



FH Salzburg
MultiMediaTechnology

***Identifying the Ideal Length of Time to Record
Smartphone Data, in Order to Obtain Distinct
Clusters to Predict Eating Crises***

Bachelor Thesis 2

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Salzburg, Austria, 10.05.2020

Affidavit

I herewith declare on oath that I wrote the present thesis without the help of third persons and without using any other sources and means listed herein; I further declare that I observed the guidelines for scientific work in the quotation of all unprinted sources, printed literature and phrases and concepts taken either word for word or according to meaning from the Internet and that I referenced all sources accordingly.

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Kurzfassung

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Abstract

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1 Introduction

Han, Pei, and Kamber (2011)[18, 32, 362, 363, 367] declare, that data mining is used to discover patterns and knowledge from data. Cluster Analysis is a type of machine learning algorithm known as unsupervised machine learning. It is used in data mining to divide data into groups (clusters). Each cluster contains data that is similar to each other, but dissimilar to the data allocated to other clusters. Cluster Analysis can be used to acquire knowledge on the distribution of the data, discover characteristics, detect outliers and reduce noise, or to pre-process data for other algorithms.

There are several different methods to create clustering. Han, Pei, and Kamber (2011)[364, 366-367, 374, 385, 392] explain, that objects are often arranged into clusters using distance measures (e.g. Euclidean or Manhattan distance measures). The authors divide the clustering algorithms into the following categories:

- Partitioning methods (examples: k-means, k-medoids)
- Hierarchical methods (examples: BIRCH, Chameleon)
- Density-based methods (examples: DBSCAN, OPTICS)
- Grid-based methods (examples: STING, CLIQUE)

Bermad and Kechadi (2016) introduce in their paper, how clustering can be used in digital forensics to provide information on all the events that led up to a certain crime. They used ascending hierarchical clustering to receive clusters of events (e.g. phone calls, SMS) ordered in time, thus creating a timeline of events leading up to the incident.

Dey and Chakraborty (2015)[1,2,6,7] give an example, where clustering was implemented to predict future weather. Air pollutant data was preprocessed and then arranged into clusters using (incremental) DBSCAN clustering. Finally, priority based protocol was used on them to predict weather conditions and a temperature range. The accuracy of the technique, based on hit and miss times, was calculated to approximately 74.5%.

SmartEater ¹ is an upcoming mHealth (mobile health) app, with the goal to provide the user with content-dependent feedback, to avert a food craving episode. The app will predict future eating crises based on the user's past behaviour. In order to reduce intense user input, the app records and uses various smartphone sensor data. With the help of data mining, machine learning algorithms, and pattern recognition, this recorded situational context data will aid in predicting stress. The following data is recorded by the app:

1. Background volume
2. Relative movement of the smartphone (gyro and accel)

1. <https://sites.google.com/site/eatingandanxietylab/resources/smarteater>

3. Time and duration of phone calls (without storing the numbers)
4. Time of messages (e.g. SMS, WhatsApp) (without collecting identifying information such as content, addresses, numbers)
5. Screen activity (so-called touch events)
6. Screen-on-time (illuminated display)
7. Ambient brightness
8. Data volume per unit of time (summary value of all smartphone activities on the internet)
9. Switch-on and switch-off times of the smartphone

This sensor data will be recorded for different lengths of time (**TODO: NAME TIME LENGTHS**). It is necessary to establish which time period will be most fitting to make accurate predictions for the future. This thesis will use cluster analysis to determine which time period is most significant.

According to Han, Pei, and Kamber (2011)[414], the above-mentioned clustering methods work well with data sets that are not high-dimensional and have less than 10 attributes. Since the SmartEater data set only has 9 dimensions, it is not considered high-dimensional. This paper will therefore utilise these clustering methods. Since different clustering algorithms can yield different results, multiple methods will be used and compared.

To reduce the size and amount of data, dimensionality reduction will be used. Han, Pei, and Kamber (2011)[93] define dimensionality reduction as a type of data reduction, which removes random attributes and creates a smaller data set with close to equal integrity. This thesis will use principal component analysis (PCA) to reduce the dimensionality. Furthermore, T-Distributed Stochastic Neighbor Embedding (t-SNE) will be employed to depict the data set in this thesis. Maaten and Hinton (2008)[2579] first introduce t-SNE, which is used to visualise data with a higher dimensionality.

The clustering methods will be implemented using a Python machine learning platform or library (e.g. Anaconda², scikit-learn³). Next, these will be implemented on the other time lengths. The resulting clusters of each time length will be compared to one another and evaluated. Rousseeuw (1987) reveals how silhouettes can be used to measure the separation between clusters and therefore evaluate the quality of the resulting clusters are.

The thesis will be structured as follows: The first section will briefly present existing work relating to this subject. The following chapter will concentrate on the theory of data mining and cluster analysis. After covering these topics, the next section will describe the conducted experiment and its results. In the final sections, the findings of the experiment will be discussed and summarised.

TODO: !!!WRITE ABOUT EATING DISORDERS...!, ALSO WRITE ABOUT MOBILE HEALTH APPS

2. <https://www.anaconda.com/>

3. <https://scikit-learn.org/stable/>

2 Related work

As introduced in section 1, SmartEater⁴ will be a mHealth (mobile health) app, that predicts future eating crises based on the user's past behaviour. The predictions are made on smart-phone sensor data, therefore reducing strenuous user input. The app will give the user content-dependent feedback, to avert a food craving episode.

