

# Master Thesis

Topic:

Unsupervised learning in decision making

<b>Author:</b>	Domagoj Fizulic Felix Gutmann
<b>Student number:</b>	125604 125584
<b>Program:</b>	M.S. Data Science
<b>E-Mail:</b>	domagoj.fizulic@barcelonagse.eu felix.gutmann@barcelonagse.eu

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## **IV List of Listings**

## V List of mathematical symbols

Symbol	Meaning
$a_t$	Action at time t
$Q(a)_t$	Value function at time t
$\epsilon$	Probability of exploration in epsilon greedy
$\alpha$	Learning rate
$\tau$	Softmax parameter
$X$	Random variable
$H(X)$	Entropy of a discrete random variable $X$
$d(\cdot, \cdot)$	Distance Function
$S(\cdot, \cdot)$	Similarity Function
$\mathbb{R}_0^+$	Positive real numbers including zero
$\mathcal{X}$	Data set
<b>W</b>	Weighted adjacency matrix
$d_i$	Degree of node $i$
<b>D</b>	Diagonal matrix of degrees
<b>L</b>	Graph laplacian

## VI List of abbreviations

Abbreviations	Description
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# 1 Introduction and conceptual approach

Learning is a complex procedure. The learning procedure can be affected due to social conditions... Due to their mental ability people should show different learning behavior. The decision making process is studied by monitoring people's sequential choices in a controlled experiment environment.

In *supervised learning* data are predicted by training a classifier based on features and corresponding categories. In comparison to that in *unsupervised learning* we don't know the ground truth. The objective is to discover natural clustering behavior in the data. [Murphy, 2012, page 9 et. seqq.] and group objects into subsets, such that objects in those subsets are more closely related to each other [Hastie et al., 2001, page 501]. A vast class of clustering algorithms based on different approaches are proposed in the literature (e.g. hierarchical, and optimization based clustering). A detailed overview of the algorithms and corresponding distance and similarity concepts is provided in section 3.3.

This paper investigates, whether such unsupervised learning techniques can be used in the context of human decision making process to identify latent grouping. This paper operates in the intersection of machine learning and cognitive science. To our knowledge this particular setting has not been studied before.

To approach this issue, we first set up a reinforcement learning based simulation framework to study theoretical boundaries of several clustering techniques and when they are applicable. Subsequently, we test our chosen methods on several real world data sets. Corresponding to our simulation framework we first apply clustering algorithms on a real n-armed bandit experiment.<sup>1</sup> A widely used approach to monitor human decision making process is the *Iowa gambling task*, where participants try to maximize rewards by choosing from different decks with different reward structures.<sup>2</sup> Within that framework we analyse data from people with different criminal profiles. Furthermore, we use data from cocaine abusers.

The report has the following structure. In section two we provide a short overview of related literature in the field.

The following section three is dedicated to the theoretical foundation and the simulation. Therefore, we first provide knowledge of reinforcement and line out our experiment design in more detail. This section also includes an overview of applied algorithms,

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<sup>1</sup>A detailed introduction is given in section 3.2

<sup>2</sup>There are existing several slightly different versions of test. [Steingroever et al., 2015] provides a data collection for from several sources giving a broad overview of different variations of the test.



similarity and distance concepts. Finally, we study their simulation performance and try to identify situations where they are applicable.

The rest of this paper is dedicated to the data sets. Our data sets are studied before from a cognitive science perspective. We introduce relevant concepts such as expectancy valence models and compare the findings of the authors to the results we obtain from the clustering algorithms.

We try to keep the scope of this paper tight and there are some open questions left. Thus we dedicated another section to discussing some possible extensions. We close this paper with a final summary of our results. A mathematical formulation of the applied algorithms, applied algorithms, similarity measures and cluster evaluation techniques.<sup>3</sup>

## 2 Relevant Literature

There exists a rich literature in cognitive science on identifying different behavioral groups. As mentioned in the introduction a commonly applied tool is the Iowa Gambling Task experiment. It has been shown that individuals with pre-frontal brain damage and decision-making defects continue to choose disadvantageously even after they learned the optimal strategy [Bechara et al., 1997].

A broad overview on various results in the field can be found in [Steingroever et al., 2013]. Several studies identify especially specific drug-user groups, e.g. cocaine addicts [Stout et al., 2004], chronic cannabis users [Fridberg et al., 2010], heavy alcohol users (heavy drinkers) [Gullo and Stieger, 2011]. Furthermore, extensive set of research is focused around particular mental disabilities, e.g. Asperger's disorder [Johnson et al., 2006], psychopathic tendencies [Blair et al., 2001], bipolar disorder [Brambilla et al., 2012], schizophrenia [Martino et al., 2007] pathological gambling disorder [Cavedini et al., 2002], attention-deficit-hyperactivity disorder [Nirit Agaya, Eldad Yechiama, Ziv Carmelb, 2010]. Most popular reinforcement learning models for identifying behavioural differences between different disorders are Expectancy Valence model [Busemeyer and Stout, 2002] and Prospect Valence Learning model [Ahn et al., 2008].

