used. This was done for every unique combination of parameters. The possible values for each parameter, that was used, is listed below.

normalized: yes, no

• preprocessed: yes, no

• window size: None, 2-51 (in steps of one)

• centered window: yes, no

• **method**: mean, median, mad, z-score, modified z-score (madn-z-score)

• common-id: "36022-ie", "39003-ie", "2386-ch", "42960105-de", "2720050000-de"

Due to the large number of unique combinations of parameters the size of the resulting files was quite large (multiple Gigabytes). The grid search was executed in parallel using multiprocessing, in order to speed up the process.

After the results of each parameter was calculated, for each file a range of thresholds was tested and the performance (confusion matrix and $F_1-score$) of this threshold and the parameters used were saved to a DataFrame. This was also conducted in parallel to decrease the runtime.

The code of the grid search for different parameters can be found in the appendix in Listing 12.

4.8 Compare different Outlier Detection Approaches

As expected, using a centered window yields the best $F_1 - score$. Furthermore the methods with the best performance are the median and the MADN z-score. While the median performed best with smaller window sizes (5-7) the modified z-score performed best with larger window sizes (22-28). Using the MAD to calculate the $\hat{x_t}$ yields the worst performance.

Table 9 shows the top 5 average $F_1-scores$ of all stations tested. When using one set of parameters for different measurement stations the median performed best. Using the mean for $\hat{x_t}$ delivered the second best performance, when comparing shared parameters bewteen all tested stations. However the average $F_1-score$ of the mean is only 0.47794, it was reached by using a centered window of size 5, a threshold of 18.87960 and not normalizing the data. Due to the heterogeneity of the fluctuations of the water levels for the different stations it is not recommended to use the same parameters for different stations. Similar or equal parameters should only be used when the water levels of two measurement stations behave similarly. Additionally when using the same parameters for different stations the performance of those parameters should be looked at per station and not as an average of the $F_1-scores$. This hinders the fact that one model performs perfectly $(F_1-score=1)$ and the other very poorly $(F_1-score=0.5)$.

window_size	center_window	normalized	threshold	model_type	average_f1_score
3.0	True	False	6.628763	median	0.725722
3.0	True	False	6.959866	median	0.725293
3.0	True	False	6.297659	median	0.723374
3.0	True	False	8.284281	median	0.719480
3.0	True	False	8.615385	median	0.719397

Table 9: Best parameters of the average F1-score of all stations tested

Using the preprocessing (described in subsection 4.7.6) usually resulted in a lower performance, when comparing the hightest $F_1-scores$ for both datasets (preprocessed and not preprocessed). The reason for this is, that the outliers removed by the two sided filter were detected as outliers anyway. So just the number of TPs was reduced. Thus resulting in a slightly lower overall performance, since the outliers were completely removed from the dataset in the preprocessing step.

Mean

Figure 16 shows the best performing outlier detection using mean. The F_1 – score is about 0.68, the Precision is about 0.73 and the Recall is about 0.65.

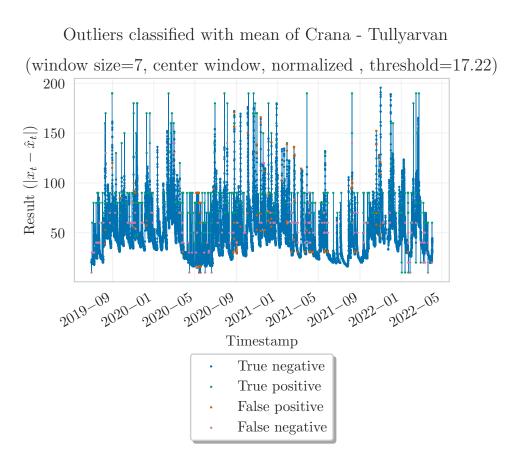


Figure 16: Best performance of outlier detection using mean (Crana - Tullyarvan)

Median

Figure 17 shows the best performing outlier detection using median. The $F_1 - score$ is about 0.91, the Precision is about 0.93 and the Recall is about 0.89.

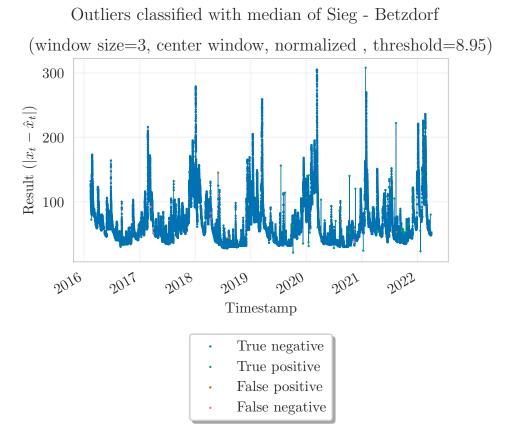


Figure 17: Best performance of outlier detection using median (Sieg - Betzdorf)

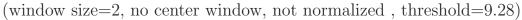
MAD

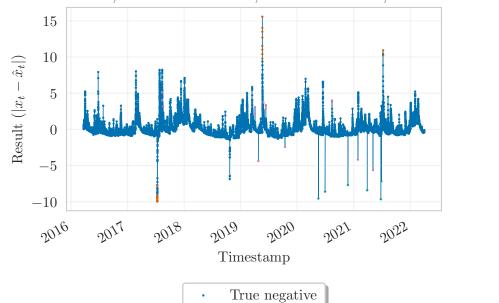
Figure 18 shows the best performing outlier detection using MAD. The F_1 – score is about 0.45, the Precision is about 0.53 and the Recall is 0.4.