Rahman et al. (2016) had a similar idea in their paper. Their goal is to predict "About-to-Eat" and "Time until the Next Eating Event" stages by using wearable sensing devices, in order to reduce serious health issues (e.g. obesity). Detecting when a person is eating is not helpful. It is more beneficial to predict moments shortly before the user is about to eat ("About-To-Eat"). Rahman et al. learnt more on how people were currently tracking their meals by conducting a survey. They asked 75 people with varied ages and body sizes. 34 of 75 participants revealed, that they had never used any type of eating tracking or food journals. The remaining 41 respondents were further asked how long they used the respective tool. 48.9% of these had used the tool for less than a month. 65 of the 75 participants revealed that they no longer use a food tracking/journaling a tool. Further questions resulted in the following revelations: 33 of the 75 respondents wished for the app to take action directly before a meal/snack ("About-to-Eat" moments), thus supporting the authors previous assumptions. Ideas for interventions, included a calorie calculator, reminders to eat balanced or of calorie allowances, visualisations of previous food eaten, or a breakdown of the nutrients taken in. The authors used a variety of different sensors, which at the time, were not all available in one device. The list of utilised sensors and the recorded data are as follows:

- Microsoft Band: physical movement (raw accelerometer, gyroscope, step count, speed), caloric expenditure, heart rate, skin temperature, etc.
- Affectiva Q sensor: measures electrodermal activity (good indicator for psychological arousal)
- Wearable microphone: chewing and swallowing sounds (for detection of current eating events)
- Android smartphone application: GPS location, recording self-reports (right before eating: "Start of Eating Event" button, current emotional state when eating, intensity of desire/craving and hunger; when finished eating: "End of Eating Event" button)

In order to predict "About-to-Eat" moments, eight participants, aged 26-54, wore these four technologies for five days. The recorded data then underwent cleaning and preprocessing, feature extraction, feature selection and machine learning. During the preprocessing, it was made sure that the raw sensor data streams were not dirty and had high accuracy. Some of these steps included resampling, normalisation, recognising chewing and swallowing sounds, extracting longitude and longitude, etc. In the feature extraction step, two parameters are used on the

4. <https://sites.google.com/site/eatingandanxietylab/resources/smart eater>

processed sensor time series to create windows. Firstly, the feature extraction window size parameter regulates the time duration in a specific window. While a short window duration could catch immediate characteristics in the sensor time series, a coarse one could be used for long term trends. The authors used a variety of window sizes, varying from 5 to 120 minutes. The prediction model results would decide the best window. The second parameter, the window shift size, establishes the time duration between two neighbouring windows, meaning window n is shifted one minute compared to window $(n - 1)$. A constant shift of one minutes was used for all window sizes. Statistical functions (e.g. min, max, mean, standard deviation, etc.) were used to extract a total of 158 window-level features. Two features were added to the sensor streams: current time (minutes since the start of the day) and time since the last eating event (minutes) and number of eating events in that day. In the feature selection step, the most relevant features were selected (e.g. the location features were not beneficial and merely represented noise). In order to train an "About-to-Eat" moment classifier, signal processing and machine learning were used on the sensor streams. The classifier was trained to recognise the two classes "About-to-Eat" and "Not-About-to-Eat". The average recall of this model resulted a a recall, precision and F score of 0.77, 0.67 and 0.69 (respectively).

According to Han, Pei, and Kamber (2011)[306-307], precision and recall are measures used in classification. Precision describes the exactness (how many of the positive selected items are positive), recall defines the completeness (how many positive items have been correctly selected). The F-score (or F_1 score) is a measure that combines precision and recall (harmonic mean).

Rahman et al. (2016)'s classifier's performance was further inspected, in order to see how the different feature extraction window sizes affected it. The small window sizes were vulnerable to noise and the coarser ones were unable to detect recent events, which were crucial in creating the classifier. As can be seen in figure 1, the smaller window sizes have a higher gap between precision and recall. The performance with window sizes between 60 and 80 minutes is higher and more consistent.

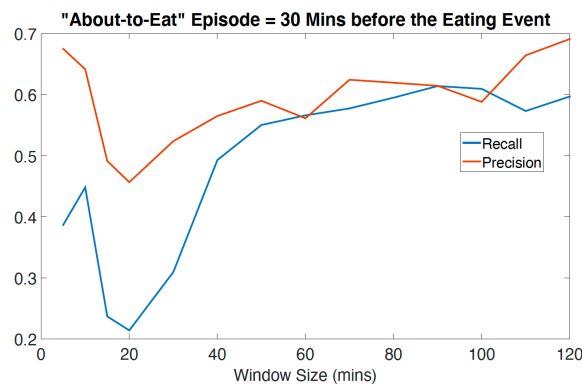


Figure 1: This graph depicts the F measure with the different feature extraction window sizes of the "About-to-Eat" classifier.

The performance for the "Time until Next Eating Event" model gained a correlation coefficient of 0.49. The most fitting feature extraction window size was assessed, the best performance

was reached with a window size of 100 minutes. The authors further claim, that both models could be improved by incorporating person-dependent data from the target user to the models (e.g. person-specific eating pattern, lifestyle).

