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Attention in Mixed-Type Clustering

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Declaration of Authorship

I hereby declare that the thesis submitted is my own unaided work. All direct or indirect sources used are acknowledged as references.
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Abstract

This document serves as a model for the development of a thesis at the Department of Database Systems at the Institute for Computer Science at the LMU Munich. The abstract should not contain more than 300 words.

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Chapter 1

Introduction

1.1 Introduction

Clustering is an unsupervised machine learning method that groups similar observations together. Due to its ability to find patterns in an unlabeled dataset, its an essential task in Data Mining and Knowledge Discovery. A *cluster* is a group of similar instances that belongs to a *centroid* (center point of a cluster). Distance-based clustering algorithms use distance measures such as Euclidean distance to calculate the similarity of datapoints. Hierarchical methods partition the instances and merge (agglomerative) or split them into bigger or smaller clusters. Many other methods exist, but this work focuses on methods for clustering *mixed-type* data. [1]

1.2 k-means

The most well known distance-based clustering method is k-means [11]. The goal is defined as follows: Suppose we have a finite set of n instances $S = \{p_1, p_2, ..., p_n\} \in \mathbb{R}^m$ for a dataset with m features, the target of k-means is to find optimal centroids $B = \{b_1, b_2, ..., b_k\} \subseteq \mathbb{R}^m$ for a given $k(\leq n) \in \mathbb{N}$ that minimize the sum of the squared Euclidean distance of each point in S to its nearest centroid. Formally

$$\sum_{i=1}^{n} d(p_i, B)$$

has to be minimized, where d is the Euclidean distance from a point $p_i \in S$ to the nearest centroid in B [12]:

$$d(p_i, B) = min_{1 \leq j \leq k} d(p_i, b_j)$$

The Euclidean distance between two points p and q in an n-dimensional Euclidean space is defined as

$$d(p,q) = ||p-q|| = \sqrt{(p_1-q_1)^2 + (p_2-q_2)^2 + ... + (p_n-q_n)^2}$$

Finding the optimal centroids is a NP-hard problem, even for $d = 2$, as shown by Mahajan et al. [12]. The most common algorithm used for the k-means problem is a iterative refinement technique proposed by Lloyd [10]. It is defined as follows

1. Randomly set k initial cluster centroids $b_1^{(1)}, ..., b_k^{(1)}$.
2. Assign each obseration p_i to the nearest centroid using squared Euclidean distance. This splits our instances into S into k sets $\{S_1^{(t)}, ..., S_k^{(t)}\}$.
3. Recalculate the optimal position of each centroid using the mean distance to each instance assigned to the centroid:

$$b_i^{(t+1)} = \frac{1}{|S_i^{(t)}|} \sum_{p_j \in S_i^{(t)}} p_j$$

4. Repeat steps 2. and 3. until the centroid assignments no longer change.

1.3 Mixed-type data

In many real-world scenarios, besides continuous, numerical data, *categorial* data exists. While Euclidean distance or other distance measures work well with continuous data, categorial data is different. Suppose we have categories $\{A, B, C\}$ of a given feature, we would encode them into numeric values to allow for computation of a distance measure:

$$\{A, B, C\} \equiv \{1, 2, 3\}$$

While A and C can share the same semantic similarity as A and B, numerically category A and Category C are now $|1-3| = 2$ apart, while Category A and B are only $|1-2| = 1$ apart. During clustering, this could lead to instances being assigned to centroids based on a wrong distance assumption.

A possible solution is to use *one-hot encoding*, also known as *dummy coding* in classical statistics. One-hot encoding turns a discrete feature containing k mutually exclusive categories into a vector x of length k, in which only one of the elements x_k equals 1 and all remaining elements equal 0 [3]. For an instance B of a feature having $k = 3$ separate categories $\{A, B, C\}$, the one-hot vector x would be represented by $x = (0, 1, 0)^\intercal$.

1.3.1 k-modes

According to Huang [6], one-hot encoding has two drawbacks:

1. In real-world applications, categorial features with hundreds or thousands of categories are encountered. This would result in a large number of binary features in the one-hot encoded representation, which will increase cost and space of computation.

2. The centroid value of a certain one-hot encoded feature, given by a real value between 0 and 1, cannot indicate the characteristics of the according cluster, since the feature only describes the presence or absence of one category.