Z-score

Figure 19 shows the best performing outlier detection using z-score. The F_1 – score is about 0.68, the Precision is about 0.80 and the Recall is about 0.59. In Figure 22 examples for TP, TN, FN and FP are shown.

Outliers classified with mad of Losse - Helsa





- · True positive
- False positive
- · False negative

Figure 18: Best performance of outlier detection using mad (Losse - Helsa)

Outliers classified with z-score of Crana - Tullyarvan (window size=26, center window, not normalized , threshold=1.99)

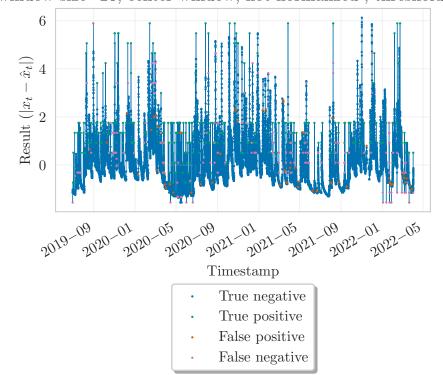


Figure 19: Best performance of outlier detection using z-score (Crana - Tullyarvan)

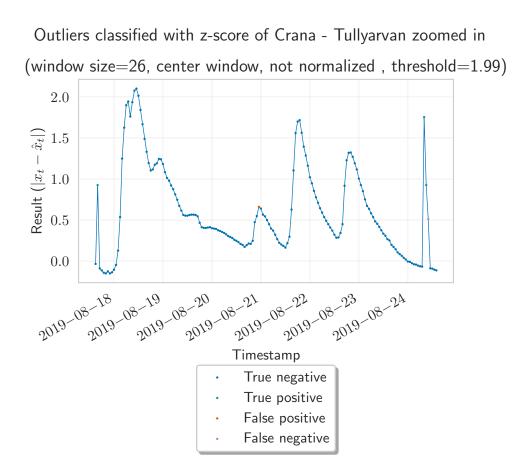


Figure 20: Best performance of outlier detection using z-score (Crana - Tullyarvan) zoomed in

MADN-z-score

Figure 21 shows the best performing outlier detection using MADN-z-score. The F_1 – score is about 0.79, the Precision is about 0.75 and the Recall is about 0.84. In Figure 22 examples for TP, TN, FN and FP are shown.

Outliers classified with madn-z-score of Aghacashlaun - Aghacashlaun (window size=24, center window, not normalized , threshold=3.65)

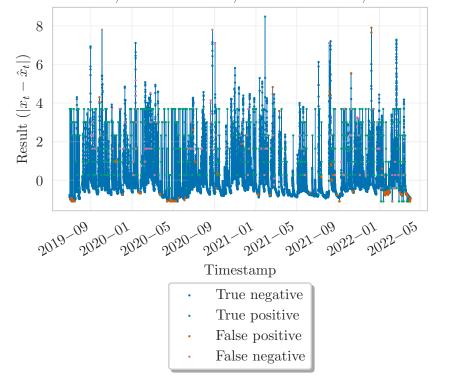


Figure 21: Best performance of outlier detection using MADN-z-score (Aghacashlaun - Aghacashlaun)

4.8.1 Station Aghacashlaun, Aghacashlaun (36022-ie)

Table 10 shows the top three predictions per model for normalized and not normalized data. It clearly pictures, that methods using a centered moving window perform better. It is also interesting to see that the MADN z-score and the regular z-score performed about equally well, regardless of the fact, that the data is normalized or not.

4.8.2 Station Murg, Frauenfeld (2386-ch)

In Table 11 the top three predictions per model for normalized and not not normalized data is shown. The outlier detection for this station has the worst performance among those tested.

Outliers classified with madn-z-score of Aghacashlaun - Aghacashlaun zoomed in (window size=24, center window, not normalized , threshold=3.65)

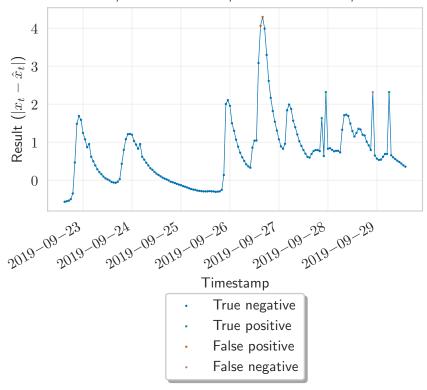


Figure 22: Best performance of outlier detection using MADN-z-score (Aghacashlaun - Aghacashlaun) zoomed in

			thus should	mandal turan	f1 22242
window_size	center_window	normalized	threshold	model_type	f1_score
5.0	True	False	7.622074	median	0.812550
5.0	True	False	8.284281	median	0.812348
5.0	True	False	7.953177	median	0.811688
24.0	True	True	3.648829	madn-z-score	0.789205
24.0	True	False	3.648829	madn-z-score	0.789205
22.0	True	True	3.648829	madn-z-score	0.787572
22.0	True	False	3.648829	madn-z-score	0.787572
26.0	True	True	4.311037	madn-z-score	0.786415
26.0	True	False	4.311037	madn-z-score	0.786415
9.0	True	True	1.000000	median	0.759430
7.0	True	True	1.000000	median	0.750670
8.0	True	True	1.000000	median	0.749358
24.0	True	False	1.993311	z-score	0.626321
32.0	True	True	2.324415	z-score	0.622718
32.0	True	False	2.324415	z-score	0.621457
23.0	True	True	1.993311	z-score	0.621359
27.0	True	True	2.324415	z-score	0.620833
27.0	True	False	2.324415	z-score	0.620833
9.0	True	False	16.892977	mean	0.619647
10.0	True	False	18.879599	mean	0.619173
10.0	True	False	19.210702	mean	0.618538
11.0	True	True	1.331104	mean	0.611993
9.0	True	True	1.331104	mean	0.611418
10.0	True	True	1.331104	mean	0.610659
24.0	True	True	1.993311	mad	0.404255
26.0	True	True	1.993311	mad	0.404000
28.0	True	True	1.993311	mad	0.403183
22.0	True	False	66.889632	mad	0.401679
22.0	True	False	67.220736	mad	0.401126
22.0	True	False	67.551839	mad	0.400856