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<sup>3</sup>Since our data are fairly small we will not discuss complexity of the algorithms.

### 3 Theoretical Background and simulation experiments

This section is dedicated to a more detailed outline of our analysis approach and the results of our simulation experiments. The data we are analysing are gathered by observing peoples decisions over time. Hence, our data set are in the form  $N \times M$  data set, where a row  $N$  is the number of individuals and  $M$  is the number of trials in the experiments. The data for each individual can be seen as a categorical time series. In terms of modeling there are two challenges. Some algorithms relying on euclidean distance while others operating on similarity concepts. On one hand we introduce how repress those data and introduce related distance and similarity concepts for the algorithms. The section has a rather qualitative character. The appendix provides in more detail a mathematical background to applied algorithms, distance concepts and related clustering evaluation techniques.

#### 3.1 Experiment design and problem formulation

Figure 1 depicts our simulation design.<sup>4</sup> The objective is to obtain a set of sequential choices for a given parameter setting of the artificial agent. We first generate a set of rewards by sampling from  $n$ -vectors from a normal distribution ("*multi arm bandit*"). The agent processes those rewards by sequentially choosing from those  $n$ -vectors. We repeat this procedure for several parameter settings for the agents and keep track of those choices which will define our data set.

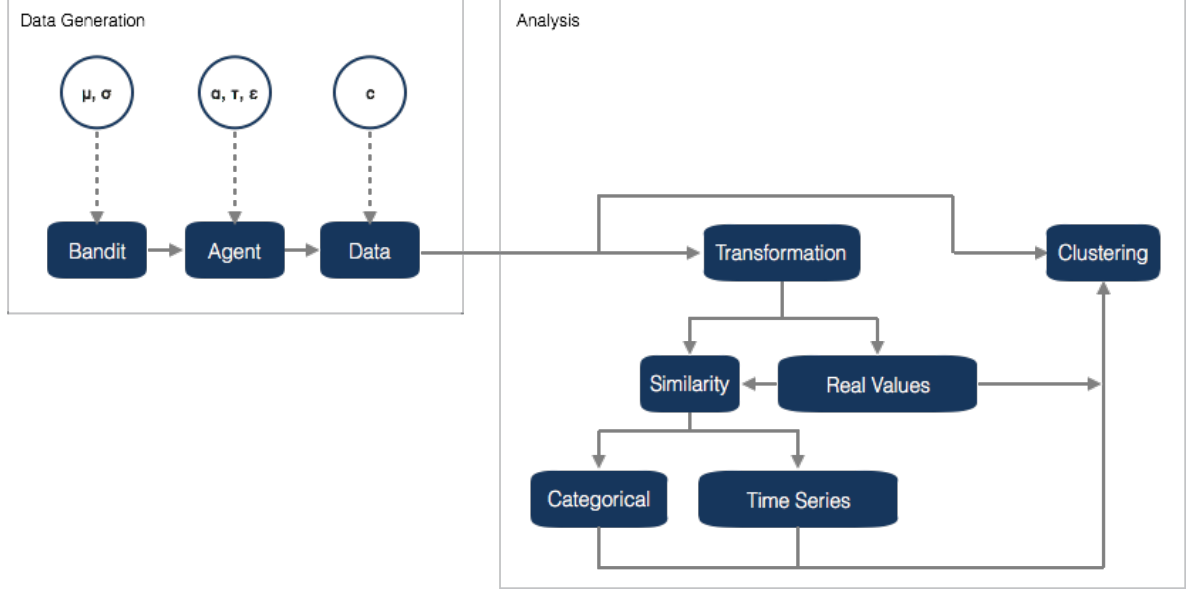
#### 3.2 Reinforcement Learning background and multi arm bandits

In the following we provide some basic background of *Reinforcement Learning* (RL). The following definitions coming from [Sutton and Barto, 2012, chapter 1 and 2]. RL is a branch of *machine learning* try model how an artificial agents interact with its environment and learns from the process over time.

In our particular setting the agent is confronted with the task of choosing sequentially from a set of possible choices. The doesn't have any knowledge about the system a priori. Therefore, it has to learn the nature of the system by sequentially interacting with its environment and keeping tack of the obtained information. Because of the lack of examples it has to explore different possible actions to identify the best action.

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<sup>4</sup> We implemented related coding for this project mainly in python. The code can be found on our github repository.



**Figure 1:** Flowchart experiment design

Hence, it is useful to deviate from time to time from the current optimal strategy. It is necessary for the agent to keep track and updates the value of a each state it discovered so far. This is done by defining a value function for each state or action  $a$ . Denote the value function of an action  $a$  as  $Q_t(a)$  and define it as:

$$Q_t(a) := \frac{R_1 + R_2 + \cdots + R_{K_\alpha}}{K_\alpha} \quad (1)$$

where  $R$  denotes rewards. Hence the value function is the average over the rewards for a given state. The main task of the agent is to balance *exploration* and *exploitation* of the environment. There are two basic approaches to model this trade-off; An "*Epsilon-Greedy*" action selection method and "*Softmax*" selection method.