Stütz et al. (2015)[240, 242-249] research, whether data collected by a user's smartphone can be used to predict stress. In their study, they used an android smartphone app called "TheStress-Collector" (TSC) to collect smartphone usage and sensor data in the background. The following data was collected:

- Activity: whether the device on the user is on foot, on a bike, in a vehicle, tilting, still or unknown.
- App Usage: apps for information, system, health, entertainment, social, or work
- Network Traffic: amount of network traffic (received and transmitted)
- Reboot Activity: power on and off events
- Calls: min, max and mean dB-values collected by the microphone
- Light: environment brightness
- Messages: timestamps of received messages
- Noise exposure: min, max and mean dB-values
- Screen Activity: duration of a user session (between screen power on and off)

15 participants installed the app on their smartphone and took part in the conducted study for two weeks. Seven times a day they would fill out questionnaires (at set times), which included the perceived stress score (PSS) and queried them on their current stress status. The stress levels were predicted by WEKA'S machine learning algorithms. The mean absolute error (MAE) and Person correlation were used for the evaluation. The results of this study presented compelling correlations between PSS and the data collected by the smartphone app. The weekly PSS average, as opposed to the daily one, included the highest correlation coefficient. Thus, it is expected, that it easier to spot longer periods of high stress than shorter ones. This paper also a team publication featured in the research project from which SmartEater was developed.

In their experiment, Ameko et al. (2018) intend to predict user's negative affect states, in order to provide targeted just-in-time mental health interventions. 65 students participated in the study. Through a smartphone app, GPS location data, accelerometer (activity) data, phone calls, SMS and ecological momentary assessments (EMA) data were collected and used to cluster participants according to their behavioural profiles. Grouping the participants this way seemed to improve the predictive model's performance.

Other related work: Pius Owoh, Mahinderjit Singh, and Zaaba (2018) use the k-means clustering algorithm to create automatic annotation of unlabelled smartphone sensor data, to observe sensitive location information of mobile crowd sensing users. Sornbootnark and Khoenkaw

(2019) who use smartphone sensor data (e.g. accelerometer) to predict excessive alcohol consumption, in order to replace breathalysers. Their algorithm produced 100% accuracy, however with 15 minute lags.

3 Theory/Literature Review

3.1 Data mining

Larose and Larose (2015)[4] declare, that data mining is used to recognise patterns and trends in large amounts of data. Han, Pei, and Kamber (2011)[16-18] explain, that the term "data mining" is a misnomer. A more suitable phrase would be "knowledge mining from data". The word "mining" represents valuable nuggets found within large amounts of raw material. Other names used to describe the same process include: knowledge discovery from data (KDD), knowledge extraction, data/pattern analysis, data archaeology, and data dredging. According to the authors, the discovery of data is an iterative process represented in the following steps: Data cleaning, data integration (combine multiple data sources), data selection (relevant data is extracted), data transformation (into applicable forms for data mining), data mining (discover patterns), pattern evaluation (determine if patterns have a meaning), and knowledge presentation. The following data forms, are typically used for mining: database data, data warehouse data, and transactional data. Other forms include data streams, ordered/sequence data, graph or networked data, spatial data, text data, multimedia data, and the World Wide Web. Data mining requires continuous human supervision for quality monitoring and evaluation, as stated by Larose and Larose (2015)[9-13, 15-16]. Software alone will serve wrong results. Data mining is used for description of patterns and trends, estimation of numerical values, prediction of future results, classification of categorical variables, clustering of similar objects and association of attributes.

Larose and Larose (2015)[160] describe the two types of data mining methods: *supervised* and *unsupervised*. Han, Pei, and Kamber (2011)[363] interpret supervised learning as *learning by examples*, whereas unsupervised learning is *learning by observation*. Larose and Larose (2015)[160-163] continue, the majority of methods are supervised. In supervised methods, there is a predefined target variable. The method receives several examples, where the target variable value is defined, thus learning which values of the target variable correspond to which values of the predictor variable. The goal of the unsupervised approach is to find patterns and structure in the inserted variables. Therefore, no target variable is established. Clustering is the most prevalent unsupervised method. As reported by Han, Pei, and Kamber (2011)[32], through using unsupervised machine learning, it is possible to detect classes within data.

Problems that can occur in data mining methods are data dredging, underfitting and overfitting. As stated in Larose and Larose (2015)[160-163], data dredging arises when false results develop in data mining due to random variations of data. Cross-validation is used to prevent data dredging, by guaranteeing that the results can be generalised to an independent data set.