Table 10: Top predictions summary of Aghacashlaun - Aghacashlaun

The result of this model is shown in Figure 23. Every value above the threshold is classified as an outlier. Every value below the threshold is classified as a regular value.

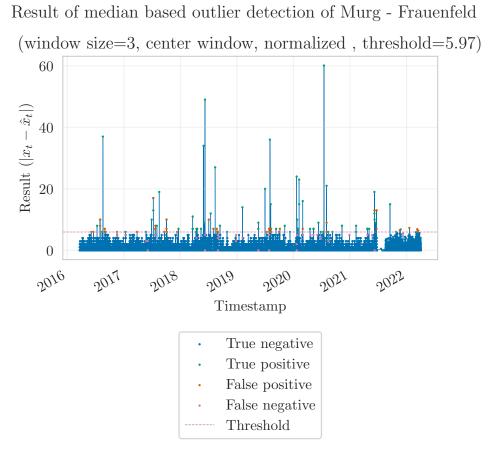


Figure 23: Result of median based outlier detection Murg - Frauenfeld

4.8.3 Station Sieg, Betzdorf (2720050000-de)

In Table 12 the top three predictions per model for normalized and not not normalized data is shown. With an $F_1-score$ of 0.905109 this station had the best performance. The result of this model is shown in Figure 24. Every value above the threshold is classified as an outlier. Between 2018 and 2019 an example of a FP can be seen (the orange values above the threshold).

4.8.4 Station Losse, Helsa (42960105-de)

In Table 13 the top three predictions per model for normalized and not not normalized data is shown.

window_size	center_window	normalized	threshold	model_type	f1_score
3.0	True	False	5.966555	median	0.657895
3.0	True	False	5.635452	median	0.649351
3.0	True	False	6.628763	median	0.639175
3.0	True	False	4.642140	mean	0.447917
3.0	True	False	4.973244	mean	0.443804
3.0	True	False	5.304348	mean	0.429907
50.0	True	True	3.979933	z-score	0.327273
50.0	True	False	3.979933	z-score	0.327273
49.0	True	True	3.648829	z-score	0.306931
49.0	True	False	3.648829	z-score	0.306931
48.0	True	False	3.648829	z-score	0.305419
50.0	True	True	3.648829	z-score	0.303922
47.0	True	True	1.000000	median	0.120690
42.0	False	True	11.926421	median	0.120690
42.0	False	True	8.946488	median	0.120690
49.0	False	True	24.177258	mean	0.120690
34.0	True	True	9.277592	mean	0.120690
34.0	True	True	6.959866	mean	0.120690
NaN	True	True	97.351171	madn-z-score	0.120690
NaN	True	True	76.491639	madn-z-score	0.120690
NaN	True	True	74.505017	madn-z-score	0.120690
NaN	True	False	97.351171	madn-z-score	0.120690
NaN	True	False	76.491639	madn-z-score	0.120690
NaN	True	False	74.505017	madn-z-score	0.120690
7.0	True	True	1.000000	mad	0.120690
11.0	True	True	1.993311	mad	0.120690
34.0	False	True	24.839465	mad	0.120690
7.0	True	False	1.000000	mad	0.004301
27.0	True	False	4.973244	mad	0.004301
27.0	True	False	5.635452	mad	0.004301