Considering epsilon greedy action selection method: The rule is to select the next action with the highest value function. However, to model exploration we introduce a random element to deviate from that greedy strategy with a certain probability denote by  $\epsilon$ . In general we can define the next action selected by the epsilon greedy strategy as:

$$a_{t+1} = \begin{cases} \text{random action} & , \text{ with probability } \epsilon \\ \arg \max_i Q_t(i) & , \text{ with probability } 1 - \epsilon \end{cases}$$

In the softmax action selection method each next action is sampled from with a certain probability coming (*Boltzmann Distribution*). The probability for action  $a$  is computed

by:

$$P(a_t|X) = \frac{e^{\frac{Q_t(a)}{\tau}}}{\sum_i^K e^{\frac{Q_t(i)}{\tau}}}$$

In each iteration the next action of the agent is drawn with probability  $p_a$ :

$$a_{t+1} \sim p_a$$

After selecting an action the agent is updating its believe of the chosen action. One can show that equation (1) can be expressed in the following way:

$$Q(a)_{k+1} = Q(a)_k + \alpha [R(a)_k - Q(a)_k],$$

where  $\alpha$  is a is the non negative *learning rate* defining how much the current action is affecting the believes.

### 3.3 Unsupervised learning methods, data handling and similarity

As mentioned we find two main challenges. First, our data have a categorical nature. Furthermore, the learning process also imposes a time series dependence on the data. A well studied approach clustering such data are *hidden markov models*. For example a decent research on that can be found in [Pamminger, 2007], [Pamminger and Fruhwirth-Schnatter, 2009] and [Pamminger and Fruhwirth-Schnatter, 2010]. However, we focus our attention only on partition based clustering algorithms.

Some of applied algorithms operate on different distance or similarity concepts. Given our data we have to think carefully think about distance and similarity measures to respect the nature of our data and algorithms.<sup>5</sup> In extension to only considering raw choices we might try to re-express our data to discriminate them according to different purposes. The first approach is to map the series of choices to a real valued series. One way is to consider *Shannon's Entropy* introduced by [Shannon, 1948] based on the empirical probability of the choices. For a discrete random variable  $X$  with probability  $p$  the entropy is defined as [MacKay, 2005, page 32]:

$$H(X) ::= - \sum_{i=1}^N p_i \log_2 p_i \quad (2)$$

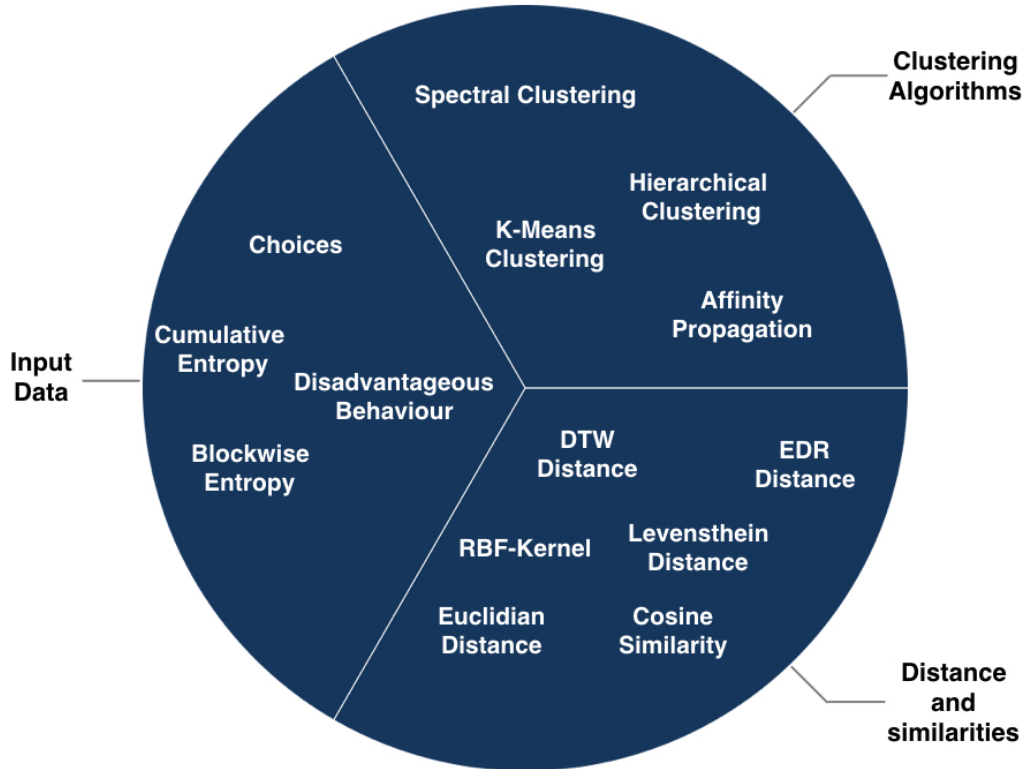
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<sup>5</sup>A formal definition of the distance and similarity can be found in the appendix

Entropy gives measure on how random a random variable behaves.<sup>6</sup> Within the entropy framework we consider to types of entropies. For each time step we compute the entropy using choices done so far. We call this *cumulative entropy*. Furthermore, we might want to observe more clearly how individuals adapt their behavior over time. Considering an experiment with 100 trials we then compute the entropy for set of ten choices. We call this *blockwise entropy*. Mapping choices to an entropy based data set is therefore aims to discriminate individuals by their level randomness in their behavior.