In their paper on attempting to balance underfitting and overfitting, Aalst et al. (2010)[87-89] clarify when these can occur. When fitting a model to a log, underfitting or overfitting the

model are main problems. Underfitting the model means not fitting the model well enough to the log, therefore allowing too much behaviour which is not present in the log ("anything is possible"). Overfitting has the opposite effect. The model is fitted too well to the log, thus reducing it to another depiction of the log. It therefore only permits the same paths present in the log. These problems can take effect, for example, in a hospital process. Each patient's path of events is most probably unique, two patients are unlikely to have the same process. Hence, the event log is always growing, therefore generalisation is required to avoid overfitting. Likewise, underfitting (allowing all possibilities) should also be averted. Larose and Larose (2015)[164-165] mention, that another way to describe the overfitting/underfitting problem is through the bias-variance trade-off. In figure 2 there are three scatter plots with data points in two different colours, which need to be separated by a line. The first scatter plot depicts a low-complexity separator (e.g. a straight line), which may have some classification errors (*high bias*), however it needn't change much to accommodate new data points. Therefore, it has *low variance*. The second scatter plot illustrates a high-complexity separator (e.g. curvy line that can separate more of the points correctly), which reduces the amount of errors (*low bias*), but has to change a lot when new data points are added. Thus, it has *high variance*. The higher the complexity of the model gets, the bias is reduced, the variance however increases. The third scatter plot shows both a low-complexity separator and a high one, with additional data. While the low-complexity separator can still classify with little change, the high-complexity one needs to be altered more. The ideal model has neither high bias or variance.

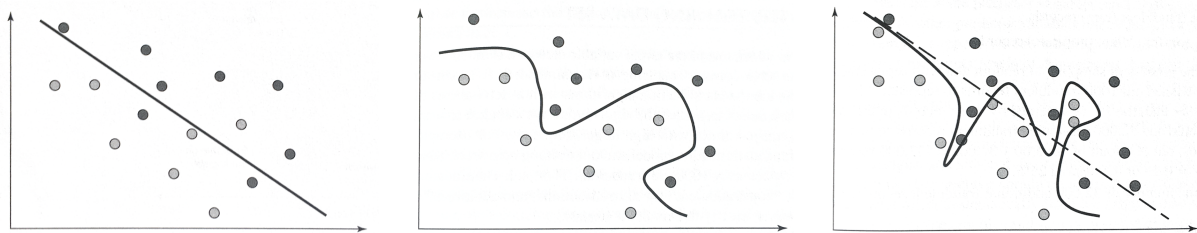


Figure 2: These three scatter plots from Larose and Larose (2015)[164-165] depict the bias-variance trade-off. The first plot portrays a low-complexity resulting in a high error rate. The second plot achieves a low error rate by using a high-complexity separator. The third graph compares the two separators.

3.2 Data preprocessing

To make data useful in data mining, Larose and Larose (2015)[20] point out, that data sets first need to undergo a data preprocessing step, including data cleaning and data transformation. Raw data extracted directly from databases can be incomplete (values are missing), noisy (contains outliers), or may contain out-dated or redundant data. García, Luengo, and Herrera (2015)[45] list the following sources of dirty data: data entry errors, data update errors, data transmission errors and bugs. Dirty data can impact the produced model, making it less reliable. The significance of its effect depends on the implemented data mining method. Larose

and Larose (2015)[20] define the goal as to decrease garbage in, garbage out (GIGO). To clarify, decreasing *garbage in* means to reduce the irrelevant data that is fed into the model, thus reducing the amount of irrelevant data received out of the model (*garbage out*). Further information to different types of dirty data and their solutions are outlined in the next sections below.

3.2.1 Noisy data

Pyle (1999)[71-72] interprets outliers, as objects that have low recurrence and that are separated from the main collection of values. These values are often mistakes and can lead to distortion of the data set. Insurance companies provide a good example of outliers. The majority of insurance claims are only for a small sum, however every so often a customer may be in need of a large claim (outlier). Han, Pei, and Kamber (2011)[28-29] mention, that in some cases, these uncommon events are of more interest. One of these instances, is detecting unusually large payments compared to the card holders normal payments, to uncover fraudulent usage of credit cards. As stated by Larose and Larose (2015)[26-27], there are some data mining algorithms that have trouble functioning correctly when fed outliers. Moreover, outliers may be data errors. Graphical methods used to identify outliers include, histograms or two-dimensional scatter plots. In order to smooth the data, Han, Pei, and Kamber (2011)[84] use binning, regression and outlier analysis (e.g. clustering).

3.2.2 Missing values

According to Pyle (1999)[81-82, 260, 264, 267], it is good practice to differentiate "empty" values from "missing" ones. Empty values do not have a comparable real-world value. Missing values, however, do have underlying values, they simply weren't recorded. The author does not recommend ignoring the record with the missing value, since it would mean wasting the data stored in the other fields of that record. These fields may contain relevant information. Substituting the value, means that the record can be used. One of the problems with not having these values, is that this missing information content (e.g. predictive or inferential) could be carried by the pattern. Another problem, is how to substitute the missing value, without adding bias to the data set. An inadequately chosen replacement value could distort the data set, by adding data which doesn't exist in the real world. A crucial focus is reserving the relationship between variables. Substitute values, if not suitable, may disrupt the between-variable variability, thus hiding or distorting patterns in the data.

Larose and Larose (2015)[23, 25] give an example, of how replacing missing values can lead to invalid results. The authors experimented with a database of cars. Substituting a missing brand with a random value (here "Japan") led to a car, that doesn't even exist. Data imputation takes into account the other attributes stored in the record and from these, calculates what the missing value would most likely be. Larose and Larose suggest, that the value can be replaced, either with a constant determined by the data analyst, with a field mean (for numerical values) or mode (for categorical values), with a random value, or with imputed values based on the different features of the record. Pyle (1999)[260, 267-269] point out, that regression can be used to find supplement values. When using regression (e.g. linear regression), one can calculate a value

with the help of another given value. There are several different methods to replace missing values. Some of which promise to generate more information. Such methods however are computationally complex.