Table 11: Top predictions summary of Murg - Frauenfeld

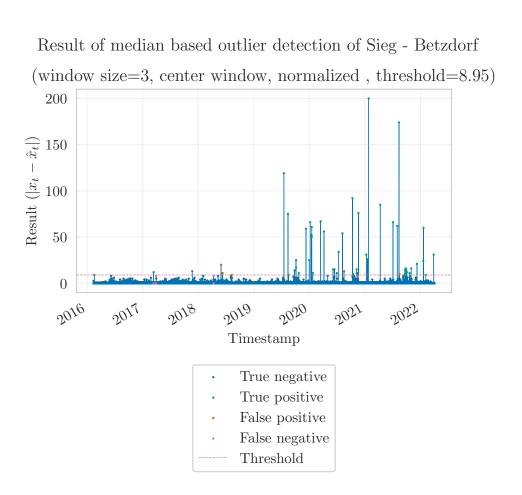


Figure 24: Result of median based outlier detection Sieg - Betzdorf

window_size	center_window	normalized	threshold	model_type	f1_score
3.0	True	False	8.284281	median	0.905109
3.0	True	False	8.615385	median	0.905109
3.0	True	False	8.946488	median	0.905109
29.0	True	False	3.648829	z-score	0.545455
23.0	True	False	3.317726	z-score	0.545455
27.0	True	False	3.648829	z-score	0.542373
22.0	True	True	3.317726	z-score	0.533333
28.0	True	True	3.648829	z-score	0.533333
20.0	True	True	3.317726	z-score	0.516667
3.0	True	False	7.290970	mean	0.510288
3.0	True	False	6.959866	mean	0.510121
3.0	True	False	6.628763	mean	0.503937
NaN	False	True	10.602007	madn-z-score	0.133333
NaN	True	True	10.602007	madn-z-score	0.133333
NaN	False	False	10.602007	madn-z-score	0.133333
NaN	True	False	10.602007	madn-z-score	0.133333
NaN	False	True	10.270903	madn-z-score	0.119048
NaN	False	False	10.270903	madn-z-score	0.119048
47.0	True	True	1.000000	median	0.108108
29.0	False	True	1.000000	median	0.108108
50.0	False	True	2.324415	median	0.108108
NaN	False	True	1.662207	mean	0.108108
NaN	True	True	1.662207	mean	0.108108
NaN	True	True	1.000000	mean	0.108108
7.0	True	True	1.000000	mad	0.108108
31.0	True	True	1.000000	mad	0.108108
25.0	False	True	2.324415	mad	0.108108
49.0	True	False	100.000000	mad	0.006390
50.0	True	False	100.000000	mad	0.006379
47.0	True	False	100.000000	mad	0.006360

Table 12: Top predictions summary of Sieg - Betzdorf

window_size	center_window	normalized	threshold	model_type	f1_score
6.0	True	True	2.655518	median	0.731707
4.0	True	False	25.170569	median	0.731707
4.0	True	False	26.494983	median	0.731707
4.0	True	False	26.163880	median	0.731707
3.0	True	True	1.000000	median	0.720000
4.0	True	True	2.324415	median	0.714286
19.0	True	True	5.966555	mean	0.571429
17.0	True	True	5.635452	mean	0.571429
15.0	True	True	5.304348	mean	0.571429
15.0	True	False	62.585284	mean	0.571429
16.0	True	False	62.585284	mean	0.571429
16.0	True	False	59.605351	mean	0.571429
2.0	False	True	9.277592	mad	0.454545
2.0	True	True	9.277592	mad	0.454545
2.0	False	True	9.939799	mad	0.439024
NaN	True	True	18.879599	z-score	0.275862
NaN	True	True	17.555184	z-score	0.275862
NaN	False	True	16.892977	z-score	0.275862
NaN	False	False	19.541806	z-score	0.275862
NaN	False	False	16.561873	z-score	0.275862
NaN	False	False	15.899666	z-score	0.275862
NaN	False	True	30.137124	madn-z-score	0.275862
NaN	False	True	32.785953	madn-z-score	0.275862
NaN	False	True	35.103679	madn-z-score	0.275862
NaN	False	False	30.137124	madn-z-score	0.275862
NaN	False	False	32.785953	madn-z-score	0.275862
NaN	False	False	35.103679	madn-z-score	0.275862
NaN	True	False	100.000000	mad	0.005068
NaN	False	False	100.000000	mad	0.005068
NaN	True	False	99.668896	mad	0.004548

Table 13: Top predictions summary of Losse - Helsa

4.8.5 Station Crana, Tullyarvan (39003-ie)

In Table 14 the top three predictions per model for normalized and not not normalized data is shown.

-					
window_size	center_window	normalized	threshold	model_type	f1_score
5.0	True	False	8.615385	median	0.859035
5.0	True	False	9.277592	median	0.858500
5.0	True	False	8.946488	median	0.857685
34.0	True	True	3.648829	madn-z-score	0.736842
34.0	True	False	3.648829	madn-z-score	0.736842
34.0	True	True	4.311037	madn-z-score	0.733962
34.0	True	False	4.311037	madn-z-score	0.733962
32.0	True	True	4.642140	madn-z-score	0.731707
32.0	True	False	4.642140	madn-z-score	0.731707
11.0	True	True	1.000000	median	0.723699
10.0	True	True	1.000000	median	0.723059
9.0	True	True	1.000000	median	0.720189
7.0	True	False	17.224080	mean	0.684211
7.0	True	False	16.230769	mean	0.683398
7.0	True	False	16.892977	mean	0.683267
26.0	True	True	1.993311	z-score	0.677668
26.0	True	False	1.993311	z-score	0.677668
27.0	True	True	1.993311	z-score	0.672489
27.0	True	False	1.993311	z-score	0.672489
25.0	True	True	1.993311	z-score	0.669633
25.0	True	False	1.993311	z-score	0.669633
8.0	True	True	1.000000	mean	0.643868
9.0	True	True	1.000000	mean	0.636678
10.0	True	True	1.000000	mean	0.633596
36.0	True	False	85.431438	mad	0.180556
34.0	True	False	85.431438	mad	0.180149
36.0	True	False	85.100334	mad	0.179840
30.0	True	True	1.662207	mad	0.173418
14.0	False	True	1.662207	mad	0.173355
29.0	True	True	1.662207	mad	0.173149

Table 14: Top predictions summary of Crana - Tullyarvan

5 Conclusion

This bachelor thesis provides an overview of the topic anomaly detection, especially on outlier detection for time series data. It provides a description for key features of data quality, and introduces the topic of data cleaning and data cleansing. Furthermore this paper provides general overview of outlier detection approaches. After a theoretical overview of different outlier detection approaches they are tested on water level data from different rivers.

