Term Paper Data Science 1

Docent: Prof. Dr. Lena Wiese
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GOETHE UNIVERSITÄT FRANKFURT AM MAIN

Institute of Computer Science
Goethe-Universität Frankfurt a. M.

Author: M. A.
⟨your Student ID⟩
⟨your.email@ddre.ss⟩
⟨branch of study (Bachelor/Master, semester count)⟩
L. B.
⟨your Student ID⟩
⟨your.email@ddre.ss⟩
⟨branch of study (Bachelor/Master, semester count)⟩
B. L.
⟨your Student ID⟩
⟨your.email@ddre.ss⟩
⟨branch of study (Bachelor/Master, semester count)⟩
J. M.
⟨your Student ID⟩
⟨your.email@ddre.ss⟩
⟨branch of study (Bachelor/Master, semester count)⟩
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Chosen Project Topic:

- T3 Clustering

Github Repository:

- https://github.com/BenLucht/DS1_term_paper

Abstract

The objective of this term paper is to provide an overview of clustering by the example of four different clustering algorithms applied to four different data sets. The algorithms used are K-Means, Mean Shift, Affinity Propagation, and Spectral Clustering. These provide different characteristics concerning e.g. metrics, handling of data set sizes and evenness of cluster size as well as the parameters driving them. Data sets on house pricing, mall customers, wheat seeds and red wine show vastly different properties in relation to the number of observations and features, types of features to exhibit the differences in clustering results for the algorithms used. Visualization of results and comparisons can be accessed through an online frontend.

Contents

1 Problem Description

Clustering is a long-known method in the field of Data Science and Machine Learning. It describes the process of grouping elements of a given dataset into a finite number of distinct segments such that the elements of one segment are as similar as possible to one another while maximizing the dissimilarity between different segments. The resulting segments are called clusters. Finding clusters is of interest to gain information on patterns or structures characterizing a given dataset [1]. Each of the given data points is interpreted as a multidimensional feature vector and clusters are found by calculating vector similarities. Similarity or dissimilarity is measured using different kinds of metrics which are chosen according to the underlying data space [2].

As no a priori knowledge about the given dataset is assumed, distinguishing it from classification contexts, clustering is an unsupervised learning method. There exist several different clustering techniques which differ in their embedded assumptions on the cluster shapes or the requirement of various parameters such as the number of clusters or the bandwidth.

There is a wide variety of applications for clustering methods in research and professional contexts ranging from social network analysis to image compression and even oil well operation.

In this report, K-Means Clustering, Affinity Propagation Clustering, Mean Shift Clustering and Spectral Clustering are investigated.

Each of these clustering algorithms is applied on each of the chosen datasets and clustering performance is evaluated using cluster validation indexes. In the end, results generated applying the different algorithms are compared to each other.

2 Description of Specific Methods and Algorithms

2.1 K-Means

written by B.L.

On the surface, the idea for K-Means clustering is straight forward: an initial grouping of observations closest to starting points whereafter the start-

ing points are updated to be placed at the center of these groupings. A new grouping step is performed and centers updated until the groupings do not change any further [3,4]. This very brief introduction requires elaboration.

One way to look at clustering mathematically is to consider an objective function, similar to [5]

$$\sum_{k=1}^{K} \sum_{x \in C_k} w_x d(x, c_k) \tag{1}$$

where $K \in \mathbb{N}$ is the number of clusters $C_k, k \in \{1, \ldots, K\}$ of which the centers are c_k. Observations are $x \in \mathcal{X}$ and their weights w_x with $\mathcal{X} = \{x_1, \ldots, x_m\}$ being the entire data set. The data in $\mathcal{X}$ lives inside a feature space $\mathcal{F}^n$ with $n \in \mathbb{N}$ the number of different features. There also exists a measure on $\mathcal{F}^n$ that allows to calculate the distance d between points.

The most common specification of K-Means and often most practical in real world applications is the feature space being a euclidean space $\mathbb{R}^n$ and used for its distance function $d : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$, fittingly, the euclidean distance (written as $\|\cdot\|$). Using these, the optimization problem presents as

$$\min \sum_{k=1}^{K} \sum_{x \in C_k} \|x - c_k\|^2 \tag{2}$$

$$= \min \sum_{k=1}^{K} \sum_{x \in C_k} \left\| x - \frac{1}{|C_k|} \sum_{y \in C_k} y \right\|^2 \tag{3}$$

The inner sum in equation 2 can be seen as the sum of squared errors (SSE) for each cluster. Notably this version omits the weighting of the points. Introducing (equal) weights for all points $(\ldots) \sum_{x \in C_k} \frac{1}{|C_k|} \|x - c_k\|^2$ will not change the clustering result but allows for it to be seen as the intra-cluster variance, its minimizaiton across clusters directly reflecting one of the objectives mentioned in section 1.

Achieving the goal described above globally is an NP-hard problem but convergence to local optima can be achieved rather efficiently. This leads to the question of how an approximation can be achieved in practice. A method similar to the one described by [5,6] works as follows:

The one parameter that has to be specified for this algorithm is K, the number of clusters one wishes to produce. Once a K is chosen, the method can

start by picking K locations in the feature space $\mathcal{F}^n$ (each feature is a column in the data set). There are more advanced methods to be explored later but for the moment we assume these locations, so called centroids, c_k to be picked randomly. For every observation (row in the data) there is a centroid with the lowest distance (for equidistant centroids there is a method in place for assignment). In this step each observation is assumed to be part of the cluster C_k whose centroid c_k is closest to it. After this assignment the centroids are relocated to the "center" of their respective first step clusters (more on this below). Hereafter the method starts again from the point of calculating the distance between all observations and centroids. Observations are newly assigned to clusters, centroids are relocated and the method starts again. This procedure is repeated until the centroids are stationary (again, a closer look into this follows below). At this point a clustering has been achieved which satisfies the described method, but cannot necessarily be assumed to be the best clustering possible given the inputs. The entire procedure shall be redone from the top, beginning with new starting points, until one is reasonably satisfied with the stability of the result given a predefined method of evaluation. This series of operations can be summarized in a short amount of pseudo-code

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Algorithm 1 Pseudo K-Means

1: place initial centroids c_i ①
2: **while** centroids **not** stationary ④ **do**
3:     **if** observations have labels **then**
4:         update centroids c_i to center of current clusters C_i ③
5:     **end if**
6:     calculate all distances d_{n,k_i} ②
7:     assign each observation to min distant centroid via label i
8: **end while**

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where each of the numbers ① to ④ refer to a topic mentioned above and further examined below.

Clustering with the described method is fast, commonly requiring fewer iterations than observations [7]. The naive upper bound is trivially $\mathcal{O}(K^n)$ (trying every possible configuration), with [8] showing worst case run time to be superpolynomial ($\mathcal{O}(m^{(K+2/n)})$) with common runtimes being polynomial.

① Initial placement of the centroids can be achieved in different ways. The most basic method is placing them at random. On singular runs of the

algorithm this can lead to problems as can be seen in the example in figure 1.

Figure 1: Example with 1 dimension and 10 points bad starting position

It can be seen that this initial placement does allow for a clustering in the end, though it does not achieve what a human would describe as a fitting result. In two ways a solution to this problem can lie in repeating the method multiple times with different initialization. Firstly a new placement of initial centroids can lead to different clustering results which can be more fitting to the observer and secondly introducing a measure of fit and comparing it across runs to select the clustering that maximizes (minimizes) the measure can objectivize the selection of the "best" clustering. Commonly used as a measure are SSE and intra-cluster variance themselves, while other methods will be discussed more thoroughly in section 5. The repetition of clustering can therefore alleviate some problems introduced by randomly selecting starting points.

While computational capabilities are ever growing and trying more initializations should provide a higher chance of achieving better clustering results, it may still be useful to attempt improving on pure randomness.

One early proposition is selecting the center of the entire data set $\frac{1}{|\mathcal{X}|} \sum_{x \in \mathcal{X}} x$ as a first centroid and then randomly going through all observations and picking the subsequent points if they exceed a predefined distance threshold [9].

To ensure that initial points cannot fall far from the data [10, 11] propose going a step further by only selecting observations as initial points by randomly selecting observations. This can save some iterations required to "pull" centroids towards the data and can prevent the formation of empty clusters. Assuming no inner logic to the ordering of data in a data set (which might of course exist and presents a problem to this method) an implementation of K-Means in SPSS [12] selects the first i observations in the data set as starting points [13].

A number of methods expand on the idea of working with observations by first selecting a single observation and then seeking to select more not too close to the first one, which appears sensible computationally as well as considering the goal of identifying seperate clusters.

One such idea is to randomly select a starting point and subsequently selecting points with the maximum minimal distance to the previously selected [14], often called *maximin*.