Therefore, Huang [6] proposed using the Kronecker-Delta as a dissimilarity measure between multiple categorial columns. Formally, if we have two instances X and Y of a dataset with m categorial features, d_1 will count the number of mismatches between the categorial features of both instances, defined as

$$d_1(X, Y) = \sum_{j=1}^{m} \delta(x_j, y_j)$$

where the Kronecker delta $\delta(x_j, y_j)$ is defined as

$$\delta(x_j, y_j) = \begin{cases} 0 & (x_j = y_j) \\ 1 & (x_j \neq y_j) \end{cases}$$

If we have a finite set of n instances $S = \{p_1, p_2, ..., p_n\}$ for a dataset with m categorial features, the goal of *k-modes* [6] is to find optimal *modes* $B = \{b_1, b_2, ..., b_k\}$ for a given $k(\leq n) \in \mathbb{N}$ that minimize

$$\sum_{i=1}^{n} d_1(p_i, B)$$

where

$$d_1(p_i, B) = min_{1 \leq l \leq k} \sum_{j=1}^{m} \delta(p_{i,j}, b_{l,j})$$

Similar to k-means, we can use an iterative algorithm for efficient computation [6]:

1. Randonly choose k instances from the dataset as initial modes for the clusters.

2. Assign each instance to their nearest mode using the proposed dissimilarity measure one by one and update the mode of each cluster after each assignment.

3. Test if each instance still belongs to its assigned mode, i.e. if each instance is assigned to its nearest mode. If the instance would belong to a different mode, reassign the instance and update the modes of both clusters.

4. Repeat step 3. until the mode assignments no longer change.

1.3.2 k-prototypes

As proposed by Huang [6], it is straightforward to combine the k-means and k-modes algorithms into the *k-prototypes* algorithm, which can be used to cluster *mixed-type* data (consisting of numerical, continuous and categorial features). The dissimilarity between two instances X and Y with features $A_1^r, A_2^r, ..., A_s^r, A_{s+1}^c, ..., A_m^c$, where features $A_1^r, ..., A_s^r$ are continuous and features $A_{s+1}^c, ..., A_m^c$ are categorial, is defined as

$$d_2(X,Y) = \sum_{j=1}^{s}(x_j - y_j)^2 + \gamma \sum_{j=s+1}^{m} \delta(x_j, y_j)$$

The first part of the equation is the Euclidean distance as used in k-means, while the second part is taken from the k-modes algorithm. Huang [6] states: "The weight γ is used to avoid favouring either type of attribute".

Again, we need to find k optimal centroids $B = \{b_1, b_2, ..., b_k\}$ and therefore have to minimize

$$\sum_{i=1}^{n} d_2(p_i, B)$$

where

$$d_2(p_i, B) = min_{1 \leq l \leq k} \sum_{j=1}^{s}(p_{i,j} - b_{l,j})^2 + \gamma \sum_{j=s+1}^{m} \delta(p_{i,j}, b_{l,j})$$

We can minimize both distance measures at the same time since they are nonnegative. Therefore, we can use the same algorithm as defined in 1.3.1. [6]

1.3.3 Gower distance

Gower distance [5] is a general similarity measurement between instances containing mixed-type features. It is defined as follows: When comparing instances x_i and x_j, for each feature k of p total features, we calculate a score

SCORES AND VALIDITY OF DICHOTOMOUS CHARACTER COMPARISONS

	Values of character k			
Individual i	+	+	−	−
j	+	−	+	−
s_{ijk}	1	0	0	0
δ_{ijk}	1	1	1	0

Figure 1.1: Score s_{ijk} and quantity δ_{ijk} of a feature k on two instances x_i and x_j. Presence of a feature is denoted by "+" and absence by "-". [5]

$s_{ijk} \in [0, 1]$. The score will be close to 1 for two instances x_{ik} and x_{jk} of a feature k if they are similar, and close to 0 they are not similar. Gower distance is also computable between instances with missing values, therefore a quantity δ_{ijk} is calculated, which is equal to 1, when feature k can be compared across the two instances x_i and x_j, and 0 otherwise (illustrated in Figure 1.1). Gower distance then is the average of the known score

$$S_{ij} = \frac{\sum_{k=1}^{p} s_{ijk}\delta_{ijk}}{\sum_{k=1}^{p} \delta_{ijk}}$$

The Score s_{ijk} is calculated differently according to the type of feature [5]:

1. For *dichotomous* (when a value is either present or absent) features, the score s_{ijk} is 1 when the value is present in both features and 0 otherwise, as shown in Figure 1.1.

2. For categorial features, the score s_{ijk} is 1 if they both instances match on feature k and 0 otherwise.

3. For continuous features the score is calculated as

$$s_{ijk} = 1 - \frac{|x_i - x_j|}{R_k}$$

   where R_k is the range of feature k in the dataset or in the sample.

Gower [5] has shown that $\sqrt{1 - S_{ij}}$ is a valid distance representation for two instances x_i and x_j. We can now convert our similarity matrix S into

a distance matrix and are able to use Hierarchical clustering methods [7]. Philip and Ottaway [19] used Gower distance with agglomerative clustering. Agglomerative clustering places each object into its own cluster and recursively merges the clusters together using the given distance matrix, until only the specified number of clusters is remaining [7].