3.2.3 Normalisation

Han, Pei, and Kamber (2011)[105-106] describes normalisation as giving the attributes of a data set equal weight. For example, it can transform the data to fall in a smaller, common range (e.g. [-1, 1]). It therefore hinders variables with large ranges from outweighing ones with smaller ranges. Income would, for instance, have a larger range than binary attributes.

García, Luengo, and Herrera (2015)[46-48] explain, that raw data is often transformed to produce new attributes with more applicable properties in the process of normalisation. These new attributes are then known as *modeling variables* or *analytic variables*. *Min-Max Normalization*, *Z-score Normalization*, and *Decimal Scaling Normalization* are methods that convert the distribution of the existing attributes. For the following examples, A is a numerical attribute from a data set, a single value of this attribute is represented with v :

- Min-max normalization scales the original numerical values to a newly defined range, with a new minimum ($newMin_A$) and maximum ($newMax_A$) (e.g. 0.0 and 1.0). The original minimum and maximum values found in A are presented as min_A and max_A respectively:

$$v' = \frac{v - min_A}{max_A - min_A} (newMax_A - newMin_A) + newMin_A$$

The intervals [0, 1] and [-1, 1] are common intervals for normalisation.

- Z-score (or zero-mean) normalization normalises the values using the mean (\bar{A}) and standard deviation σ_A of the values A .

$$v' = \frac{v - \bar{A}}{\sigma_A}$$

After this transformation, the mean equals zero and the standard deviation is one. The advantages of this normalisation method take effect, when the min and max values of A are not known, or when there are outliers that could bias the min-max method.

- The decimal scaling method moves the decimal point enough spaces, so that the maximum absolute attribute value of A is below one. The smallest required number of digits to move the decimal point, so that the largest absolute number in A is below zero, is represented by j :

$$v' = \frac{v}{10^j}$$

3.2.4 Data transformation

NOT REALLY SURE WHAT TO DO HERE - LEAVE OPEN, WAIT AND SEE WHAT HAVE TO DO IN THE EXPERIMENT

As reported by Larose and Larose (2015)[39-41, 45], flag variables can be used to transform categorical variables into numerical. A flag variable can take on one of two values: 0 and 1 (e.g. female = 0, male = 1). When $k \geq 3$ (k being the amount of categorical predictors), the variables can be transformed into $k-1$ flag variables. Assigning categorical variables numerical values is not advised, since this orders the categorical variables. For example, if North = 1, East = 2, South = 3 and West = 4, West would be closer to South than to North, etc.

ID fields should be removed from the dataset, since the value is different for each record and not helpful.

3.3 Dimensionality reduction

Bellman (1957)[20-22] first introduces the *curse of dimensionality*. The curse effects a mathematical model, when there are a large number of variables. The real world is complex and by trying to incorporate as many real world features into a mathematical model as possible, it becomes complicated. A too simple model, however, will not be suitable for prediction. Bellman (1961)[94] further details the results of *the curse of dimensionality*. Functions with one variable can be visualised as curve in a 2D space and a function with two variables in a 3D space. Depicting functions with more variables however, is more problematic (both for visualisation and tabulation). According to Larose and Larose (2015)[93], high quality visualisation methods usually cannot depict more than five dimensions. Bellman (1961)[94, 198] further gives the following example: Imagine if the variables of a function take on the values between 1 and 100. While a function with one variable would need to tabulate 100 values, a function with 2 variables would need to tabulate $100 \times 100 = 10^4$ values and a function with 3 variables 10^6 . Each additional variable adds more complexity.

According to Larose and Larose (2015)[92, 93], a high amount of predictor variables in data mining can lead to overfitting and overlooking crucial relationships between predictors. Dimensionality reduction techniques have the ability to reduce the number of predictor items, aid in ensuring that these predictor items are independent, and present a framework for interpretability of the results. As stated by Han, Pei, and Kamber (2011)[93], dimensionality reduction is a data reduction method. Data reduction is utilised to attain a smaller, more concentrated data set, whilst mostly keeping the integrity of the initial data set. Principal components analysis is a dimensionality reduction technique.

Principal Components Analysis was first proposed by Pearson (1901) and Hotelling (1933). Pearson's approach is to identify a line or plane that best fits the collected variables plotted to a plane. In order to determine the best fitting line or plane, means, standard-deviations, and correlations are used (Pearson 1901)[559-560]. Hotelling (1933)[5] introduces his method as *the method of principal components*. In his paper, Jolliffe (2002)[7] clarifies, that while these two papers used different methods, the standard algebraic derivation was announced by Hotelling (1933).

!!!TODO: IF USE PCA, GO MORE INTO DETAIL AND TAKE IT FROM jolliffe2002PCA (=pdf) INSTEAD OF han2011data.

Han, Pei, and Kamber (2011)[95-96] lists the first step of PCA is to standardise the input data, therefore making the data-range identical. Larose and Larose (2015)[94] declares, that after standardising the data, the mean is zero and the standard deviation is one. Han, Pei, and Kamber (2011)[95-96] describes the next step, which entails calculation k orthonormal vectors, the so called *principal components*. These unit vectors present a basis for the input data, which are a linear combination of the principal components. Larose and Larose (2015)[94] explain, that the principal components can be discovered, by rotating the initial coordinate system to the direction of maximum variability. These then create a new coordinate system.