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A popular method going by the name *kmeans++* developed by [15] extends the idea by [13] described above. After arbitrarily selecting a first observation, the remaining $K - 1$ initial points are picked in a random process. Instead of assuming an even distribution all observations are assigned probabilities proportional to the squared distance to their nearest previously picked initial centroid. Despite the additional computational aufwand in the beginning, this method shows reductions in terminal errors as well as time to convergence of up to half compared to naive random selection on $\mathcal{F}^n$. There are implementations of *kmeans++* for most popular machine learning implementations, including the one described in section 4.

This selection of methods is by no means exhaustive but something something ..

② In theory the practical application of the algorithm described above can be adapted to a plethora of distance measures to varying degrees of success. As described the most natural is the euclidean distance as it maps directly to variance minimization. It has been shown by [16] that other L^p norms than L^2 (like euclidean) can be used successfully, L^1 proving particularly good when applied for high dimensional cases. It can be shown by [17], though, that using metrics other than euclidean distances may cause the method to fail to converge. This may in some cases be alleviated by a clever selection of thresholds as described in ④. The choice of distance function will affect the clustering result. Opting for the euclidean distance will lead to clusters tending towards *n-spherical* shapes, applying Manhattan distance *hypercubes* and so on. Befitting the K-Means designation the ideal use case is data containing mostly contiguous subsets distributed around a finite number of means. Illustration 2 depicts examples of data suitable (1-3) and not suitable (4-6) for K-Means application.

Figure 2: Data shapes and K-Means-clustering success

③ The K-Means name makes it sufficiently clear that the selected method of calculating the position of centroids is by taking the mean of the observations grouped in the particular cluster. However, other interpretations of the concept of a mean have been devised in order to tackle specific limitations of the described method. One of the best known is *K-Medoids*. A method described similar to K-Means by [18] proposes to always select the most central observations of each cluster by minimizing the sum of pairwise dissimilarities.

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This method is generally more robust to outliers and can perform better when incorporating categorical data.

④ An important question to answer is when to stop iterating. There are mainly three options (cf. [19]): Execution can be stopped once the centroids stop changing. It is possible though to construct examples where this is unlikely to happen. Then this criterion can be expanded to stopping when the distance of centroids between iterations is below a threshold like [6] suggests. Another idea is to stop execution when intra-cluster variance (or another measure) stops improving, respectively improves less than a threshold, for a defined number of iterations. The third option is to stop when points remain in the same cluster for multiple iterations. In many software implementations there is an option to hard cap the number of iterations to prevent excessively long execution times or simply in place of one of the described criteria.

The elephant in the room remains: how to choose K? Looking at equation 2 makes it obvious that optimization improves when increasing K. It is also obvious that simply adding more clusters is not the goal. Domain knowledge about the data set can inform the decision but the application case for an unsupervised method like K-Means typically lacks this type of information. A brief overview of methods to determine K by [20, 21] include among others: visualizing the clustered data, density, internal validation measures (see section 5), gap statistic, or their own distortion measure. One common method of determining K from these statistical methods is then to apply the so-called *elbow rule*: clustering is performed for multiple different K and the corresponding statistics are calculated. The results are then plotted against each other. Often the resulting plot exhibits a "kink" at a certain point after which its trajectory flattens out. Its position then is used as an approximation of K. Viability of this method varies depending on the underlying data.

2.2 Affinity Propagation

by Jonas Mertens

Affinity Propagation is a machine learning algorithm which is used to create clusters. It was developed by Brendan J. Frey and Delbert Dueck in 2007. This algorithm does not require an input which specifies how many clusters are created. The algorithm finds the clusters by itself. Like

other clustering algorithms, Affinity Propagation iteratively sends "messages" between data points. In detail, the algorithm calculates responsibility and availability in each iteration (this will be explained later on). It iterates until all data points converge. After this, the algorithm has found the clusters for the input dataset. A disadvantage of Affinity Propagation is the computation complexity. Assume there are n data points, it results in a complexity of $O(n^2)$ because of the loop through all data points in every iteration. The runtime depends on the number of iterations T until the algorithm converges. Because of this, the runtime is $O(T * n^2)$.

Algorithm description:

$x_1, x_2, \ldots, x_n$ is a set of datapoints and the input of the algorithm. s[i,k] describes the similarity between x_i and x_k. In the Scikit-Learn (sklearn) implementation, similarity is measured using the negative Euclidean distance, but this algorithm also works with other type of similarities.

The responsibility describes how is k suitable to be an exemplar for i:

$$r(i, k) \leftarrow s(i, k) - max\left[a(i, k') + s(i, k') \forall k \neq k'\right] \tag{4}$$

The availability describes what happens if i should be chosen k as an exemplar.

$$a(i, k) \leftarrow min\left[0, r(k, k) + \sum_{i' s.t. i' \notin \{i,k\}} r(i', k)\right] \tag{5}$$

I am making use of the sklearn implementation of the Affinity Propagation algorithm. An important parameter is the preference where you can chose which how many exemplars are used.

The values for r(i,k) and a(i,k) are updated that after t iteration they are convergent:

$$r[i, k] = (1 - \lambda)r[i, k] + \lambda r'[i, k] \tag{6}$$
$$a[i, k] = (1 - \lambda)a[i, k] + \lambda a'[i, k] \tag{7}$$

λ is a dumping factor to avoid numerical oscillation. λ can be a float between 0.5 and 1.0. In my implementation the damping factor is 0.9.

2.3 Mean Shift

written by Leonie Bender

Mean Shift is an algorithm which can be used to find distinct clusters within a given dataset. The method was first proposed in 1975 by Fukunaga and Hostetler [22] and is categorized as density based clustering. It is assumed that data points of a given dataset are sampled from a distribution, the probability density function. The main idea is to define clusters in dense regions of the feature space. These clusters are defined around centroids corresponding to peaks, so-called *modes*, of the underlying probability density function. One can imagine that each data point is shifted to its nearest local peak of the density function and all the data points located at the same maximum are assigned to the same cluster around this mode. As the underlying distribution which determines the cluster centroids is not given, Mean Shift makes use of the concept of kernel density estimation. Local structures of the estimated probability density function determine both, the number of resulting clusters as well as which data points are assigned to which cluster [23].

The only input the user has to provide for Mean Shift Clustering is the *bandwidth* or *scale* [24]. The bandwidth parameter $h > 0$ determines the kernel's radius. The larger the bandwitdh is chosen, the larger is the kernel's radius, resulting in a smoother estimated density surface. Analogously, the smaller the bandwidth is chosen, the smaller is the kernel's radius and hence this results in an estimated density surface containing a peak for each point. Accordingly, if the bandwidth parameter value is chosen too small, Mean Shift will assign each data point to it's own cluster. In contrast to that, if the bandwidth parameter is chosen too big, Mean Shift will assign all data points to one single cluster.

For a given dataset consisting of n data points in the d-dimensional space, the kernel density estimator, using kernel $K(x) = c_{k,d} \cdot k\left(||x||^2\right)$ with bandwidth $h > 0$, is given through

$$\hat{f}_{h,K} = \frac{c_{k,d}}{n \cdot h^d} \sum_{i=1}^{n} k\left(\left|\left|\frac{x - x_i}{h}\right|\right|^2\right).$$

As explained above, modes of this density have to be found as each mode determines one cluster centroid. Modes correspond to stationary points which fulfill the requirement that $\nabla \hat{f}(x) \overset{!}{=} 0$. Computing the gradient of the estimated density function $\hat{f}$ and afterwards performing some further

algebraic manipulations yields the following formula:

$$\hat{\nabla} f_{h,K}(x) = \underbrace{\frac{2 \cdot c_{k,d}}{n \cdot h^{d+2}} \left[\sum_{i=1}^{n} g \left(\left\| \frac{x - x_i}{h} \right\|^2 \right) \right]}_{\text{proportional to } \hat{f}_{h,K}} \underbrace{\left[\frac{\sum_{i=1}^{n} x_i \cdot g \left(\left\| \frac{x - x_i}{h} \right\|^2 \right)}{\sum_{i=1}^{n} g \left(\left\| \frac{x - x_i}{h} \right\|^2 \right)} - x \right]}_{\text{mean shift}}.$$

While the first term is proportional to the above stated density estimate at point x, the second term describes the actual mean shift. It denotes the shift of point x, on which the kernel center is located, to the weighted mean of all the neighboring data points within the kernel's bandwidth. It can be shown that the mean shift vector always points in the direction of maximal increase of density of data points [23]. Local peaks of the probability density function are thus found by iteratively performing the mean shift as a gradient ascent method.

The iterative mean shift approach provides a way to determine modes without having to estimate the complete density function beforehand [23].

Initially, each of the given data points is chosen to be a candidate cluster centroid. In each iteration, all the candidate centroids are updated by shifting them to the mean of their respective neighboring data points. As the mean shift vector always points into the direction of maximal increase, repeating this procedure finally locates local maxima in the density function. The lower the density of data points, the larger the mean shift steps get. This means that data point density automatically regulates the step size and therefore, mean shift is an adaptive form of a gradient ascent method. After the mean shift of each data point is performed, the next iteration starts by placing the kernel on the shifted data point and again shifting it to the mean of its respective neighbors [25].