The overall bes performance, across different water level measurement stations, was achieved by using the median threshold based outlier detection method with a centered window with the size of three and a threshold of about 6.6. The median threshold based outlier detection also delivered the hightest $F_1 - score \ (0.905)$. Using the mean to calculate \hat{x}_t is not recommended since the mean is not robust against outliers. Using the MAD with the threshold based outlier detection resulted in the lowest $F_1 - score$, with the best score only being about 0.45. The second best result was achieved by using the modified z-score described in section 3.5. For the stations tested the approach using the median delivered the best performances. However this does not mean, that this will be true for all stations. It has to be assessed for each station individually which model is able to detect best. Furthermore it depends on the use case if higher precision or recall is required. Depending on that, β for the F_{β} – score needs to be chosen accordingly. For the tests the $F_1 - score$ was used since precision and recall are equally important. In addition preprocessing the data by setting upper and lower boundaries and removing datapoints which exceed those limits, did not improve the performance of the models, on the contrary the performance was worse. Because the extreme outliers were mostly detected anyways, thus fewer outliers were detected when setting upper and lower limits, which resulted in a lower performance.

6 Future Work

Chapter about which additional approaches could be tested:

- setting a maximum gradient for both directions (one for rising and falling values) for each measurement station.
- · ANNs with LSTM or GRU maybe also autoencoder architecture
- · Prediction vs classification ANN

Ich schlage hier vor auch einen Teil der quanitativen Analyse zusammenzufassen. Dabei sollten die Methoden und die Ergebnisse kurz skizziert werden. Vielleicht lassen sich auch Entscheidungen ableiten wann welche Methode besser greift.

• 1.5 times the IQR

Should I also include this or is this not common for a bachelor thesis? -> YES

Die Methode wollte ich auch vorschlagen, aber der Umfang ist so schon gross genug.

7 Appendix

Basically include the whole repo: https://github.com/cellularegg/bachelor-thesis-code

7.1 Python Code

7.1.1 Manual outlier detection

```
import json
   import numpy as np
4
   import pandas as pd
   import plotly.express as px
   from dash import Dash, dcc, html
   from dash.dependencies import Input, Output
9
   app = Dash(__name__)
10
11
   stations_dict = pd.read_csv('./data/stations.csv').groupby(
12
        ['common_id']).first().to_dict('index')
13
   common_id = '2736731000100-de'
   df = pd.read_parquet(f'./data/{common_id}_outliers_classified.parquet')
15
   fig = px.scatter(df, x='timestamp', y='water_level',
17
                     title=f'{common_id}', color='is_outlier')
18
19
   fig.update_layout(
     xaxis=dict(
20
          rangeselector=dict(
21
22
              buttons=list([
                   dict(count=1,
23
                         step="day",
24
                         stepmode="backward"),
25
                ])
          ),
           rangeslider=dict(
28
29
               visible=True
30
           ),
           type="date"
31
32
33
   app.layout = html.Div([
34
       html.H1('Manual Outlier Selection'),
35
36
       dcc.Graph(
37
           id='water-level-graph',
            figure=fig
       html.Button('Refresh', id='refresh-btn', n_clicks=0),
```

```
41
        html.Div([
42
            dcc.Markdown('Clicked value:'),
            html.Pre(id='click-data'),
43
        1),
44
    ])
45
46
47
48
    def toggle_outlier(timestamp: str):
49
        df.loc[(df['timestamp'] == timestamp), 'is_outlier'] = np.invert(
            df.loc[(df['timestamp'] == timestamp), 'is_outlier'])
50
51
52
    @app.callback(
53
        Output('click-data', 'children'),
54
        Input('water-level-graph', 'clickData'))
55
    def display_click_data(clickData):
56
57
        if clickData is not None:
58
            toggle_outlier(clickData['points'][0]['x'])
59
        return json.dumps(clickData, indent=2)
60
61
    @app.callback(
62
        Output('water-level-graph', 'figure'),
63
        Input('refresh-btn', 'n_clicks'))
64
    def update output(n clicks):
65
        fig = px.scatter(df, x='timestamp', y='water_level',
66
                          title=f'{common_id}', color='is_outlier')
67
        df.to_parquet(f'./data/{common_id}_outliers_classified.parquet')
68
        fig.update_layout(
69
            xaxis=dict(
70
                rangeselector=dict(
71
72
73
                rangeslider=dict(
74
                     visible=True
75
                type="date"
76
            )
77
78
        fig.update_layout(
79
            yaxis_range=[df.loc[df['is_outlier'] == False,
80
                                  'water_level'].min() - 5,
81
                          df.loc[df['is_outlier'] == False,
82
                                  'water_level'].max() + 5])
83
84
        return fig
85
86
    if __name__ == '__main__':
88
        app.run_server(debug=True)
```

Listing 9: Manual Outlier Detection Webapp using Dash [30]

7.1.2 Preprocessing

```
1 # %%
2 import os
```

```
3
   import numpy as np
4
   import pandas as pd
   random\_seed = 1
8
   np.random.seed(random_seed)
10
   stations_df = pd.read_csv('./data/stations.csv')
11
12
   stations_dict = stations_df.groupby(['common_id']).first().to_dict('index')
   stations_dict['2386-ch']['lower_limit'] = 38_000.0
13
   stations_dict['2386-ch']['upper_limit'] = 40_000.0
14
   stations_dict['2720050000-de']['lower_limit'] = 20.0
15
   stations_dict['2720050000-de']['upper_limit'] = 500.0
16
   stations_dict['36022-ie']['lower_limit'] = 20.0
17
   stations_dict['36022-ie']['upper_limit'] = 175.0
18
   stations_dict['39003-ie']['lower_limit'] = 10.0
19
   stations_dict['39003-ie']['upper_limit'] = 225.0
20
   stations_dict['42960105-de']['lower_limit'] = -10.0
21
   stations_dict['42960105-de']['upper_limit'] = 275.0
   stations_dict['auto-1003803']['lower_limit'] = -10.0
   stations_dict['auto-1003803']['upper_limit'] = 275.0
25
26
   for common id, station dict in stations dict.items():
27
        fp = f'./data/classified_raw/{common_id}_outliers_classified.parquet'
28
        if not os.path.exists(fp):
29
30
            continue
        raw_classified_df = pd.read_parquet(fp)
31
        print(f'Removing for {common_id}, lower limit '
32
              f'{station_dict["lower_limit"]}, upper limit '
33
34
              f'{station_dict["upper_limit"]}')
35
       print('Removing following rows:')
36
       mask = (raw_classified_df['water_level'] < station_dict['lower_limit']) | (</pre>
37
                raw_classified_df['water_level'] > station_dict['upper_limit'])
       print(raw_classified_df[mask])
38
       raw_classified_df[~mask].to_parquet(
39
            f'././data/classified/{common_id}_outliers_classified.parquet')
40
        print()
41
```