In the following step, as stated by Han, Pei, and Kamber (2011)[95-96], the principal components are selected.

Hotelling (1933)[4, 5, 15, 18] When choosing the calculated components, they are chosen with the decreasing amount of variance. Therefore, the one with the highest variance (γ_1) is chosen first. The next highest (γ_2) is chosen orthogonal to γ_1 and so on, until the number n dimensions are reached (γ_n). The components left with small variance are disregarded, since they are trivial.

Han, Pei, and Kamber (2011)[93, 95-96] stated, in data mining the vectors with the lowest variance that are removed, reduce the amount of data and number of dimensions. Despite the loss of data, the components with higher variance can approximate the original data. The authors suggested wavelet transforms (e.g. discrete wavelet transform (DWT)) as another method of dimensionality reduction.

3.4 Cluster Analysis

Hartigan (1975)[1] describes clustering as a means to group similar objects together. For example, two planets are considered similar, if (given measurement error) it is probable they could be perceived as the same planet. Romesburg (2004)[2] gives the gathering of a variety of pebbles and sorting them into piles of similar attributes (e.g. shape, size, colour) as an example of cluster analysis. Hartigan (1975)[1-3, 6] further explains, that it can be expected from similar objects, for them to act and be treated the same. Clustering is also used to name, display, summarise, predict, and require explanation of the objects in the cluster. If some of the objects assigned to a cluster exhibit certain properties, it is expected that the other objects in this cluster will exhibit them as well. Clustering is almost equivalent to classification. Real-world examples of clustering include classifications of animals, plants and diseases.

Han, Pei, and Kamber (2011)[361-363] state that cluster analysis is another term for clustering. It divides a data set of objects into subsets (clusters). The objects placed into one cluster are dissimilar to the objects assigned to other clusters. Therefore, such a cluster can also be defined as an implicit class. For this reason, clustering is occasionally referred to as automatic classification. The fact that cluster analysis can find groups by itself, gives it its unique advantage. As mentioned in section 3.1, clustering is a type of unsupervised machine learning. It is unsupervised, since the class label for each group is unknown and needs to be discovered. In data mining, it is utilised to understand the distribution of the data and inspect the distinctions between clusters. Moreover, it can be used as a preprocessing tool for other data mining methods, for example characterisation, attribute subset selection and classification. Cluster analysis is

used in various fields, including: biology, security, business intelligence, image pattern recognition, and web search. It can be used to place customers into groups, organise projects into categories in project management and to sort web search results into concise groups. Furthermore, it can be used to detect outliers, since these are located outside of clusters. The detection of outliers is useful in credit card fraud and for identifying criminal activity in e-commerce.

According to Hartigan (1975)[9-10], there are usually five different types of variables used in practice in clustering:

- Counts: no arbitrary scale (e.g. number of legs on a spider)
- Ratio scale: only defined in proportion to a standard volume (e.g. volume of a liquid in a glass)
- Interval scale: chosen from a standard position in a standard unit (e.g. height of a building)
- Ordinal scale: ordered classification, can be changed by a monotonic transformation (e.g. socio-economic status)
- Category scale: classification that can be adjusted by a one-to-one transformation (e.g. religion)

A data set can be comprised of various variable types (*mixed*), of the same type but with different ranges (*heterogeneous*), or of variables with the same range (*homogenous*). There are also methods for conducting type or scale conversions.

Larose and Larose (2015)[524-525] explain, that data should be normalised before being put into a clustering algorithm, thus optimising the performance. Min-max normalization or Z-score standardization can be used to do so.

3.4.1 Overview of clustering algorithms

Han, Pei, and Kamber (2011)[363-365] There are several different clustering methods, each one must meet certain requirements:

- Scalability: clustering algorithms need to work on large databases, which may contain millions or billions of entries
- Ability to work with different attribute types: The algorithm must be able to handle various data types, for example: binary, nominal (categorical), and ordinal data. More complex data types include graphs, sequences, images, and documents.
- Recognising clusters with arbitrary shapes: Methods that use distance measures (e.g. Euclidean or Manhattan) to compute clusters, usually find clusters of spherical shape. The size and density also tend to be similar. Clusters however could be of any shape, therefore the algorithms need to be capable of detecting any shape.

- Requirements for domain knowledge: For some clustering algorithms, parameters (e.g. desired number of clusters) need to be determined. These can affect the cluster results. Parameters are hard to define, if the data is not understood.
- Ability to handle noise
- Incremental clustering: The method should be able to integrate incremental data updates into existing structures, without recomputing the clustering.
- Insensitivity to the order of the input: The clustering results should be the same, regardless of the order the objects are inserted into it.
- Ability to cluster high-dimensional data
- Capability to cluster under certain constraints
- Interpretability and usability of the results

Han, Pei, and Kamber (2011)[366-396] present different clustering algorithms. They state, that it is not easy to divide these into distinct categories, since some algorithms share features from other categories. The general categories are partitioning methods, hierarchical methods, density-based methods and grid-based methods.