The algorithm stops if the shift of centroids falls below a predefined threshold. All data points that reside at the same stationary point are summarized into the same cluster where the local maximum of the underlying density function is used as the cluster centroid.

The procedure of Mean Shift Clustering can be summarized by the following pseudocode.

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Algorithm 2 Mean Shift Clustering

1: **for** i=1,2,..., N **do**
2:     **while** *mean shift exceeds threshold* **do**
3:         $m(x_i) \leftarrow$ *compute mean of neighboring data points of* x_i
4:         $x_i \leftarrow m(x_i)$
5:     **end while**
6:     Store $z_i \leftarrow x_i$
7: **end for**
8: Identify clusters $\{C\}_{1...m}$ grouping together all nearby z_is
9: Return clusters $\{C\}_{1...m}$

As the search for all the neighboring data points is computationally costly and in each iteration a large number of such searches has to be performed, the algorithm is not highly scalable. While in lower dimensions, complexity tends towards $O(T \cdot n \cdot log(n))$, in higher dimensions complexity tends towards $O(T \cdot n^2)$, where n denotes the number of samples and T denotes the number of data points. If all given data points are used as samples, this results in a complexity of $O(n^2 \cdot log(n))$ in lower dimensions and analogously to a complexity of $O(n^3)$ in high dimensions. This complexity can be improved by initializing only a fraction of data points as candidate cluster centroids or by only taking a subset of all the given data points as samples [26]. Details on this are provided in section 4.3.

Unlike other clustering algorithms, Mean Shift is a nonparametric method, meaning it neither makes any assumption on the number of resulting clusters nor on their shape. The algorithm can thus be used to find clusters of arbitrary, even non-elliptical shapes. This makes Mean Shift applicable to real world datasets where clusters of convex shapes would possibly introduce severe artifacts [23].

In addition to that, Mean Shift Clustering is robust against outliers. This can be verified as outliers would only lead to the definition of a cluster consisting of a single data point instead of shifting the centroid of another cluster. At the same time, this can also be seen as a disadvantage of the Mean Shift algorithm. The resulting clusters caused by outliers are not meaningful and do not have any reasonable interpretation when analyzing the resulting clustering. The rationale of another drawback of Mean Shift algorithm is based on the concept of kernel density estimation. In high dimensions, kernel density estimation may react sensitively to changes in the bandwidth parameter value. Therefore,

Mean Shift Clustering is better applicable to low-dimensional datasets [27].

2.4   Spectral Clustering

written by M.A.

Spectral clustering is an unsupervised learning algorithm. It treats each data point as a graph-node and performs the clustering problem into a graph-partitioning problem. The affinity rather then the absolute location (i.e. k-means) determines what points are set in which cluster. The algorithm consists of four basic steps:

1. The construction of a similarity graph:
During this step the Similarity Graph is being built in the form of an adjacent matrix, which is presented by A. The adjacency matrix can be built as an Epsilon-neighbourhood Graph, K-Nearest Neighbours strategy or a fully-connected graph.

The Epsilon-neighbourhood Graph sets the parameter epsilon already. Afterwards each point is connected to all the points which lie in the epsilon -radius. The graph which is built in this case is an undirected and unweighted graph.

By using the k-nearest neighbours strategy a parameter k is set as well. Then, for two vertices u and v, an edge is directed from u to v only if v is among the k-nearest neighbours of u. To build the fully-connected graph, each point is connected with an undirected edge-weighted by the distance between the two points to every other point. Since this approach is used to model the local neighbourhood relationships thus typically the Gaussian similarity metric is used to calculate the distance.

2. Projecting the data onto a lower Dimensional Space: This step is done to account for the possibility that members of the same cluster may be far away in the given dimensional space. Thus the dimensional space is reduced so that those points are closer in the reduced dimensional space and thus can be clustered together by a traditional clustering algorithm. It is done by computing the Graph Laplacian Matrix . To compute it though first, the degree of a node needs to be defined. The degree of the ith node is given by

(Formel noch einfügen)

Note that $w_{i,j}$, is the edge between the nodes i and j as defined in the adjacency matrix above. The degree matrix is defined as follows (noch einfügen)

This Matrix is then normalized for mathematical efficiency. To reduce the dimensions, first, the eigenvalues and the respective eigenvectors are calculated. If the number of clusters is k then the first eigenvalues and their eigenvectors are taken and stacked into a matrix such that the eigenvectors are the columns.

3. Clustering the Data: This process mainly involves clustering the reduced data by using any traditional clustering technique – typically K-Means Clustering. First, each node is assigned a row of the normalized of the Graph Laplacian Matrix. Then this data is clustered using any traditional technique. To transform the clustering result, the node identifier is retained.

3 Data Set Description

3.1 Boston House Pricing Data

written by L.B.

The Boston House Pricing Dataset was originally published in 1978 by Harrison and Rubinfeld [28]. In their study the authors used the dataset to investigate how people's willingness to pay for clean air is correlated to different measurements of house data around the area of Boston. In total, 506 samples are included within the dataset, containing fourteen different attribute columns. Six of those attribute values originate from the U.S. Census Service, the remaining originate amongst others from the FBI, the Metropolitan Area Planning Commission, the Massachusetts Taxpayers Foundation, the Massachusetts Department of Education and the MIT Boston project. All data was sampled in 1970. The attributes of each data can be separated into different types, providing information on structure, neighborhood, accessibility or air pollution.

Structural attributes yield information on the state of the house in terms of year of construction or spaciousness. While the *RM* variable holds the

numeric value for the average number of rooms, the AGE attribute describes the proportion of houses that were built before 1940. Both values are assumed to have a positive correlation on housing values since owning more rooms or owning houses with modern structures is perceived as increasing life quality.

Neighborhood attributes hold details about the socioeconomic status of the environment. This includes the fraction of colored people in the whole population as well as the $LSTAT$ attribute, which denotes the amount of people being of a lower educational status. In addition to that, crime rate is included for neighborhoods of the Boston area. The latter attribute is supposed to have a negative effect on housing values as crime rate influences people's level of danger. Another neighborhood attribute stands for the sum of square feet available for residential zoning where constructing buildings like factories is prohibited. Next, the $INDUS$ attribute comprises the proportion of industry which comes along with noise, traffic and dirt and is therefore negatively correlated with housing values. Moreover, property tax rate as well as the ratio between pupils and teachers are included. The last socioeconomic attribute classifies whether the respective city area adjoins Charles River.

Accessibility attributes characterize the infrastructure measured by closeness to employment centers and to radial highways.

In order to estimate air quality, the concentration of Nitrogen Oxid in parts per hundred million is measured.

The last attribute is the dependent variable which describes the median value of houses that are occupied by private owners.

While the index of highway accessibility is an integer value and the closeness to Charles River is measured using a boolean variable, all the other attributes are float numbers. The dataset does not contain any empty columns, thus no elimination or preprocessing of the available data is necessary.

3.2   Mall Customer Segmentation

by J. M.

The Data Set Mall Customer Segmentation Data includes basic customer data. It contains a unique Id for each customer, gender, age, the annual income, and the spending Score. In this Score you can have a value between 1 and 100. The distribution of gender of the customer is 56% female and 44 % male. In the preprocessing every entry of the gender column gets a number 0 or 1 depending on the gender is male or female. I do this because than every

entry of this dataset contains only numbers. The Age of the Customers is between 18 und 70. The Annual Income of the customers is between 15 and 127.

3.3 Seeds Data

written by B.L.

This data set has been used in the work of [29]. The data comprises information on different features of wheat kernels. There are seven species with a total of about 20 varieties of which three can be found in the data: Kama, Rosa and Canadian wheat. The kernels for which data was collected were selected randomly. They were then examined through X-ray imaging. A software called *GRAINS* for this specific application [30] was used to extract the features for each observation:

- area A
- perimeter P
- compactness $C = 4\pi A/P^2$
- length (along groove)

- width
- asymmetry coefficient
- length of kernel groove
- label

A brief look into the data set confirms this.