Listing 10: Data preprocessing code in Python [30]

7.2 Outlier Detection Methods Implementation

```
12
        :param input_df: the input dataframe where the values are stored
13
                         in the column water_level
        :param window: the size of the window, None if no window should
14
                       be used
15
        :param center_window: whether the window should be centered or not
16
        :return: a copy of the input dataframe where the column result
17
18
                 should be compared to a threshold to detect outliers
19
        od_df = input_df.copy()
20
21
        if window is None:
22
            od_df['x_hat'] = od_df['water_level'].mean()
23
        else:
            od_df['x_hat'] = \
24
                od_df['water_level'].rolling(window=window,
25
                                              center=center_window,
26
                                              min_periods=1).mean()
27
28
        od_df['result'] = np.abs(od_df['water_level'] - od_df['x_hat'])
29
        return od df
30
31
   def median_outlier_detection(input_df: pd.DataFrame,
32
                                  window: Union[int, None],
33
34
                                  center_window: bool):
35
        Detects outliers in a dataframe using a (moving) average.
36
        :param input_df: the input dataframe where the values are stored
37
                         in the column water_level
38
        :param window: the size of the window, None if no window should
39
                       be used
40
        :param center_window: whether the window should be centered or not
41
        :return: a copy of the input dataframe where the column result
42
43
                 should be compared to a threshold to detect outliers
44
45
        od_df = input_df.copy()
46
        if window is None:
            od_df['x_hat'] = od_df['water_level'].median()
47
48
        else:
            od_df['x_hat'] = \
49
                od_df['water_level'].rolling(window=window,
50
51
                                               center=center_window,
                                              min_periods=1).median()
52
        od_df['result'] = np.abs(od_df['water_level'] - od_df['x_hat'])
53
54
        return od_df
55
56
57
   def mad_outlier_detection(input_df: pd.DataFrame,
                               window: Union[int, None],
58
59
                               center_window: bool):
60
        Detects outliers in a dataframe using a (moving) average.
61
        :param input_df: the input dataframe where the values are stored
62
                         in the column water_level
63
        :param window: the size of the window, None if no window should
64
65
                       be used
66
        :param center_window: whether the window should be centered or not
67
        :return: a copy of the input dataframe where the column result
                 should be compared to a threshold to detect outliers
```

```
69
70
        od_df = input_df.copy()
        if window is None:
71
             od_df['x_hat'] = np.median(
72
                 np.abs(od_df['water_level'] - np.median(
73
                     od_df['water_level'])))
74
75
         else:
             od_df['x_hat'] = \
76
77
                 od_df['water_level'].rolling(window=window,
78
                                                center=center_window,
79
                                                min_periods=1).apply(
                     lambda x: np.median(np.abs(x - np.median(x))))
80
         od_df['result'] = np.abs(od_df['water_level'] - od_df['x_hat'])
81
         return od df
82
83
84
    def z_score_outlier_detection(input_df: pd.DataFrame,
85
86
                                    window: Union[int, None],
87
                                    center_window: bool):
88
         Detects outliers in a dataframe using a (moving) average.
89
         :param input_df: the input dataframe where the values are stored
90
                          in the column water_level
91
         :param window: the size of the window, None if no window should
92
                        be used
93
         :param center_window: whether the window should be centered or not
94
         :return: a copy of the input dataframe where the column result
95
                  should be compared to a threshold to detect outliers
96
97
        od_df = input_df.copy()
98
        if window is None:
99
100
             od_df['mean'] = od_df['water_level'].mean()
101
             od_df['std'] = od_df['water_level'].std()
102
         else:
             od_df['mean'] = \
                 od_df['water_level'].rolling(window=window,
104
105
                                                center=center window.
                                                min_periods=1).mean()
106
             od_df['std'] = \
107
                 od_df['water_level'].rolling(window=window,
108
                                                center=center_window,
109
                                                min_periods=1).std()
110
         od_df['result'] = \
111
112
             (od_df['water_level'] - od_df['mean']).divide(od_df['std'])
113
         return od_df
114
115
116
    def delta_z_score_outlier_detection(input_df: pd.DataFrame,
117
                                          window: Union[int, None],
                                          center window: bool):
118
119
        Detects outliers in a dataframe using a (moving) average.
120
121
         :param input_df: the input dataframe where the values are stored
                          in the column water_level
122
         :param window: the size of the window, None if no window should
123
124
                        be used
        :param center_window: whether the window should be centered or not
125
```

```
126
         :return: a copy of the input dataframe where the column result
127
                  should be compared to a threshold to detect outliers
128
         od_df = input_df.copy()
129
         od_df['water_level_delta'] = od_df['water_level'].diff().fillna(0)
130
         if window is None:
131
132
             od_df['mean'] = od_df['water_level_delta'].mean()
133
             od_df['std'] = od_df['water_level_delta'].std()
134
         else:
             od_df['mean'] = \
135
                 od_df['water_level_delta'].rolling(window=window,
136
137
                                                       center=center window.
                                                       min_periods=1).mean()
138
             od_df['std'] = \
139
                 od_df['water_level_delta'].rolling(window=window,
140
141
                                                       center=center_window,
142
                                                       min_periods=1).std()
143
         od_df['result'] = \
144
             (od_df['water_level_delta'] - od_df['mean']).divide(
145
                 od_df['std'])
         return od_df
146
147
148
149
    def madn_z_score_outlier_detection(input_df: pd.DataFrame,
                                          window: Union[int, None],
150
                                          center window: bool):
151
         ....
152
         Detects outliers in a dataframe using a (moving) average.
153
         :param input_df: the input dataframe where the values are stored
154
                           in the column water_level
155
         :param window: the size of the window, None if no window should
156
157
                         be used
158
         :param center_window: whether the window should be centered or not
159
         :return: a copy of the input dataframe where the column result
160
                  should be compared to a threshold to detect outliers
161
         od_df = input_df.copy()
162
         if window is None:
163
             od_df['median'] = od_df['water_level'].median()
164
             od_df['mad'] = np.median(
165
                 np.abs(od_df['water_level'] - od_df['median']))
166
             od_df['madn'] = od_df['mad'] / 0.6745
167
168
         else:
169
             od_df['median'] = \
                 od_df['water_level'].rolling(window=window,
170
171
                                                min_periods=1,
                                                center=center_window).median()
172
             od_df['mad'] = \
173
                 od_df['water_level'].rolling(window=window,
174
175
                                                min_periods=1,
176
                                                center=center_window).apply(
                     lambda x: np.median(np.abs(x - np.median(x))))
177
             od_df['madn'] = od_df['mad'] / 0.6745
178
         od_df['result'] = \
179
             (od_df['water_level'] - od_df['median']).abs() \
180
                 .divide(od_df['madn'])
181
         return od_df
182
```