A second approach is based on the experimental setting. We know within the framework there are a set of choices which are disadvantageous for the participant. Following e.g. [Yechiam et al., 2008] or [Ahn et al., 2008], we then compute block wise the ratio of disadvantageous choices. We call this *disadvantageous choice*.

Within our analysis we consider a broad selection of several clustering techniques and similarity concepts. Figure 2 shows an overview of the algorithms and their corresponding distance/similarity requirements. A technical description for all of them is provided in the appendix. According to our different data types and for our different algorithms



**Figure 2:** Input data, algorithms and proximity measures

<sup>6</sup>In case we get a value for  $X$  such that  $p_i = 0$ , we set  $H(X) = 0$  [Bishop, 2006, page 49]

we apply the following distance and similarity concepts.<sup>7</sup>

### 3.4 Simulation results

The following table shows a snippet of our simulation results. We have a broad range of similarity measures. Some of them are task specific meaning being designed for either categorical or time series data or both.<sup>8</sup>

We also considered some specialised articles. [Garcia-Magarinos and Vilar, 2014] provide an algorithm to cluster categorical time series.

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<sup>7</sup>Note that distance and similarity can be converted according to equation (3) in the appendix

<sup>8</sup>For example Levenstein distance (or edit distance) is a basic way to measure similarity between categorical sequences [?, page 1]Richter or [Gabadinho et al., 2009, page 2], however some authors stating that it might perform poorly in their task [Ren et al., 2011, page 3] or a poor measure at all [Morzy et al., , page 5]

Specification	$\mu$	$\sigma$	CL Size	SD	Decision	$\alpha$	$\tau$	N	ALG	TRNS	MI	NMI	AMI	CS	HS	VMS
1	-	-	-	-	-	-	-	-	-	-	-	-	-	-		

Table 1: Overview Outcome

## 4 Data Analysis

Our simulation result suggested that we can cluster the decision behavior under some give constraints. We apply our approach to different real data sets. In total we are considering three different data sets. As mentioned in the introduction the Iowa gambling task is popular way to monitor decision and learning process of individuals. In the simulation setting we initially define participants with a certain set of parameters. There exist techniques to estimate those parameters from actual data.

### 4.1 Recover cognitive parameters

### 4.2 Prison data and approach

With acknowledgment to [HERE WE ADD THE GUY] we were provided with experimental data from [Yechiam et al., 2008]. We try to apply our methods to cluster different groups in the data. The participants had to perform the Iowa gambling task (detailed description see later on). [Steingroever et al., 2015] assembled a collection of data of healthy individuals performing the IGT test from various sources. We extended the data set we got with a set of healthy people, which we hope will behave significantly different than the individuals with criminal profile.

#### 4.2.1 Data summary and experimental design

In particular we have data of 96 individuals with different criminal profile. Table 2 gives a broad summary of some demographics.

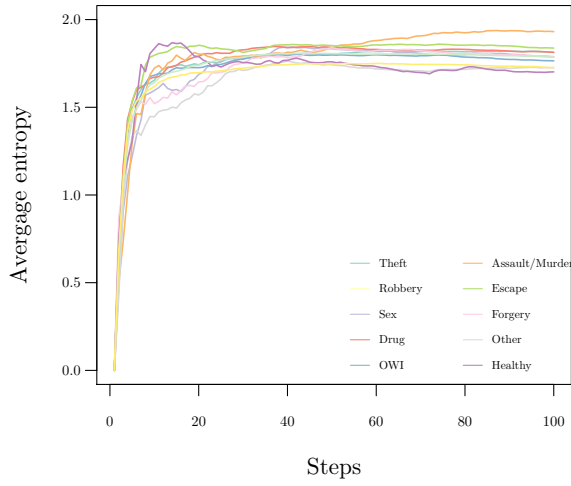
Propositi had to perform the *Iowa gambling task* (IGT), where they have to pick sequentially a card from four different decks. Two decks have distributions with negative expectations while two have positive. However, they different according to their variance.

Figure 3 (a) shows the average cumulative entropy averaged across groups. We observe a random behavior independent from group affiliation. However, normal people show the least random behavior. Furthermore, Figure 3 (b) shows the average people of negative choices people chose over steps of ten periods averaged across groups.