1.4 Methodology

In this work we use 8 mixed-type datasets from the UC Irvine Machine Learning Repository [13]. The Abalone dataset [16] contains physical measurements from abalones. It has 4177 instances, one categorial feature and seven continuous features. The Auction Verification dataset [17] has 2043 instances that contain verification runs of multi-round auctions. It is composed of six categorial and one continuous feauture. The Bank Marketing dataset [15] is related to a direct marketing campaign of a portuguese banking institution. It has 49732 instances. The "age", "day" and "month" features were removed, which results in eight categorial and five continuous features. The Breast Cancer dataset [23] contains 699 instances and 9 categorial features. The Census Income dataset [9] has a total of 48842 instances. It is composed of eight categorial and 6 continuous features. The Credit Approval dataset [20] contains information of applications for credit cards. It has 690 instances, nine categorial features and six continuous features. The Heart Disease dataset [8] is composed of four datasets and has 920 instances in total. It has seven categorial features and six continuous features. The Soybean (Large) Dataset [16] consists of 683 instances from soybeans with a certain disease and has 35 categorial features.

All instances containing missing values were removed. Duplicate instances were explicitly not removed, since there is no information available if they are duplicates by accident, or real duplicates. Categorial columns were standardized by removing the mean and scaling to unit variance, using the scikit-learn Python API [18]. Formally, the standardized score z of a sample x from a feature is calculated as

$$z = \frac{(x - \mu)}{\sigma}$$

where μ is the mean of the samples $x_1, ..., x_N$ from a feature of length N, defined as

$$\mu = \frac{1}{N} \sum_{i=1}^{N} x_i$$

	Naive k-means	k-means one-hot	k-prototypes	Gower distance
Abalone	0.171795	**0.173982**	0.171639	0.161416
Auction Verification	**0.016172**	0.007087	0.007667	0.006170
Bank Marketing	0.019781	**0.026060**	0.019522	0.001334
Breast Cancer	**0.746818**	0.736310	0.592480	0.553707
Census Income	0.108029	**0.184979**	0.141737	0.004259
Credit Approval	**0.313076**	0.171038	0.116579	0.003465
Heart Disease	**0.204577**	0.164486	0.189264	0.140792
Soybean Disease	0.672229	**0.710164**	0.567635	0.669526

Figure 1.2: Comparsion of Normalized Mutual Information of various classical methods on clustering mixed-type datasets.

	Naive k-means	k-means one-hot	k-prototypes	Gower distance
Abalone	0.135265	0.131434	0.134307	**0.195356**
Auction Verification	0.664709	0.576114	0.580519	**0.800783**
Bank Marketing	0.779600	0.786600	0.787200	**0.884200**
Breast Cancer	**0.960469**	0.950220	0.915081	0.900439
Census Income	0.608200	0.697600	0.625600	**0.768400**
Credit Approval	**0.808576**	0.705972	0.666156	0.548239
Heart Disease	0.334448	0.321070	0.424749	**0.565217**
Soybean Disease	0.576512	**0.599644**	0.471530	0.501779

Figure 1.3: Comparsion of Cluster Accuracy of various classical methods on clustering mixed-type datasets.

and σ is the standard deviation of the samples of a feature, defined as

$$\sigma = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(x_i - \mu)^2}$$

The datasets were shuffled. For all random operations, a random state of integer value 0 was used to ensure reproducibility.

1.5 Comparison of classical Clustering methods

Chapter 2

Neural Networks

The idea of computation by neurons inspired by the human brain was first formalized into a mathematical model by McCulloch [14]. A *neuron* was defined as a element that takes multiple boolean inputs and has one boolean output. The neuron *fires*, meaning the output is set to true, when the sum of the input values extends a certain threshold.

The single-layer *perceptron*, the first neural machine learning algorithm, was invented by Rosenblatt in 1957 [21]. Formally, the binary valued output o_j given an input vector x_i is calculated as

$$o_j = \begin{cases} 1 & \sum_i w_{ij} x_i + b > 0 \\ 0 & otherwise \end{cases}$$

where w is the learnable weight matrix, and b is a predefined bias. For training, the weights w are simply incremented when the output is 0 but the ground truth is 1, and decremented if the output is 1 but should be 0. If the output was predicted right, no weights are changed.