	Area	Perimeter	Compactness	Length	Width	Asymmetry	Groove	Label
1	15.26	14.84	0.871	5.763	3.312	2.221	5.220	1
2	14.88	14.57	0.881	5.554	3.333	1.018	4.956	1
3	14.29	14.09	0.905	5.291	3.337	2.699	4.825	1
4	13.84	13.94	0.896	5.324	3.379	2.259	4.805	1
5	16.14	14.99	0.903	5.658	3.562	1.355	5.175	1

Table 1: Seeds Data Set First Observations

Figure 3: Seeds pairplot WIP
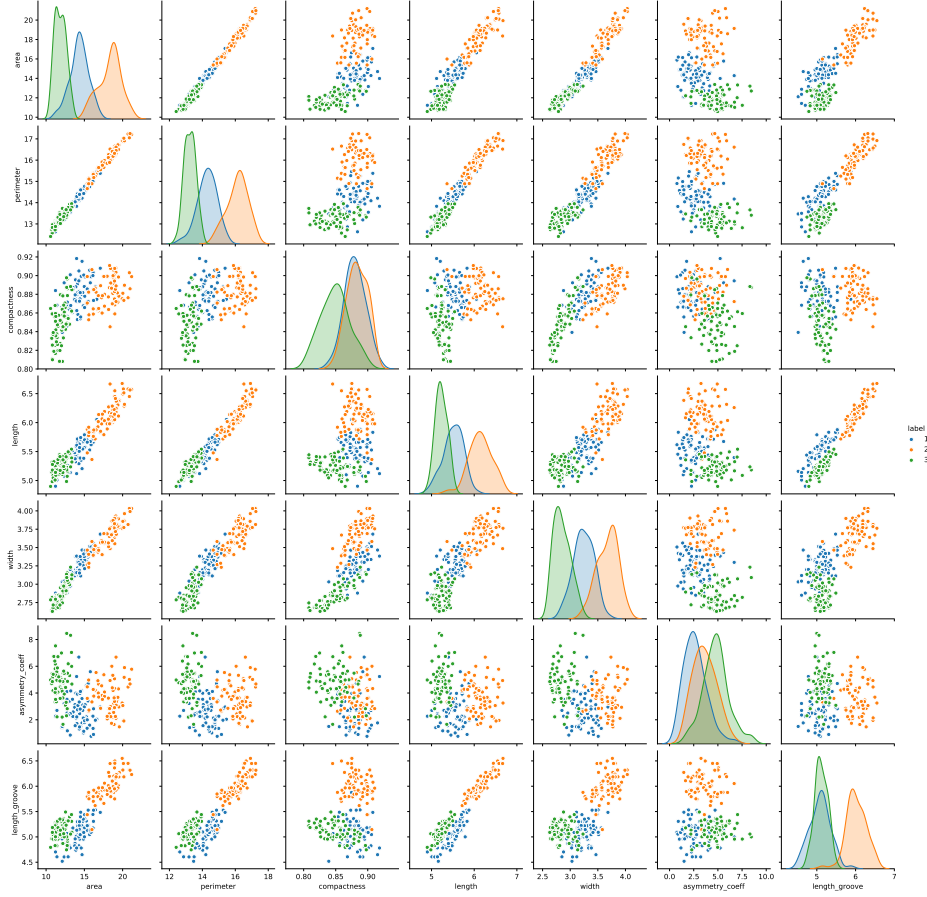
A few things can be noted: compactness is linearly dependent on two other features in the data set, calling into question what value this information can bring to a clustering method. Furthermore the area is not computed from other measurements, but is correlated with width and length and the perimeter. These relationships among others can be seen in figure 3. Note that these plots have been colored according to their original labels. Density plots on the diagonal for example already show distinct characteristics for the different varieties of kernels for certain features.

Some key insights on the data set as a whole can be found in table 2 with information on the observation count, mean, standard deviation (std), minimum and maximum as well as 25, 50 and 75% quantiles as rows for each

feature in columns. There are a total of 210 observations which is on the lower end for clustering applications. The data is balanced at 70 observations for each kernel variety. There is no missing data in any of the features.

	Area	Perimeter	Compactness	Length	Width	Asymmetry	Groove
Count	210	210	210	210	210	210	210
Mean	14.848	14.559	0.871	5.629	3.259	3.700	5.408
Std	2.910	1.306	0.024	0.443	0.378	1.504	0.491
Min	10.590	12.410	0.808	4.899	2.630	0.765	4.519
25%	12.270	13.450	0.857	5.262	2.944	2.561	5.045
50%	14.355	14.320	0.873	5.524	3.237	3.599	5.223
75%	17.305	15.715	0.888	5.980	3.562	4.769	5.877
Max	21.180	17.250	0.918	6.675	4.033	8.456	6.550

Table 2: Seeds Data Set Statistics Summary

A few more things can be noted here: Rosa wheat kernels exhibit a mean area more than one standard deviation above the mean area for the entire data. Similarly, Canadian wheat kernels have a mean asymmetry coefficient far beyond one standard deviation above the overall mean. For each variety of wheat a normality test [31] has shown that the hypothesis of normality cannot be rejected at a 99% level for most features. This might bode well for at least K-Means clustering.

For the clustering step of course the labels are removed from the data (this data set was included despite not being the typical application of clustering in part because it can serve as a sort of "control" for the clustering methods when looking at evaluation and conclusions).

4 Description of Python libraries used

4.1 Scikit-Learn KMeans

written by B.L.

For K-Means clustering we use the implementation provided from [26] in version 0.24.2 which is the latest stable release as of June 18, 2021.

One of the parameters of this function is the choice of algorithm used for the optimization: `full` provides the option to run a method mimicking [6]

described exhaustively in section 2.1, while `elkan` has become the default which uses a more efficient algorithm described by [32] to improve run time. This method takes advantage of the triangle inequality in multiple ways, most prominently by reducing the number of distance calculations for each iteration. After updating, distances between centroids are calculated. Then, starting with the previously assigned centroid, distances from observations to centroids are calculated. In the `full` case, this would be done for all observations with all centroids. With the `elkan`, thanks to triangle inequality, the algorithm knows it is not necessary to perform more distance calculations for a particular observation if its distance to the current centroid is below half the distance between the centroid and next closest centroid.

Another option is to specify how to initialize the algorithm. It is possible to specify `random` which selects random observations from the data, to provide a list of starting positions, a custom function, or to use the default which is `kmeans++` as described in section 2.1. Implementing a custom initialization function or providing a list of starting points is possible as well.

Stopping condition for the algorithm is movement of centroids below a certain threshold, as described in section 2.1, determined by calculation of the Frobenius norm of the difference in position of centroids of two consecutive iterations. The threshold can be set as a parameter. There is also the possibility to specify how many runs with new initializations will be run as well as a maximum number of iterations per run.

4.2 Scikit-Learn Affinity

4.3 Scikit-Learn MeanShift

written by L.B.

For Mean Shift Clustering we use the implementation provided from [26] in version 0.24.2 which is the latest stable release as of June 18, 2021. The implementation offers the possibility to enter several additional parameters supplementary to the required bandwidth. Three related additional parameters can be used to speed up the clustering procedure as mentioned in section 2.3. These parameters are called seeds, `bin_seeding` and `min_bin_freq` and allow to define which of the given data points should be used for the initialization of candidate centroids. Exclusively if no array of initial seeds is passed over, the algorithm checks the `bin_seeding` parameter value. If

this parameter is `False`, all given data points are used to initialize kernels. In contrast to that, if the `bin_seeding` parameter is `True`, the algorithm creates a grid with cell size defined by the bandwidth parameter. The number of points within the created bins defines which data points are used as seeds. Therefore, `min_bin_freq` defines the minimum number of data points that have to occur in a bin to define a candidate centroid. Running the algorithm in its default mode, as it is done in this work, all the given data points are initialized as candidate centroids and hence used as initial kernel locations. In addition to that, the algorithm provides a parameter called `cluster_all`, which defines whether all the given data points have to be assigned to a cluster. If the parameter is `True`, all data points are clustered, even if they are not placed within any kernel. Those outliers are assigned to their nearest kernel. If the parameter is `False`, outliers outside any kernel's radius are not assigned to any cluster, but instead their label is `-1`. A technical parameter is called `n_jobs`. Users can pass an integer to determine the number of jobs which should be used for the computation.

In theory, the algorithm stops the mean shift iteration for each seed if it converges. The `max_iter` parameter can be used to fix a maximum number of iterations if a seed does not converge. In the default mode, the maximum number of iterations is set to 300.

If no value for the required bandwidth parameter is provided, the bandwidth is estimated using a built-in `estimate_bandwidth` function. This function calculates the median of all pairwise distances and ascertains a suitable bandwidth based on the underlying dataset.

The algorithm performs the mean shift procedure for all the seeds in parallel. In each iteration, all the neighbors within the kernel's radius are found by executing a nearest neighbor search. The seed is shifted to the mean of all the neighboring data points until it either converges or the maximum number of iterations is reached. After shifting seeds, some post processing steps are performed. The algorithm searches for seeds whose distance is smaller than the bandwidth. If duplicates like these are found, the one with fewer data points is removed. If `cluster_all` is `True`, each of the given data points is assigned to the cluster defined by the seed that is closest to the respective data point. If `cluster_all` is `False`, only those data points that are located within a kernel's bandwidth are assigned to the cluster defined by the nearest seed and the remaining data points are assigned to the artificial cluster with label `-1`.

4.4 Scikit-Learn Spectral Clustering

5 Description of Evaluation Module

Due to the nature of clustering as an unsupervised machine learning method, it is typically applied to datasets lacking prior information on grouping. Therefore measuring the performance of each method can only be performed on the data and the labeling produced by each clustering algorithm. These types of calculations are commonly called *internal cluster validation* indices.