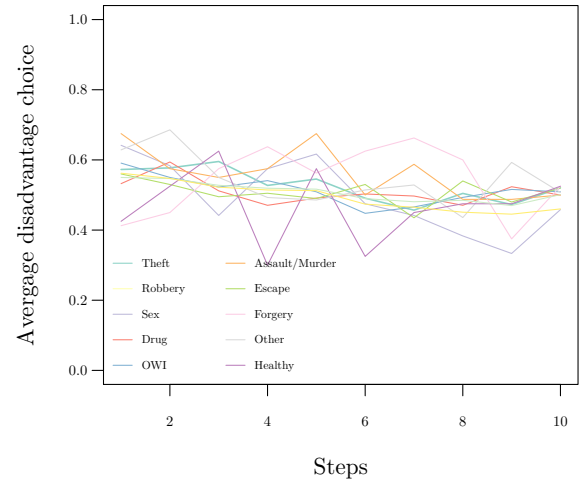
#### 4.2.2 Prison results

Following the last section we provide a summary of our results.

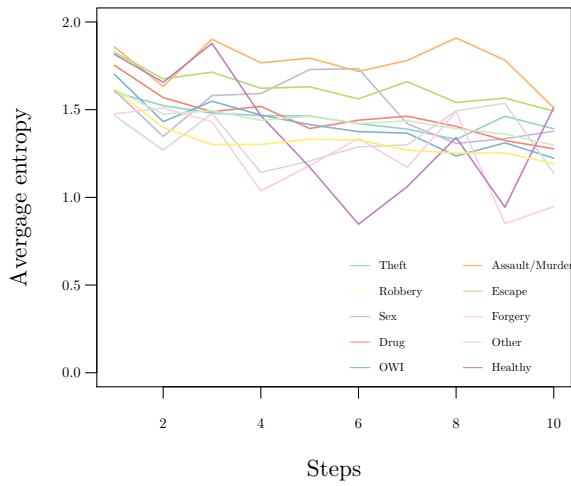




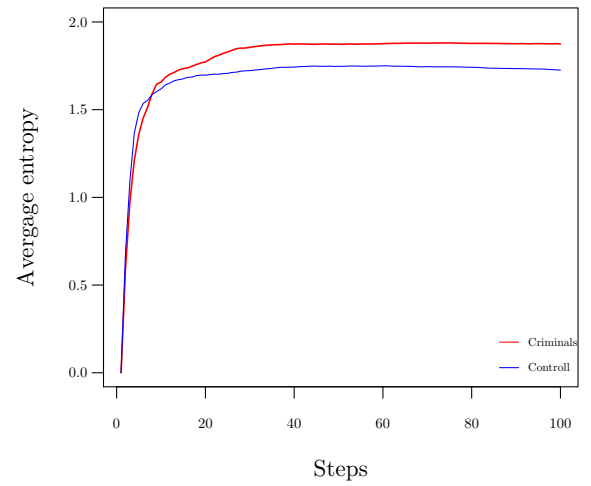
(a) Average Entropy across groups



(b) Blockwise picks from disadvantageous deck



(c) Average Entropy across groups



(d) Blockwise picks from disadvantageous deck

**Figure 3:** Average py and disadvantageous behavior

Crime	Count	Age	TABE Score	Education	Beta IQ
Theft/Burglary	22	25.36 (7.03)	11.09 (1.29)	7.38 (3.34 )	92.91 (14.37)
Robbery	6	24.17 (9.83)	11.00 (0.63)	9.22 (3.30)	96.50 (7.58)
Sex	17	33.41 (13.59)	10.97 (1.47)	9.15 (2.98)	99.65 (11.74)
Drug	22	30.91 (10.11)	11.64 (1.85)	9.06 (2.70)	100.36 (12.92)
OWI	4	38.75 (7.27)	10.88 (1.93)	7.12 (1.17)	94.25 (10.40)
Assault	10	27.20 (8.77)	12.30 (2.41)	7.62 (2.28)	94.50 (11.29)
Escape/ Failure To Appear	4	2.008 (5.60)	11.00 (1.35)	7.78 (3.21)	96.50 (14.18)
Vandalism	1	18.00 (NA)	11.00 (NA)	9.40 (NA)	90.00 (NA)
Forgery	7	34.57 (13.14)	10.93 (5.15)	9.83 (3.82)	100.71 (11.01)
Probabition	1	38.00 (NA)	12.00 (NA)	6.30 (NA)	92.00 (NA)
Other	2	35.00 (9.90)	11.50 (0.00)	9.20 (4.67)	95.00 (5.66)

**Table 2:** Summary prision data (means with standard deviation in parenthesis)

### 4.3 Multi-arm Bandit Data

The second data set we are considering are related to [Stojic et al., 2015]. In this setting we consider a 20-arm bandits situation. The data were gathered online were users were compensated with small amount of money. Four different distributional settings were given to different people. In total the data sets consists of 429 participants divided in 199 female and 229 male participants.<sup>9</sup> The average age 33.04 with standard deviation 11.75. Furthermore, the participants overall have a stronger higher education background where 261 participants have college degree and and 39 with graduate degree and Phd. 127 have a high school degree and 2 declined to answer.