TODO: ONLY EXPLAIN IN DETAIL, WHICH METHODS ARE USED IN THE EXPERIMENT

3.4.1.1 Partitioning Methods

Partitioning methods are the easiest and most significant types of clustering methods. The data is divided into k (generally pre-defined) number of groups (clusters). The data consists of n objects, thus $k \geq n$. Each group must contain at least one object. A data object can only be classified into one group (*exclusive cluster separation*). Fuzzy partitioning methods relax this condition. Many of the partitioning methods use distance measures to calculate their clusters. If the number of clusters (k) is pre-defined, then the clustering algorithm will create an initial segregation into k clusters. Objects are then relocated to improve the partitioning. The partitioning is considered good, when objects assigned to the same cluster are "similar" and "dissimilar" from the objects in the other clusters. Traditional partitioning methods can also be applied onto subspaces (for many attributes and sparse data).

Examples: k-means, k-medoids

3.4.1.2 Hierarchical Methods

The data is grouped into a hierarchy ("tree") of clusters. Depending on how the hierarchical decomposition is constructed, there are two different approaches: *agglomerative* or *divisive*. In the *agglomerative* or *bottom-up* approach, each object creates its own cluster. Step by step it is

then merged into its closest neighbours until all objects belong to one cluster, or a termination condition comes true. In the *divisive* or *top-down* approach, all objects initially form one cluster. Step by step, each cluster is divided, until each object is contained in its own cluster, or a condition is met to terminate the process. Once a merge or split step has been performed, it cannot be reversed. Once merged/split, the objects also cannot swap cluster. Each merge or split decision influences the quality of the resulting clusters and must therefore be well chosen. Hierarchical methods can be used in subspaces and can use distance measures, or can be density- and continuity-based.

COULD GO MORE INTO DETAIL ABOUT AGGLOMERATIVE AND DIVISIVE CLUSTERING, SEE PAGES 375-377 - but not sure if need, depends if being used

Examples: BIRCH, Chameleon

3.4.1.3 Density-Based Methods

The majority of clustering methods (e.g. partitioning and hierarchical methods) use distance-based approaches which leads to them only finding clusters with spherical shapes. Density-based methods have the ability to find clusters with random shapes. In these methods, the cluster keeps adding objects, so long as the number of objects/data points (density) close by is larger than a given threshold. The clusters are comprised of high-density areas of objects. These are separated by spaces with low-density. Accordingly, this method is also useful for removing noise and outliers. These methods can also be used to cluster sub spaces.

Examples: DBSCAN, OPTICS, DENCLUE

3.4.1.4 Grid-Based Methods

The previously mentioned clustering methods are data-driven (they accommodate the distribution of the data objects). Grid-based methods are space-driven (they do not rely on the distribution of the data objects). The data objects are quantised into grid cells on a multiresolution grid. The actions required for clustering are performed on the grid structure. The processing time depends on the grid size (number of cells) in each dimension and not on the number of objects and is more accelerated than other clustering methods.

Examples: STING, CLIQUE

Han, Pei, and Kamber (2011)[414, 416] clarify, that the clustering methods mentioned above have a good functionality, when used on a dataset with fewer than 10 attributes. Other ways to cluster high-dimensional data include *subspace clustering*. Subspaces (subset of attributes) are investigated to find clusters. The CLIQUE method is used for subspace clustering.

3.4.2 Evaluating clustering results

The resulting clusters received from the previously mentioned clustering algorithms are assessed in the *cluster evaluation* step. Han, Pei, and Kamber (2011)[396] describe this stage as

assessing the quality of the results. There are different steps to be taken in evaluating clusters.

3.4.2.1 Assessment of the cluster tendency

As explained by Han, Pei, and Kamber (2011)[396-397], the tendency must be assessed, meaning it is tested, whether structures exist that aren't random. Running a clustering algorithm on any data set will return clusters. However, only nonrandom structures are significant and not misleading. For example, if a data set consists of data points that are uniformly distributed, if a clustering algorithm delivers clusters, these will be random and have no purpose. Spatial randomness tests (e.g. Hopkins Statistic) can be used to measure how likely the data was created by uniform data distribution.

3.4.2.2 Evaluation of the cluster quality

Lastly, Han, Pei, and Kamber (2011)[399, 401] mentions, that the cluster quality needs to be evaluated. Generally, there are two ways to measure the quality of clustering: extrinsic methods and intrinsic methods. In extrinsic methods, there is a ground truth available, therefore these are also referred to as supervised methods. This ground truth is usually produced by experts (humans). Intrinsic methods are used, when there is no ground truth available. In intrinsic methods, the clusters are evaluated by how well they are separated from one another and how compact they are (e.g. *silhouette coefficient*).