Differentiating by the way compactness and separation are measured [33] split indices into two groups. There are graph based indices: C Index, Dunn, Gamma, G+, McClain-Rao, Point Biserial, Silhouette, Tau, and there are prototype based indices: Calinski-Harabasz, Davies-Bouldin, Pakhira-Bandyopadhyay-Maulik (PBM), Ratkowski-Lance, Ray-Turi, Xie-Beni, Wemmert-Gancarski.

We have decided to use two indices from each group: Dunn Index (DI) and Silhouette Score (SI), Calinski-Harabasz Index (CH), Davies-Bouldin Index (DB).

5.1 Dunn Index

written by M.A.

The Dunn Index (in short DI) is a metric for evaluating clustering algorithms. Its aim is to identify sets of clusters [34]. It is used for measuring an internal validation of clustering results [35].

For each cluster, compute the distance between each of the objects in the cluster and the objects in the other clusters. Use the minimum of this pairwise distance as the inter-cluster separation (min. separation). For each cluster, compute the distance between the objects in the same cluster. Use the maximal intra-cluster distance (i.e maximum diameter) as the intra-cluster compactness. Calculate the Dunn index (D) as follow:

$D = \frac{min.separation}{max.diameter}$ [35]

The higher the value of the resulting Dunn index, the better the clustering result is considered, since higher values indicate that clusters are Compact.

That means the greater the better [36].

5.2 Calinski-Harabasz Index

written by B.L.

The Calinski-Harabasz criterion [37] is defined as a poportional measure of within cluster variance to between cluster variance. That is why it is also known as the Variance Ratio Criterion (VRC). Mathematically this means

$$CH = \frac{S_B}{S_W} \frac{m-K}{K-1} = \frac{\sum_{k=1}^{K} |C_k| \left\| c_k - \sum_{x' \in X} x' \right\|^2}{\sum_{k=1}^{K} \sum_{x \in C_k} \|x - c_i\|^2} \frac{m-K}{K-1} \tag{8}$$

utilizing the same notation as equation 3. Between-cluster variance is divided by within-cluster variance. Dividing the data into more partitions of course reduces within-cluster variance, which is why there is also a scaling factor (second fraction representing degrees of freedom) to account for it. In comparison to DB between-cluster variance is calculated in relation to the center of the data set in place of between individual cluster centers themselves.

Due to its construction (distance measure) this index performs well when clusters form mostly convex shapes. This can lead to mis-evaluation if the underlying data does not comprise of such globular clusters so a method capturing this might score lower while actually fitting the data better. It may therefore be better suited to compare different parameters for the same algorithm instead of comparing different algorithms. A comparative study of 30 cluster validation indices [38] ranks CH performance in evaluating fit near the top in many applications, particularly when evaluating K-Means results as expected.

5.3 Davies-Bouldin Index

written by J.M.

The Davies-Bouldin index is a metric to evaluate clustering algorithms and it was developed by David Davies and Donald Bouldin in 1979 [39]. It is used to check the validity of the clusters. To reach this, the Davies-Bouldin Index tries to maximize the intern-cluster distance and on the other side tries

to minimize the intern cluster distance. The Davies-Bouldin index is defined as

$\bar{R} \equiv \frac{1}{N} \sum_{i=1}^{N} R_i$

where N is the number of cluster and R_i is the maximum of R_{ij} where i≠j

$R_{ij} \equiv \frac{S_i + S_j}{M_{ij}}$

where M_{ij} is the Minkowski metric which can be descibed as:

$M_{ij} = \{\sum_{k=1}^{N} |a_{ki} - a_{kj}|^p\}^{\frac{1}{p}}$

$S_{ij} = \{\frac{1}{T_i} \sum_{j=1}^{T_i} |X_j - A_i|^q\}^{\frac{1}{q}}$

If q =1 S_{ij} is the Euclidean distance between centroids.

For our evaluation we use the implementation from sklearn of this metric. This metrics calculate a score. Zero is the lowest score that can be reached. If a score is closer to zero, it related that there is a better seperation between the calculated clusters.

5.4   Silhouette Score

written by L.B.

Cluster validation indexes are used to assess clustering quality. That means it is investigated whether the resulting clusters reflect natural structures in the data or whether clusters rather determine artificial groups. In general, the ratio of dissimilarity between data points within the same cluster to dissimilarity between data points in different clusters is a measurement for clustering quality. The Silhouette Score is one of such cluster validation indexes which can be applied to evaluate clustering results if Euclidean distance measures can be calculated on the underlying dataset. According to that, a clustering result as well as proximity scores between all data points have to be provided to be able to apply the Silhouette Score. For a single data point, distances to all the data points assigned to the same cluster are calculated. Here, the mean of all these distances is called *a*. After that, the nearest cluster for each data point has to be found. This can be done by iteratively calculating the mean of distances between the single data point and all data points within another cluster until distances for all clusters have been computed. The minimum average distance determines the nearest cluster for

the single data point. The minimum average distance is called b here. The Silhouette Score for data point i is calculated using the following formula:

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

The mean of all the Silhouette Scores for each individual data point determines the Silhouette Score for the whole dataset. As the nearest cluster has to be found for each of the included data points, the Silhouette Score can only be computed as soon as more than one cluster exists [40]. Taking a closer look at extreme cluster results determines how to interpret the Silhouette Score values. Given a partition where the mean intra-cluster distance a is extremely low while the mean inter-cluster distance b is high, the Silhouette Score would tend to be `1`. Hence, a Silhouette Score of `1` corresponds to a well-partitioned dataset because the mean of distances between single points and other clusters than the one it is assigned to is large. Analogously, a value of `-1` corresponds to a partition where the inter-cluster distance b is much larger than the intra-cluster distance a. Thus, the data points are not assigned to their nearest clusters, resulting in a misclassification. If the Silhouette Score is equal to zero, means of inter- and intra-cluster distances are close to each other and it is unclear which cluster the point should be assigned to. In this case, the partition can also contain overlapping clusters [40]. For the calculations of Silhouette Scores, we make use of the implementation provided from sklearn [26]. We make use of the Silhouette Score as it can be applied on cluster results generated with any clustering technique. It therefore provides an intuitive way of comparing the results of different algorithms to each other. One disadvantage is that Silhouette Scores are higher for convex clusters. As some density-based clustering algorithms like Mean Shift explicitly allow the creation of non-convex clusters, the obtained Silhouette Scores could possibly be lower than results created applying other clustering techniques. This is further investigated in the evaluation part.

5.5 Results

In the following there is a discussion of the results of all clustering efforts in detail. A brief overview of the evaluation results can be found in table 3. For each data set there is a row for each algorithm used. In columns are the results for each index. The cells represent the highest (lowest for DB respectively) value achieved by applying various parameter configurations.

It should be noted that comparing results across different methods does not show the entire picture but it can yield indications on performance. MORE WHEN RESULTS.

Data and Method	CH	DB	SI	DI
Housing				
K-Means	1621.90	1.014	0.721	0.525
Mean Shift	1.567	2.346	3.457	4.856
Affinity	1.567	2.346	3.457	4.856
Spectral	1.567	2.346	3.457	4.856
Mall				
K-Means	301.02	0.901	0.479	0.843
Mean Shift	1.567	2.346	3.457	4.856
Affinity	1.567	2.346	3.457	4.856
Spectral	1.567	2.346	3.457	4.856
Seeds				
K-Means	369.55	0.979	0.492	0.091
Mean Shift	1.567	2.346	3.457	4.856
Affinity	1.567	2.346	3.457	4.856
Spectral	1.567	2.346	3.457	4.856
Wine				
K-Means	3116.82	0.901	0.603	0.049
Mean Shift	1.567	2.346	3.457	4.856
Affinity	1.567	2.346	3.457	4.856
Spectral	1.567	2.346	3.457	4.856

Table 3: Comparing everything example

5.5.1 Seeds K-Means

written by B.L.

K	CH	DB	SI	DI
2	351.235	0.688	0.519	0.038
3	375.804	0.753	0.471	0.085
4	327.439	0.825	0.412	0.020
5	310.331	0.915	0.361	0.091
6	302.344	0.917	0.366	0.106
7	294.385	0.939	0.350	0.077
8	297.502	0.937	0.362	0.083

Table 4: K-Means Seeds Dataset Indices by Number of Clusters

Table 4 contains the index scores for each of the indices selected as columns and the number of clusters as rows. An easier representation of this data is a line chart which can be seen in figure 4 and in the following description of results. More than simply a tool to compare scores between methods, these can help in identifying the number of clusters (or other parameters below) best fit to represent the data. So what can be learned from the data: If there is a clear maximum value for an index it indicates looking at that value to gain insight on the fit. If there is no clear maximum value, one can try to employ the so called elbow criterion (see section 2.1) where a distinct change in direction for a graph might indicate a value worth examining. If there is neither there seems to be no information gain at hand from that particular index for this application.