7.3 Parameter Grid Search

```
import itertools
1
2
   import multiprocessing as mp
   import os
   from datetime import datetime
   from typing import List
   import numpy as np
   import pandas as pd
8
   from sklearn.preprocessing import StandardScaler
10
   import outlier_detection_methods as odm
11
12
   random\_seed = 1
13
14
   np.random.seed(random_seed)
15
16
17
   def threshold_outlier_prediction(input_df, window, center_window,
18
                                      method):
19
        od_df = input_df.copy()
        if method == 'mean':
20
            od_df = odm.mean_outlier_detection(od_df, window,
21
                                                center window)
22
        elif method == 'median':
23
            od_df = odm.median_outlier_detection(od_df, window,
24
                                                   center_window)
25
26
        elif method == 'mad':
27
            od_df = odm.mad_outlier_detection(od_df, window,
28
                                               center_window)
        elif method == 'z-score':
29
            od_df = odm.z_score_outlier_detection(od_df, window,
30
31
                                                    center_window)
        elif method == 'delta-z-score':
32
            od_df = odm.delta_z_score_outlier_detection(od_df, window,
33
34
                                                          center window)
        elif method == 'madn-z-score':
35
            od\_df = odm.madn\_z\_score\_outlier\_detection(od\_df, window,
36
37
                                                         center window)
38
        else:
            raise ValueError(f'Method ({method}) not supported')
39
        # od_df['result'] = od_df['result'].replace(np.inf, np.nan)
40
        # od_df['result'] = od_df['result'].replace(-np.inf, np.nan)
41
        od_df['result'] = od_df['result'].fillna(0)
42
        od_df['result'] = od_df['result'].replace(np.inf, np.finfo(
43
            np.float64).max)
44
        od_df['result'] = od_df['result'].replace(-np.inf, np.finfo(
45
            np.float64).min)
46
        return {'window_size': window, 'center_window': center_window,
47
                'method': method, 'df': od_df}
48
49
50
   def run_grid_search_parallely(df: pd.DataFrame, windows: list,
```

```
52
                                    center windows: list,
53
                                   methods: List[str],
                                    target_dir: str):
54
        with mp.Pool(processes=12) as executor:
55
            results = executor.starmap(threshold_outlier_prediction,
56
57
                                         itertools.product([df], windows,
                                                            center_windows,
58
                                                            methods))
        if not os.path.exists(target_dir):
61
            os.makedirs(target_dir)
62
        for res in results:
63
64
            res['df'].to_parquet(
                 f'{target_dir}{res["window_size"]}_'
65
                 f'{"cw" if res["center_window"] else "nocw"}_'
66
                 f'{res["method"]}.parquet')
67
68
69
    stations_df = pd.read_csv('./data/stations.csv')
70
71
    stations_dict = stations_df.groupby(['common_id']).first().to_dict(
         'index')
72
73
    common_ids = ['36022-ie', '39003-ie', '2386-ch', '42960105-de',
74
                   '2720050000-de']
75
    methods = ['median', 'mean', 'mad', 'z-score', 'madn-z-score', 'delta-z-score']
76
    windows = [None] + list(range(2, 51))
77
    center_windows = [False, True]
78
    for common_id in common_ids:
79
        print (
80
            f'{datetime.now().isoformat()} - Processing {common_id} (regular, not preprocessed)')
81
82
        tex_plots_path = f'../bachelor-thesis/plots/pdfs/{common_id}/'
83
        df = pd.read_parquet(
             f'data/classified_raw/{common_id}_outliers_classified.parquet')
85
        run_grid_search_parallely(df, windows, center_windows, methods,
86
                                    f'./data/predictions/raw/regular/{common_id}/')
87
        print (
88
            f'{datetime.now().isoformat()} - Processing {common_id} (regular, preprocessed)')
89
        df = pd.read_parquet(
            f'data/classified/{common_id}_outliers_classified.parquet')
90
        run_grid_search_parallely(df, windows, center_windows, methods,
91
92
                                    f'./data/predictions/raw_preprocessed/regular/{common_id}/')
93
        print(
94
95
            f'{datetime.now().isoformat()} - Processing {common_id} (normalized, not preprocessed)')
        df = pd.read_parquet(
96
97
            f'data/classified_raw/{common_id}_outliers_classified.parquet')
98
        scaler = StandardScaler()
99
        df['water_level'] = scaler.fit_transform(df[['water_level']])
100
        run_grid_search_parallely(df, windows, center_windows, methods,
                                    f'./data/predictions/raw/normalized/{common_id}/')
101
102
        print (
            f'{datetime.now().isoformat()} - Processing {common_id} (normalized, preprocessed)')
103
        df = pd.read_parquet(
104
             f'data/classified/{common_id}_outliers_classified.parquet')
105
106
        scaler = StandardScaler()
        df['water_level'] = scaler.fit_transform(df[['water_level']])
107
        run_grid_search_parallely(df, windows, center_windows, methods,
```