The experiment described in this paper will use the intrinsic method silhouette coefficient, since there is no ground truth for comparison. In his paper, Rousseeuw (1987)[53-57, 59] proposes a new graphical display using silhouettes, to help determine how well objects belong to their assigned clusters. It can be used to interpret and validate the results of clustering. It is also utilised to compare the resulting clusters with those output using alternative algorithms (the input data being the same). In an example, where countries are assigned a value of how dissimilar they are to another country, the results are listed in a table. A structure contained in the results (consisting of 66 numbers), is hard to identify. Therefore, the countries are categorised into clusters using k-median. It is however uncertain, whether the clusters follow a specific structure, or if the groups are simply artificial. With the use of silhouettes, the author's goal is to answer the following questions: Is the quality of the clusters high, therefore the dissimilarities of the objects within a cluster are small, and large compared to the objects in other clusters)? Are the objects well-classified, misclassified and which ones were not classified (between clusters)? Is it possible to perceive which "natural" clusters are available in the data set? The silhouettes are ideal when the distance between objects are on a ratio scale (e.g. Euclidean distances) and when the goal is to receive clear and compact clusters. For each object i (in cluster A) the value $s(i)$ is calculated. $a(i)$ contains the average dissimilarity of the object i to each other object in the same cluster. If there are no other objects in the cluster, $s(i)$ is set to zero (most neutral value). $b(i)$ is determined, by firstly calculating the average dissimilarity, for each neighbouring cluster that isn't A . The shortest of these values, therefore the next closest cluster to A , is then assigned to $b(i)$. This cluster can so to say be seen as the next best choice for i . $b(i)$ can only be

calculated, if there are other clusters beside A. The formula is as follows:

$$s(i) = \frac{b(i) - a(i)}{\max\{a(i), b(i)\}}$$

The resulting value $s(i)$ is a number in the range of $-1 \leq s(i) \leq 1$:

$$s(i) = \begin{cases} 1 - a(i)/b(i) & \text{if } a(i) < b(i) \\ 0 & \text{if } a(i) = b(i) \\ b(i)/a(i) - 1 & \text{if } a(i) > b(i) \end{cases}$$

A $s(i)$ value close to 1 reveals, that the dissimilarity within a cluster is smaller than the dissimilarity to the neighbouring cluster. Therefore it suggests, that the assignment of that object is good, since it is the most likely the most suitable cluster for i (well-classified). A $s(i)$ value close to 0 means that $a(i)$ and $b(i)$ are almost equal and it is unclear whether A or the neighbouring cluster is a more suitable fit. If $s(i)$ is close to -1, then the dissimilarity within a cluster is larger than the dissimilarity to the neighbouring cluster. Thus, it would have been more natural to assign i to the neighbouring cluster, since it is closer to it (misclassified). The function can also be adapted to work with similarities. The *average silhouette width* for each cluster is received by calculating the average of all objects that belong said cluster. The higher the average silhouette width, the more pronounced the cluster is. An average score can also be calculated from each object i for the entire plot (data set), the so called *overall average silhouette width*.

Aranganayagi and Thangavel (2007)[15] use the silhouette coefficient in their proposed clustering algorithm which clusters categorical data. The coefficient was used assess the quality of the clusters and to relocate objects to more fitting clusters. The cluster efficiency in their algorithm was therefore enhanced.

3.4.2.3 Establishing the number of clusters

Han, Pei, and Kamber (2011)[398] states, that the number of clusters (k) found in the data set needs to be established. For some clustering methods (e.g. k -means), this number is defined before the clustering process. This number can be challenging to determine and depends on the shape and scale of the input data. A good number of clusters creates a balance between *compressibility* and *accuracy*. Having only one cluster would have maximum compression, but no value. Contrarily, if each data object formed its own cluster, the clusters would be most accurate, but not allow for summarisation of the data. Rousseeuw (1987)[59] describes, how silhouettes can be used to determine the ideal amount of clusters. Picture a data set with dense clusters which each have large distances to the other clusters. When k is chosen too small, naturally occurring clusters must be artificially joined, to satisfy the value k . Implementing the silhouette calculation will result in high within-cluster dissimilarities ($a(i)$) leading to a narrow silhouette (small $s(i)$). Likewise, if k is chosen too large, natural clusters will have to be artificially split, in order to gain k clusters. The objects in a split natural cluster will however still be very close to the other half of their cluster, therefore resulting in low dissimilarities between clusters ($b(i)$) and a small $s(i)$. This logic denotes, that silhouettes should be capable of finding the most 'natural' number of clusters in a data set.

3.5 Data Visualisation with t-SNE ?????

4 Experiment/Method?

in experiment

4.1 Preparation of the data set

in prep of data set

4.2 Clustering

in clustering

4.3 Clustering after dimensionality reduction

in clustering after dim red

4.4 Comparison and evaluation of clusters of different time lengths

in comparison of diff time lengths

4.4.1 Mathematical evaluation

4.4.2 User evaluation

5 Discussion

in discussion.tex

6 Conclusion

in conclusion

References

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Appendices

Anhänge löschen, die nicht verwendet werden.

A git-Repository

Das Repository dient zur Dokumentation und Nachvollziehbarkeit der Arbeitsschritte. Stellen Sie sicher, dass der/die BetreuerIn Zugriff auf das Repository hat. Stellen im Sinne des Datenschutzes sicher, dass das Repository nicht für andere zugänglich ist.

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- alle Webseiten als pdf

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- Vorlagen für Studienmaterial (Fragebögen, Einverständniserklärung, ...)
- eingescanntes, ausgefülltes Studienmaterial (Fragebögen, Einverständniserklärung, ...)
- Rohdaten und aufbereitete Daten der Evaluierungen (Log-Daten, Tabellen, Graphen, Scripts, ...)

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B Vorlagen für Studienmaterial

Vorlagen für Studienmaterial müssen in den Anhang.

C Archivierte Webseiten

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