Figure 4: K-Means Seeds Dataset Indices by Number of Clusters
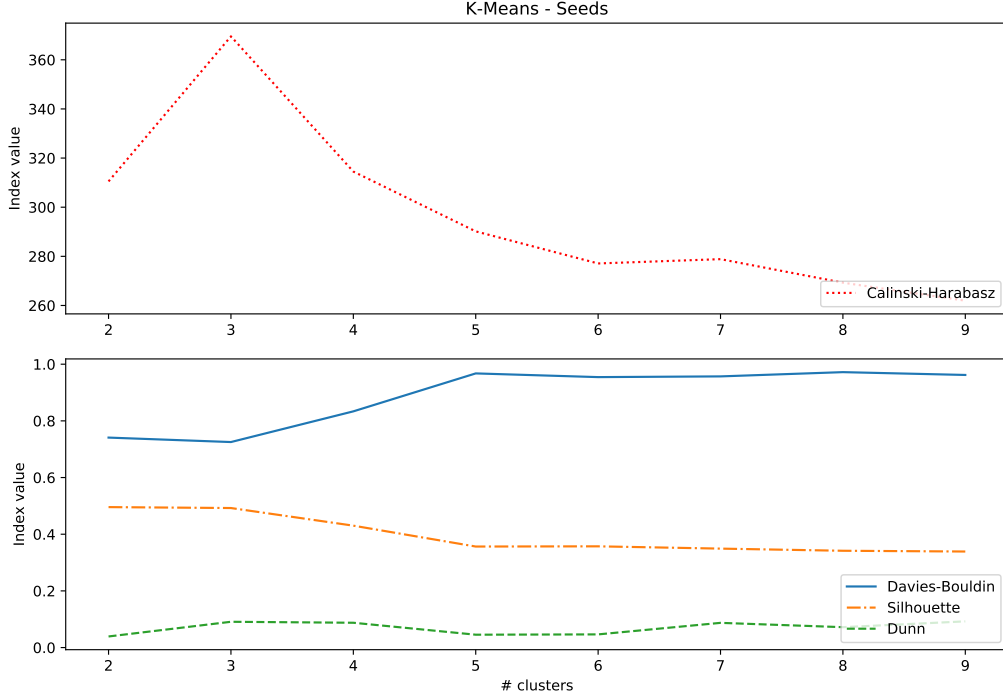
Looking at figure 4 (one line for each index, two panels because of the vastly different scale of CH) one can see a clear maximum in CH value and a local maximum in DI as well as a change in slope for SI at three clusters each. Following the described logic, DB suggests also considering five clusters as an option.

As mentioned in section 3 this dataset originally comes with labels which allows to use them as a benchmark to see how the clustering performs. Plotting (figure 5) two dimensional representations (see t-SNE in section 6) of the K-Means clustered result and the original data shows a few things: the algorithm has, as expected, produced non-overlapping mostly contiguously shaped clusters in contrast to the original data. However using three clusters has generally produced a reasonably good fit, as is supported by an accuracy of 89.5%, precision of 90% and recall of 89.5% to name a few standard metrics.

Figure 5: Seeds Data Set Comparison Clustering and Original Labels
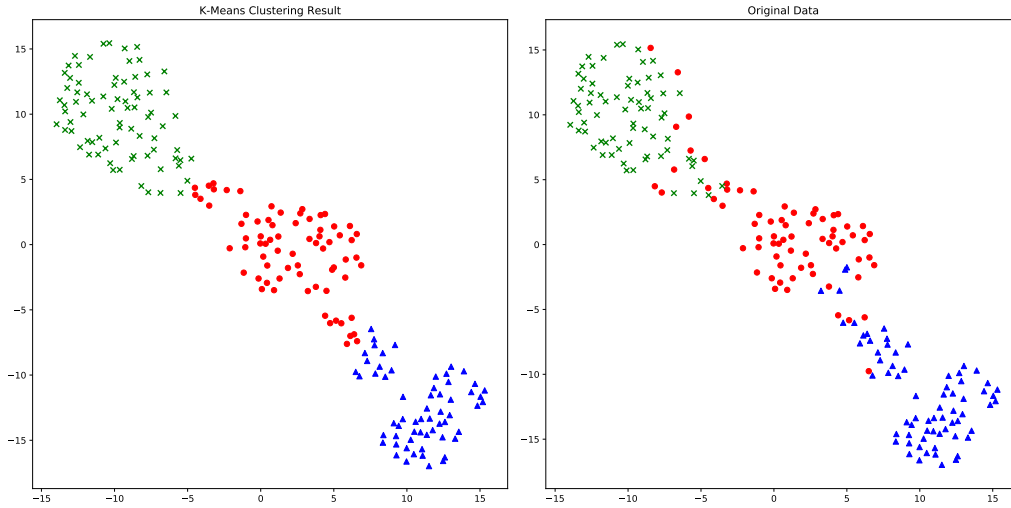
5.5.2 Mall Customers K-Means

written by B.L.

As one of the features is categorical (gender), this is not an ideal application of the K-Means clustering method. The categories can be resolved into discrete values so that calculations can be run, but the arbitrary nature of this does not really allow for good interpretation of the results. An exemplary three dimensional plot 5.5.2 shows the issue:

gender is represented on the z-axis and the two manifestations simply rip the data into two partitions. When gender is encoded as 0 and 1, this showed almost no effect. When using 0 and 100, it leads to a doubling in the index-recommended number of clusters. One attempt to deal with this is to scale all data between 0 and 1 but this aggravated the problem instead of improving on it. Exten-
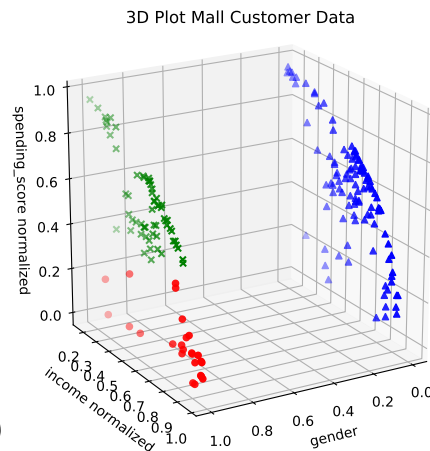
Figure 6: Split Data Due To Categorical Feature

sions of the K-Means method have
been devised to deal with this type
of data (as described in section 2.1)
but their application here seems be-
yond the scope of this work. Using
the gender feature also does not im-
prove scores in the evaluation meth-
ods used. Given these circumstances, considering plot 7 suggests considering
the results for 2 (CH, DB, SI), 7 (DB) or 8 (CH) clusters.

Figure 7: K-Means Mall Customers Dataset Indices by Number of Clusters
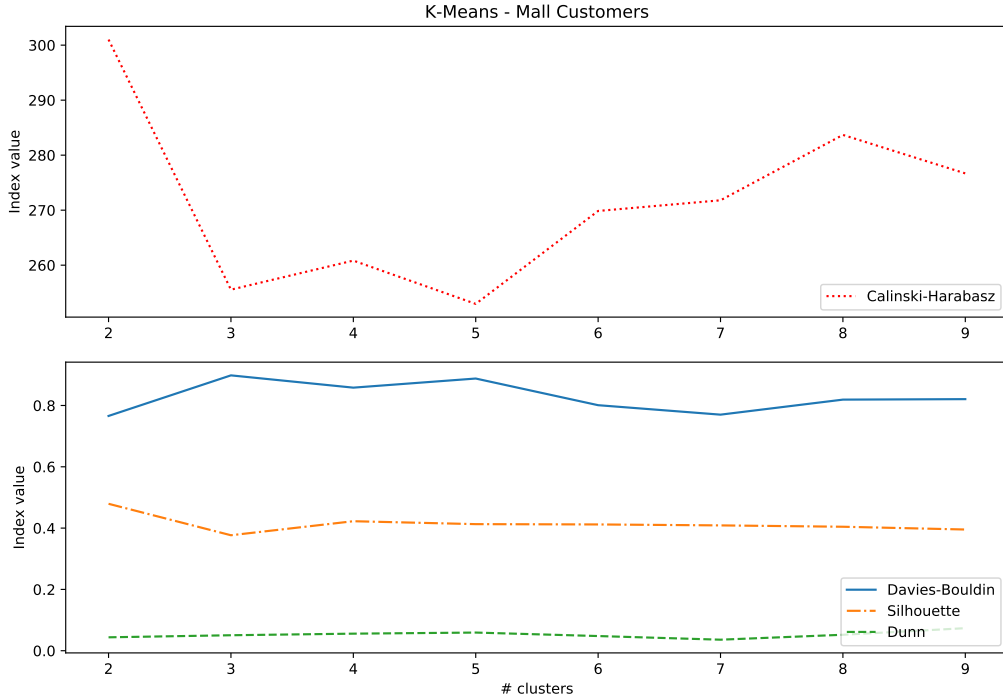
The dataset contains four features, three of which have a measurable and
interpretable impact on clustering, which lends itself to a visual comparison
in three dimensional space. Figure 8 shows three plots, one for each suggested
number of clusters. The highest overall evaluation scores were achieved for
two clusters and purely from a visual standpoint this seems to hold up.