We tried to identify different clusterings according to demographics within those four sub experiments. Our results show not a significantly different behavior.

### 4.4 Huntington Data

[Stout et al., 2001] conducted research on behavior of patients with Huntington disease (HD) and Parkinson disease (PD).<sup>10</sup> In the study there were considered 14 participants

<sup>9</sup>One did not wish to answer

<sup>10</sup>The Huntington Disease is an illness of the central nervous system. The are are a wide range of associated symptoms including physical symptoms like uncontrollable muscular movements and clumsiness and psychological symptoms like minored concentration, short term memory lapses etc . Moreover a related possible symptom is Parkinson disease [Huntington's-Disease-Association, 2016]. Parkinson is chronic and progressive movement disorder. Also Parkinson goes along with

with HD and 22 participants with PD. They participants are required to don't have ongoing drug problems (including alcohol), free of other major diseases (physical or psychological nature). A group of 33 people serves as a control group. This group can further distinguished in younger (YHC) and older control participants (OHC). Table 3 gives a basic summary of the demographic of the participants.

Demographic	Hunting Disease	Parkinson Disease	YHC	OHC
Age	44.60 (11.70)	66.00 (8.30)	45.30 (10.60)	65.50 (10.70)
Education (years)	15.30 (2.30)	14.20 (2.90)	14.30 (2.10)	14.70 (2.40)
Sex	130.60 (10.10)	131.70 (7.60)	139.50 (2.20)	138.00 (4.60)
Years since diagnosis	4.10 (2.80)	7.70 (5.50)	NA (NA)	NA (NA)
Estimated age at diagnosis	40.50 (10.80)	58.30 (7.60)	NA (NA)	NA (NA)

**Table 3:** Shortened summary of HD, PD and control people (means with standard deviations in parenthesis)

**Source:** Summary of [Stout et al., 2001, page 3]

## 4.5 Cocaine Abusers data

We have data from several individuals of cocaine abusers. There are 12 individuals performing the IGT. The control group consist out of 14 participants. Candidates among the drug abusers were selected as active users with additional drug abusing past and without any known additional mental illness [?]. Table ?? gives a summary of demographic profile.

demographic	Drug abusers	Control Group
Share of men	79%	100%
Age	36.90 (10.30)	30.00 (6.10)
Estimated IQ	105.00 (7.62)	93.70 (10.30)

**Table 4:** Demographic summary of cocaine abusers (means with standard deviations in parenthesis)

## 5 Discussion of results and possible extensions

Our analysis so far showed that people are not separate themselves. In general we assume that healthy participants and those with assumed decision making deficits show significantly different behavior. However, we observe that their behavior seem to be quite similar given our data and applied mappings. Furthermore , in most of the

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physical, such as tremors and rigidity and psychological symptoms, such as memory problems, minored speed of thinking fear and anxiety (among others) [Parkinson's-Disease-Foundation, 2016]

applied unsupervised techniques we as analysts have to set the number of clusters we assume to be in the data (so in our case two for control group and patients with habits). We apply another algorithm called affinity propagation, which identifies the number of clusters itself (algorithm formulation see appendix). In general we find that the algorithm is assign , which suggest that there more natural clusters in the data than the one we assume due to their status labeled as healthy and ill.

## **6 Conclusion**

## 7 List of Literature

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## Appendix

### Metrics and Similarities

This part of the appendix formally defines metrics and similarities and dissimilarities (proximity) used in this paper. We first define some basic general concepts followed by a description of the applied distance and similarity concepts.

#### Distances vs. Similarities

Let  $\mathcal{X}$  be a dataset and let  $\mathbf{x}_i, \mathbf{x}_j$  be two datapoints, such that  $\mathbf{x}_i, \mathbf{x}_j \in \mathcal{X}$ .

A distance function assign for pairs a points a non negative real number as distance.  $d : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}_0^+$ . Formally if the following properties are additionally staisfied the distance is also metric [Shirali and Vasudeva, 2005, page 28].

1.  $d(\mathbf{x}_i, \mathbf{x}_j) \geq 0$
2.  $d(\mathbf{x}_i, \mathbf{x}_i) = 0$
3.  $d(\mathbf{x}_i, \mathbf{x}_j) = d(\mathbf{x}_j, \mathbf{x}_i)$
4.  $d(\mathbf{x}_i, \mathbf{x}_j) \leq d(\mathbf{x}_i, \mathbf{x}_k) + d(\mathbf{x}_k, \mathbf{x}_j)$

A distance can be seen as a measure for dissimilarity of two points [Everitt et al., 2009, page 35]. Besides distance some algorithms operate on a *similarity* matrix. Formally a similarity is a function  $S : \mathcal{X} \times \mathcal{X} \mapsto [0, 1]$ . Also for similarity we can define the following properties [Fratev et al., 1979, page 3]:

1.  $0 \leq S(\mathbf{x}_i, \mathbf{x}_j) \leq 1$ , for  $i \neq j$
2.  $S(\mathbf{x}_i, \mathbf{x}_i) = 1$
3.  $S(\mathbf{x}_i, \mathbf{x}_j) = S(\mathbf{x}_j, \mathbf{x}_i)$

Once we have computed distance or a similarity we can compute for two data points we can use this information to transform it to a similarity or the distance vice versa [Boriah et al., 2008, page 4]:

$$S(\mathbf{x}_i, \mathbf{x}_j) = \frac{1}{1 + d(\mathbf{x}_i, \mathbf{x}_j)} \quad \Leftrightarrow \quad d(\mathbf{x}_i, \mathbf{x}_j) = \frac{1}{S(\mathbf{x}_i, \mathbf{x}_j)} - 1 \quad (3)$$

### .0.1 Similarity measures for time series data

We use three different similarity measures for time series. E.g. [Wang et al., 2013] or [Serra and Arcos, 2014] provide an overview and empirical evaluation on common similarity measures for time series. The following definitions are taken from the latter. Empirical research suggest that simple euclidean distance for time series performs quite well and is hard to beat. Hence, the first distance measure for time series is simply euclidean distance between two time series. They might be converted to similarity based on equation 3. Let  $\mathbf{x}, \mathbf{y}$  be two time series over N-periods. Then the  $L_2$  distance between two time series is define as:

$$d_E(\mathbf{x}, \mathbf{y}) := \sqrt{\left( \sum_{i=1}^N (x_i - y_i)^2 \right)} \quad (4)$$

## .0.2 Similarity measures for categorical data

Referring to equation 4 we define a simple measure for the categorical aspect of the data. Note that [SOURCE] defines the simplest measure for categorical data. However, since the probability that two people behave exactly the same in our context is arguably zero we modify this concept slightly. So we relax that and define the overlap similarity just as the count of overlapping instances. This serves as a benchmark similarity for categorical data.

$$d_O(\mathbf{x}, \mathbf{y}) := \sum_{i=1}^N \mathbb{1}_{(x_i=y_i)} \quad (5)$$

In [Borish 2008] we find a rich class of further categorical measures. To keep it concise we considered two of them. The first one is *Eskin* similarity measures.

$$d_O(\mathbf{x}, \mathbf{y}) := \begin{cases} 1 & , \text{if } \mathbf{x} = \mathbf{y} \\ \frac{n_k^2}{n_k^2+2} & \text{otherwise} \end{cases} \quad (6)$$

Furthermore, we consider *lins* similarity

$$d_{lin}(\mathbf{x}, \mathbf{y}) := \begin{cases} 2 \log \hat{p}_k(X_k) & , \text{if } \mathbf{x} = \mathbf{y} \\ 2 \log (\hat{p}_k(x_k) + \hat{p}_k(y_k)) & \text{otherwise} \end{cases} \quad (7)$$

## Clustering Evaluation

In this section we formally derive and explain the applied clustering metrics. Evaluating clustering performance has some issues. The algorithm is producing labels. Nevertheless we generated the "true" labels the might not be comparable. A simple example we might consider the following situation. Let  $y$  denote the labels of data the data and  $y'$  the corresponding prediction such that  $y, y' \in \{0, 1\}$ . In a small example let our data points be like  $y = (1, 1, 0, 0)$  and the corresponding prediction  $y' = (0, 0, 1, 1)$ . Obviously the clustering worked perfectly, however comparing "labels" would produce an accuracy of zero.

There are several clustering metrics, which respect such a situation. We consider a bunch of information based metrics. Most of the measures use some sort of entropy. The following concepts can be found in [Rosenberg and Hirschberg, 2007] and [Vinh et al., 2010] and as additional reading [Hubert and Arabie, 1985].

First we might introduce the contingency table.

	$V_1$	$V_2$	$\dots$	$V_c$	$\Sigma$
$U_1$	$n_{1,1}$	$n_{1,2}$	$\dots$		$a_1$
$U_2$	$n_{2,1}$	$\ddots$			$a_1$
$\vdots$	$n_{1,1}$	$\dots$			$a_1$
$U_R$	$n_{1,1}$	$\dots$			$a_1$
	$b_1$	$b_2$	$\dots$	$b_c$	$N$