Listing 12: Threshold based outlier detection [30]

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List of Figures

Figure 1	Examples of three point outliers	7
Figure 2	Examples of three subsequence outliers	8
Figure 3	Examples of four local point outliers	8
Figure 4	Examples of six local subsequence outliers	9
Figure 5	Examples of four global point outliers	9
Figure 6	Standard Score in a normal distribution [18]	12
Figure 7	Dash Webapp to classify outliers	19
Figure 8	Class distribution of Aghacashlaun - Aghacashlaun	21
Figure 9	Boxplot of Aghacashlaun - Aghacashlaun	22
Figure 10	Histogram of the water level of Aghacashlaun - Aghacashlaun	23
Figure 11	Histogram of the water level delta of Aghacashlaun - Aghacashlaun	24
Figure 12	Histogram of the time delta (in hours) of Aghacashlaun - Aghacashlaun	25
Figure 13	Line chart of Aghacashlaun - Aghacashlaun (whole data)	26
Figure 14	Line chart of Aghacashlaun - Aghacashlaun (2019-10-16 - 2019-10-19)	26
Figure 15	Precision vs Recall [31]	28
Figure 16	Best performance of outlier detection using mean (Crana - Tullyarvan)	37
Figure 17	Best performance of outlier detection using median (Sieg - Betzdorf)	38
Figure 18	Best performance of outlier detection using mad (Losse - Helsa)	39
Figure 19	Best performance of outlier detection using z-score (Crana - Tullyarvan)	40
Figure 20	Best performance of outlier detection using z-score (Crana - Tullyarvan)	
	zoomed in	41
Figure 21	Best performance of outlier detection using MADN-z-score (Aghacashlaun -	
	Aghacashlaun)	42
Figure 22	Best performance of outlier detection using MADN-z-score (Aghacashlaun -	
	Aghacashlaun) zoomed in	43
Figure 23	Result of median based outlier detection Murg - Frauenfeld	45
Figure 24	Result of median based outlier detection Sieg - Betzdorf	47

List of Tables

Table 1	Example of IoT sensor data	5
Table 2	Example of IoT sensor data after cleaning	6
Table 3	Example of IoT sensor data after cleansing	6
Table 4	Seven number summary of Aghacashlaun - Aghacashlaun (all values)	20
Table 5	Seven number summary of Aghacashlaun - Aghacashlaun (regular values)	20
Table 6	Seven number summary of Aghacashlaun - Aghacashlaun (outlier values)	20
Table 7	Example of binary confusion matrix	27
Table 8	First 9 values of Aghacashlaun - Aghacashlaun	31
Table 9	Best parameters of the average F1-score of all stations tested	36
Table 10	Top predictions summary of Aghacashlaun - Aghacashlaun	44
Table 11	Top predictions summary of Murg - Frauenfeld	46
Table 12	Top predictions summary of Sieg - Betzdorf	48
Table 13	Top predictions summary of Losse - Helsa	49
Table 14	Top predictions summary of Crana - Tullyarvan	51

List of source codes

1	Request body to get API key	15
2	Example response of the list endpoint	16
3	Example response of historical water level data for one station	17
4	First step of classifying outliers using the mean	30
5	First step of classifying outliers using the median	31
6	First step of classifying outliers using the MAD	32
7	First step of classifying outliers using the z-score	33
8	First step of classifying outliers using the modified z-score (MADN-z-score)	34
9	Manual Outlier Detection Webapp using Dash [30]	55
10	Data preprocessing code in Python [30]	56
11	Implementation of Outlier Detection Methods [30]	59
12	Threshold based outlier detection [30]	62

List of Abbreviations

ANN Artificial Neuronal Network

ARIMA AutoRegressive Integrated Moving Average

CSV Comma Separated Values

FN False Negative

FP False Positive

GP Gaussian Process

GRU Gated Recurrent Unit

HMAC Keyed-Hashing for Message Authentication

IQR InterQuartile Range

IoT Internet of Things

JSON Java Script Object Notation

KPI Key Performance Indicator

LSTM Long Short-Term Memory

Lat Latitude

Long Longitude

MADN Normalized Median Absolute Deviation

MAD Median Absolute Deviation

N Negative

P Positive

TN True Negative

TP True Positive