Figure 8: Mall Customers 3D Plot Clustering Options
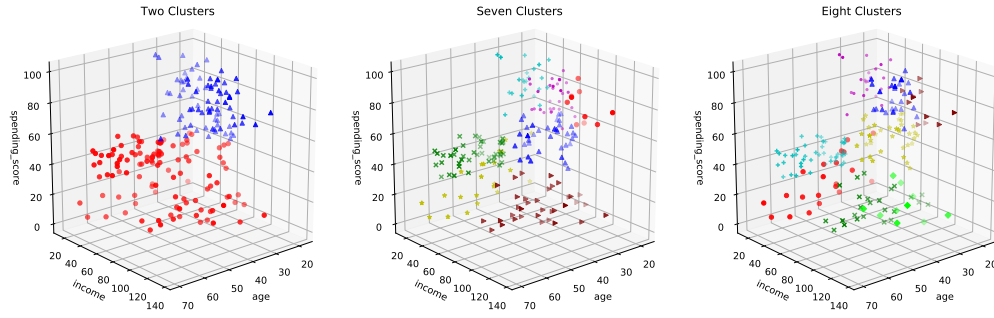
5.5.3 Housing K-Means

written by B.L.

This dataset is challenging for K-Means clustering due to the high number of features. As described in section 2.1 the concept of distance does not hold up well in high dimensional cases. Attempts to transform the data into lower dimensional representations through principle component analysis did not yield an improvement in clustering performance. Data in figure 9 suggests to consider 2 (DI), 3 (SI, DB) or 4 (CH) clusters.

Figure 9: K-Means Housing Dataset Indices by Number of Clusters
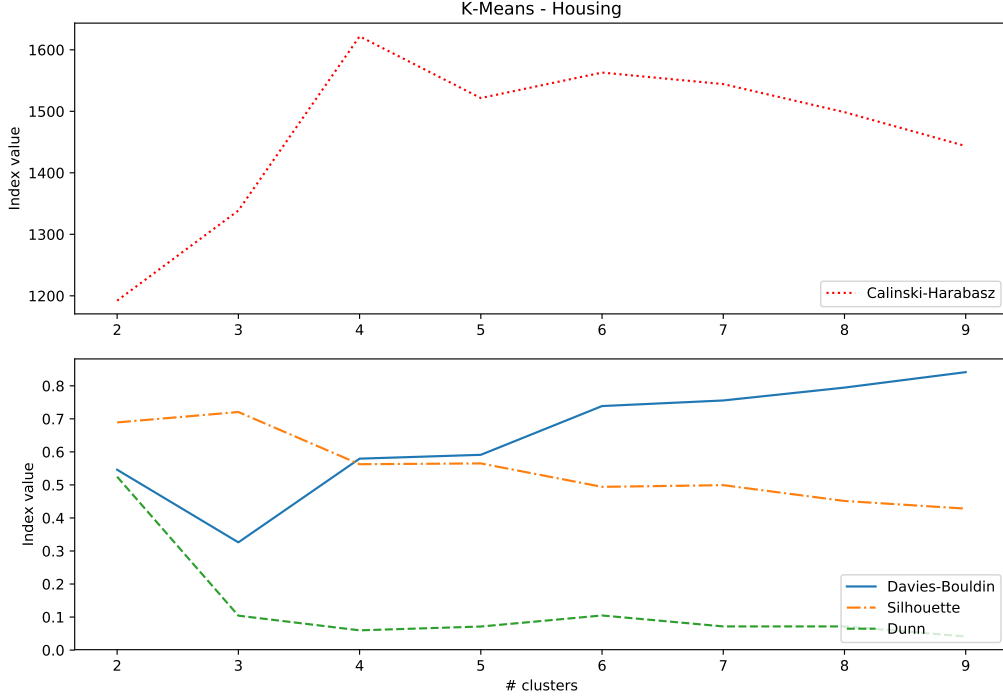
Due to the high dimensionality of the data, looking at different angles in three dimensions to get an understanding is not feasible. Therefore a two dimensional transformation (t-SNE, see section 6) will help. Figure 10 shows the case of two, three and 15 as representation for a significantly higher number of clusters. From a visual standpoint, two and three clusters seem to capture the visibly separation of parts of the data quite well, while the high cluster count suggests it might be reasonable to consider the idea of there being a much more complex underlying structure to the data which is not well captured through the method at hand.

Figure 10: K-Means Housing Dataset t-SNE Transformed Data Plot
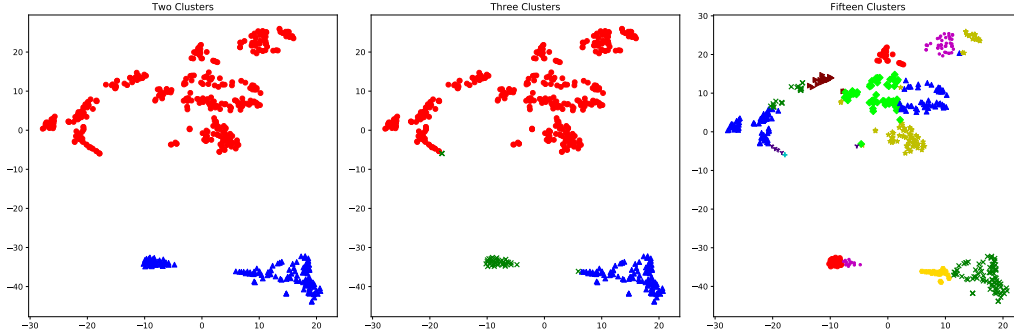
5.5.4 Wine K-Means

written by B.L.

The wine dataset again presents a challenge due to its high feature count, the highest of all the datasets in this comparison as well as having one discrete feature. Dimensionality reduction helps to speed up calculation but does not show an improvement in evaluation index performance. The plot of evaluation indices in figure 11 gives an indication for 2 (SI, DB), 3 (CH), or 6 (CH, DB) clusters but looking at the two dimensional transformed data in figure 12 does not allow for any visual evaluation concerning the quality of fit.

Figure 12: K-Means Wine Dataset Indices by Number of Clusters
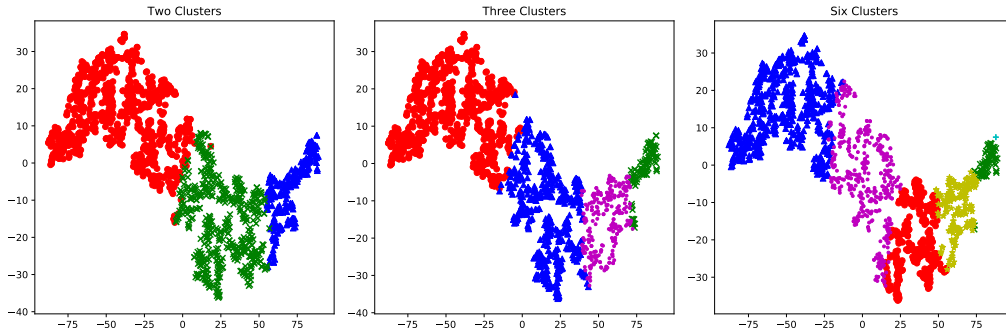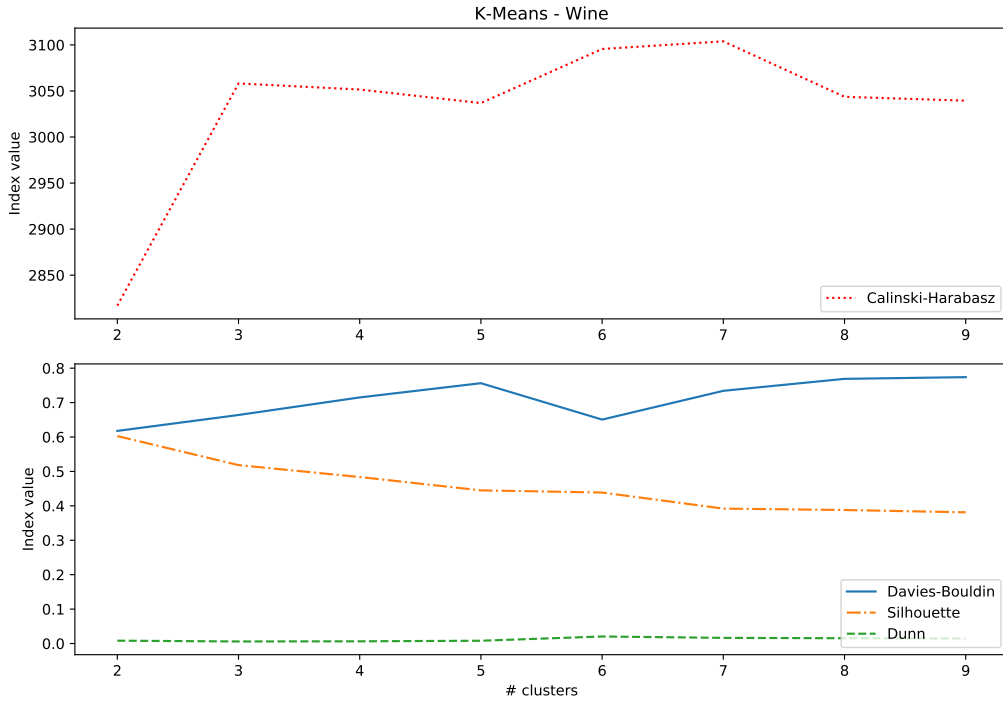
Figure 11: K-Means Wine Dataset Indices by Number of Clusters