**Table 5:** Contingency Table

- $N_{11}$ : Number of pairs in the same cluster
- $N_{00}$ : Number of pairs that are in different clusters in both  $v$  and  $u$
- $N_{01}$ : Number of pairs that are in the same cluster in both  $u$  but different in  $v$
- $N_{10}$ : Number of pairs that are in the same cluster in both  $v$  but different in  $u$

$$RI(u, v) = \frac{N_{00} + N_{11}}{\binom{N}{2}} \quad (8)$$

$$ARI(u, v) = \frac{2(N_{00}N_{11} - N_{01}N_{10})}{(N_{00} + N_{01})(N_{01} + N_{11}) + (N_{00} + N_{10})(N_{10} + N_{11})} \quad (9)$$

$$H(u) = - \sum_{i=1}^R \frac{a_i}{N} \log \frac{a_i}{N} \quad (10)$$

$$H(v) = - \sum_{i=1}^C \frac{b_i}{N} \log \frac{a_i}{N} \quad (11)$$

$$H(u, v) = - \sum_{i=1}^R \sum_{j=1}^C \frac{n_{i,j}}{N} \log \frac{n_{i,j}}{N} \quad (12)$$

$$H(u|v) = - \sum_{i=1}^R \sum_{j=1}^C \frac{n_{i,j}}{N} \log \frac{n_{i,j}/N}{b_j/N} \quad (13)$$

$$H(v|u) = - \sum_{i=1}^C \sum_{j=1}^R \frac{n_{i,j}}{N} \log \frac{n_{i,j}/N}{b_j/N} \quad (14)$$

$$I(u, v) = \sum_{i=1}^R \sum_{j=1}^C \frac{n_{i,j}}{N} \log \frac{n_{i,j}/N}{a_i b_j / N} \quad (15)$$

$$(16)$$

Normalized Info Score:

This is one example of a normalized version

$$NMI_{max}(u, v) = \frac{I(u, v)}{\max(H(u), H(v))} \quad (17)$$

$$\begin{aligned} AMI_{max}(u, v) &= \frac{NMI_{max}(u, v) - \mathbb{E}[NMI_{max}(u, v)]}{1 - \mathbb{E}[NMI_{max}(u, v)]} \\ &= \frac{I(u, v) - \mathbb{E}[I(u, v)]}{\max(H(u), H(v)) - \mathbb{E}[I(u, v)]} \end{aligned} \quad (18)$$

$$\mathbb{E}[I(u, v)] = \sum_{i=1}^R \sum_{j=1}^C \sum_{n_{i,j}=\max(a_i+b_j-N, 0)}^{\min(a_i, b_j)} \frac{n_{i,j}}{N} \log \left( \frac{N n_{i,j}}{a_i b_j} \right) \frac{a_i! b_j! (N - a_i)! (N - b_j)!}{N! n_{i,j}! (a_i - n_{i,j})! (b_j - n_{i,j})! (N - a_i - b_j + n_{i,j})!} \quad (19)$$

Homogeneity:

$$h = \begin{cases} 1 & ,\text{if } H(u, v) = 0 \\ 1 - \frac{H(u|v)}{H(u)} & \text{otherwise} \end{cases} \quad (20)$$

Completeness:

$$c = \begin{cases} 1 & ,\text{if } H(v, u) = 0 \\ 1 - \frac{H(v|u)}{H(v)} & \text{otherwise} \end{cases} \quad (21)$$

V Measure Score:

$$V_\beta = \frac{(1 + \beta)hc}{\beta h + c} \quad (22)$$

## .1 Algorithms

### Principal Components and Multidimensional Scaling

Coming to principal component analysis. [Shlens, 2014] provides an excellent contribution considering both practical applications and theoretical background. The following derivations are from this source.

## Spectral Clustering

For the spectral clustering algorithm we formally introduce some graph notation. If not stated otherwise the following derivation follows [Luxburg, 2007]. In the following we consider a weighted and simple undirected graph.

$$G = \{V, E\} \quad (23)$$

$$V = \{v_1, \dots, v_n\} \quad (24)$$

$$E = \{e_1, \dots, e_n\} \quad (25)$$

Furthermore let the graph has a weighted and symetric  $(|V| \times |V|)$  adjacency matrix, such that:

$$\mathbf{W} = \begin{cases} w_{i,j} & , \text{if } v_i v_j \in E \\ 0 & \text{otherwise} \end{cases} \quad (26)$$

The *degree* of a node is defined as the sum of edge weights of connected nodes. Formally we denote the degree of node  $i$  as:

$$d_i := \sum_{j=1}^n w_{ij} = \sum_{i=1}^n w_{ij} \quad (27)$$

Using the last expression we define matrix  $\mathbf{D}$  as the diagonal matrix of the degrees

$$\mathbf{D} := \text{diag}(\mathbf{d}) \quad (28)$$

The algorithm works on the *Laplacian* matrix defined by:

$$\mathbf{L} := \mathbf{D} - \mathbf{W} \quad (29)$$

Former versions of the algorithm are applied on the graph laplacian. However, there were proposed newer versions using the so called *normalized laplacian*. Since also the python version is using this package we will focus on this version of the algorithm. Following that the normalized graph laplacian is defined as:

$$\mathbf{L}_{norm} := \mathbf{D}^{1/2} \mathbf{L} \mathbf{D}^{1/2} = \mathbf{I} - \mathbf{D}^{1/2} \mathbf{W} \mathbf{D}^{1/2} \quad (30)$$

## **A Affinity Propagation**

[Brusco and Köhn, 2008]