The idea of neural networks was revived three decades later, using multiple perceptron layers and a differentiable error function [22]. In a multi-layer neural network, we have an input layer, an output layer and multiple hidden layers. Each layer is a collection of neurons, that acquire the outputs of each neuron from the previous layer (or from the input in case of the input layer) as their input, and produce a new output. Formally, the output a_j of the jth neuron of layer n that gets d input values from the previous layer is defined as

$$a_j = \sum_{i=1}^{d} w_{ji}^{(n)} x_i + b_j^{(n)}$$

where $w_{ji}^{(n)}$ is the learnable weight of the input x_i going through neuron j in layer n [2]. A bias b_j is also added. This output is commonly refered to as

an *activation* of a neuron [2]. Because every neuron is a linear function, in order to avoid the collapse of each neuron from all layers into a single linear function, we pass the activation a_j into a non-linear activation function f

$$z_j = f(a_j)$$

before being passed to the next layer of neurons [4].

As shown in a recent survey [4], there are many different activation functions used in neural networks. A simple example for an activation function, which naturally alligns with the idea of a biological neuron firing is the *step function* (also known as *Heaviside step function*) [2], that ouputs 0 for negative values and 1 for positive values:

$$\text{step function}(x) = \begin{cases} 1 & x \geq 0 \\ 0 & otherwise \end{cases}$$

In order to stay between 0 and 1, but also utilize all real values inbetween, another activation function that has historicaly been popular is the *logistic sigmoig* function [4], that squashes any input in $]0, 1[$:

$$\text{logistic sigmoid}(x) = \frac{1}{1 + e^{-x}}$$

Because the ouputs are in a range close to 0, it is prone to the *vanishing gradient problem*. In the vanishing gradient problem, a gradient that is very close to 0 leads to almost no update in the weights of the network during training. Moreover, using a exponential value naturally leads to a greater computational complexity. [4]

The current state-of-the-art activation function, the *Rectified Linear Unit* (ReLU) [4], is not limited by the above disadvantages. It is simple and computationally performant. It is defined as the identity for positive values and as 0 for negative values:

$$\text{ReLU}(x) = max(0, x) = \begin{cases} x & x \geq 0 \\ 0 & otherwise \end{cases}$$

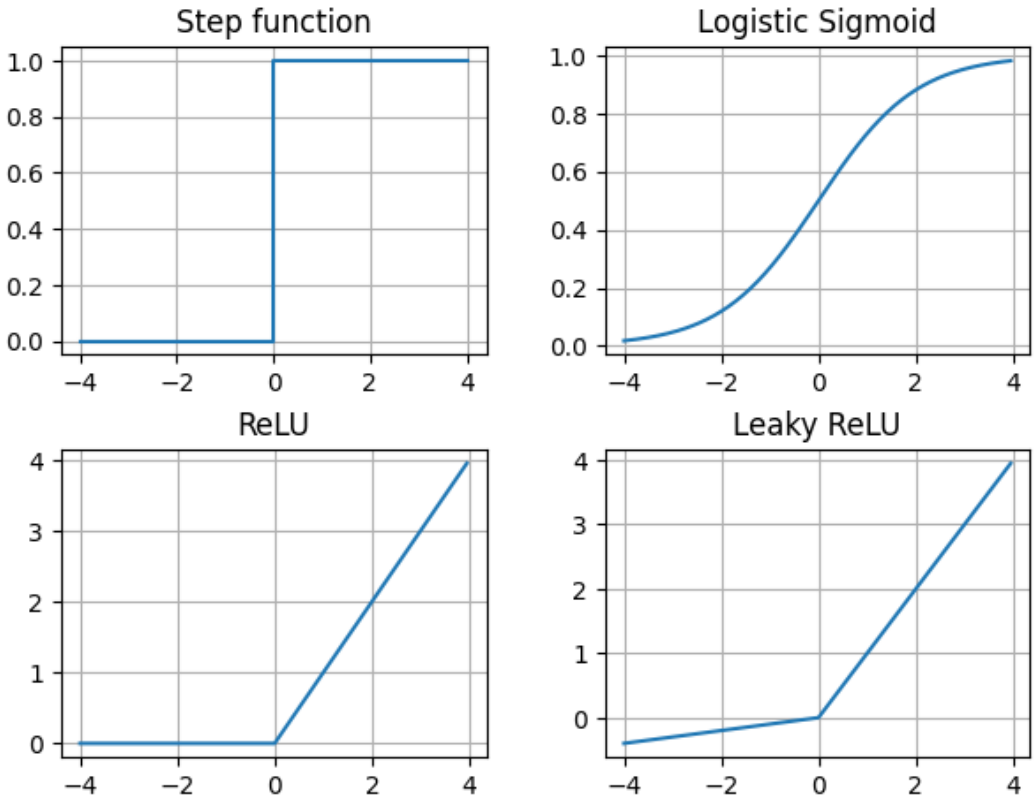

Figure 2.1: An illustration of the step function, the logistic sigmoid, the ReLU and the Leaky ReLU activaiton functions.

Chapter 3

Autoencoders

Chapter 4

Deep clustering methods

Chapter 5

Attention

5.1 Comparison of deep clustering methods

Chapter 6

Conclusion

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