Looking back at the PCA step mentioned before, the picture becomes clearer when utilizing it as a visualization support and looking at a three dimensional representation of the transformed data in figure 13 gives a clearer understanding of how the clustering has worked out. The component driving the differentiation between clusters called *PCA 1* captures 94% of the variance and loadings show it being driven in large part by the two *sulfur* concentration features.

Figure 13: Wine Dataset 3D Plot Clustering Options
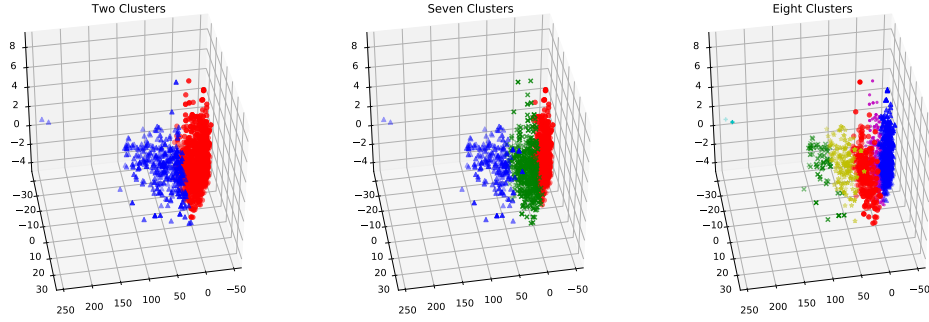
Looking at the original labeling of the data however shows the limitations of clustering and especially K-Means clustering for this data set. Figure 5.5.4 shows the same projection as figure 13 but this time with the original labeling. The math on accuracy and recall at 19.8% and precision somewhat better at 58.2% also shows the less than optimal performance. However this is not unexpected when considering the strengths and weaknesses of K-Means described in section 2.1: contiguous, non-overlapping, convex clusters can be captured well while at least this representation of the data displays a lack of these characteristics in the data set.
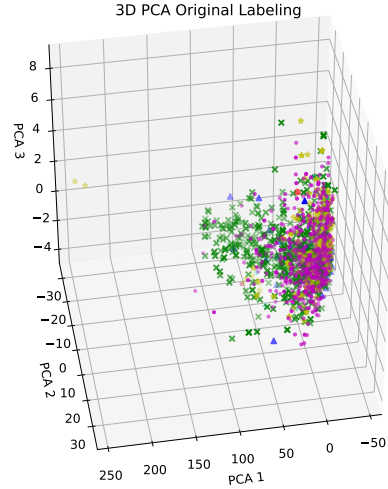

Figure 14: Wine 3D Original Labeling

6 Web Frontend and User Manual

The frontend has been developed in Streamlit [41] in its latest version as of June 18, 2021, 0.82.0 and can be accessed at `https://clustering.goethe.tech`). It provides a sidebar menu containing two dropdown lists. While the upper dropdown list can be used to select the dataset to be clustered, the second dropdown contains four different clustering algorithms to be

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applied: K-Means, Mean Shift, Spectral Clustering and Affinity Propagation. According to the selected clustering algorithm, the required input parameter can be set by dragging the slider on the respective widget. For this purpose, a message displays which kind of input parameter is required for the selected algorithm. Default values for different parameters vary with regard to the chosen dataset. We therefore provide slider widgets with different value ranges and varying default values according to the dataset to be clustered. Once dataset and clustering technique are chosen, the `Calculate` button can be clicked to run the clustering procedure. For convenience, selected dataset and algorithms are listed above the result part once again. After the dataset is clustered, a two-dimensional projection plot of all data points is displayed, distinguishing between different clusters with the help of distinct symbols and colors.

In addition to that, we provide an evaluation module which can be used to compare different clustering strategies to each other.

Our implementation is divided into segments to isolate clustering procedures from projecting the data into 2D and from visualizing the results.

Each of the clustering techniques that can be selected for grouping data points is implemented in a separate file which is named according to the technique. To run one of the clustering algorithms, the dataset has to be handed over in form of an n x m matrix consisting of n data points with m features. Moreover, a value for the algorithm specific parameter has to be provided. The `returns` parameter can be used to defined what output format is expected. We provide the possibility to distinguish between returning the fitted estimator, an n x (m+1) - matrix consisting of n data points with m features and a column containing a label for each data point or an n x 1 vector, which only includes a label for each data point. Running the clustering in its default mode, each technique returns the n x 1 label vector. For the K-Means algorithm, the additional parameter state can be chosen. This value is used to initialize the random number generator such that always the same results are yielded [26].

In the `app.py` file, we implement all the functionalities concerning the frontend elements as well as choice of dataset and clustering technique. After reading the four different datasets using the `read_csv` method provided by pandas [42,43], we calculate a cached version of the datasets projected into 2D to speed up all the following interactions. To project the datasets into 2D, we make use of the t-distributed Stochastic Neighbor Embedding (t-SNE) method provided by sklearn [26]. `t-SNE` is a method that facilitates displaying high-

dimensional data in a 2D or 3D plot and nevertheless preserving local and global structures. This is done converting Euclidean distances between all data points in high dimensions into conditional probabilities such that high probabilities are allocated to similar data points while dissimilar data points are assigned a low probability. Afterwards, the same is done for all the data points projected into lower dimensions. The optimal projection of high-dimensional data points is finally found by minimizing the mismatch between calculated probabilities between points in high and in low dimensions [**?**].

As described earlier, we not only provide dropdown lists to enable the choice of a dataset as well as a clustering technique, but also adapt the slider widget label according to the required input parameter for the chosen algorithm. We define parameter value ranges along with default values appropriate to the chosen dataset. To run the clustering procedure, we implement an event handler checking for click events on the Calculate button. According to the selected clustering algorithm, we call the respective clustering function and hand over the dataset as an n x m matrix as well as the technique specific parameter value which was selected with the help of the slider widget. In order to plot the resulting clusters, we call the `plot_tsne_2` function which we, again, implement in a separate file. In this method, we define a variety of symbols and colors to be able to distinguish between different clusters. For each data point, we check which cluster it was assigned to and connect it to the respective symbol and color. We finally create the plot showing the 2D clusters with the help of the Matplotlib visualization function `pyplot` [44]. Some screenshots like image 15 with explanation etc.

Figure 15: Frontend example screenshot
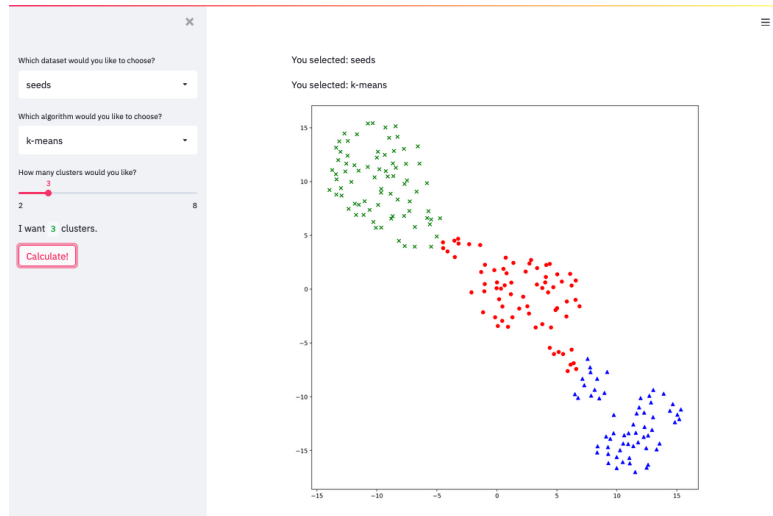
7 Conclusion

- Summarize the main points and achievements

- Add your own assessment/criticism on the topic

Acronyms

CH   Calinski-Harabasz Index.

DB   Davies-Bouldin Index.
DI   Dunn Index.

SI   Silhouette Score.
sklearn Scikit-Learn.

VRC   Variance Ratio Criterion.

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