

Master Thesis

Topic:

Unsupervised learning in decision making

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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
ϵ	Probability of exploration in epsilon greedy
α	Learning rate
τ	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
W	Weighted adjacency matrix
d_i	Degree of node i
D	Diagonal matrix of degrees
L	Graph laplacian

VI List of abbreviations

Abbreviations	Description
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1 Introduction and conceptual approach

SHUT UP DOM

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.

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 and we try to discover natural clustering behavior in the data. [Murphy, 2012, page 9 et. seqq.]. A vast class of clustering algorithms are proposed in the literature. In this paper we are investigating whether we can use unsupervised learning methods to cluster different groups of people with respect to their behavior. This paper is therefore in the intersection of machine learning and cognitive science. To our knowledge this particular setting was not studied before.

We first used a reinforcement learning based approach to simulate data and study theoretical boundaries of our methods and under which conditions they might be applicable. We then apply our methods to two real world data sets. In particular we have data of people with different criminal profiles performing a standardized test. Furthermore, we have data of people with different sex, level of education and age doing a simple n-armed bandit experiment.

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. We first provide a basic knowledge of reinforcement and line out our experiment design. Since this is a pioneer work we address the topic in a broad manner. Hence, this section includes an overview of applied similarity concepts and algorithms. Finally we present the results of our simulation and a short interim conclusion.

After that we provide results for the real world data. Since this is a first research on this subject we can only address a small part of the problem. Therefore, we close the paper with discussion of possible extensions and summary of found results. The appendix contains the theoretical foundation of the applied algorithms, similarity measures and cluster evaluation techniques. Since our data are fairly small we will not discuss complexity of the algorithms.

2 Relevant Literature

There exists a rich literature on identifying behavioral groups using 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 is given in [Steingroever et al., 2013]. Several studies identify 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]. 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].

3 Theoretical Background and simulation experiments

This section is dedicated to the a more detailed outline of our analysis approach and the results of our simulation experiments. We find that our data are not immediately suitable for common unsupervised learning methods. Hence, we also discuss how we approach this problem. Besides the introduction to reinforcement learning this section will be rather a qualitative discussion. 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

Before analyzing real data we run some simulation experiments to identify adequate approaches to model our data. To generate data artificially we follow a reinforcement learning and multi arm bandit approach where we let an agent learn the distribution of a simulated data set. The procedure is illustrated in figure 1. To keep things simple we draw a set of rewards from a normal distribution. We let several agents with different parameter setting process the reward data. From this procedure we obtain for each agent a time series of choices.

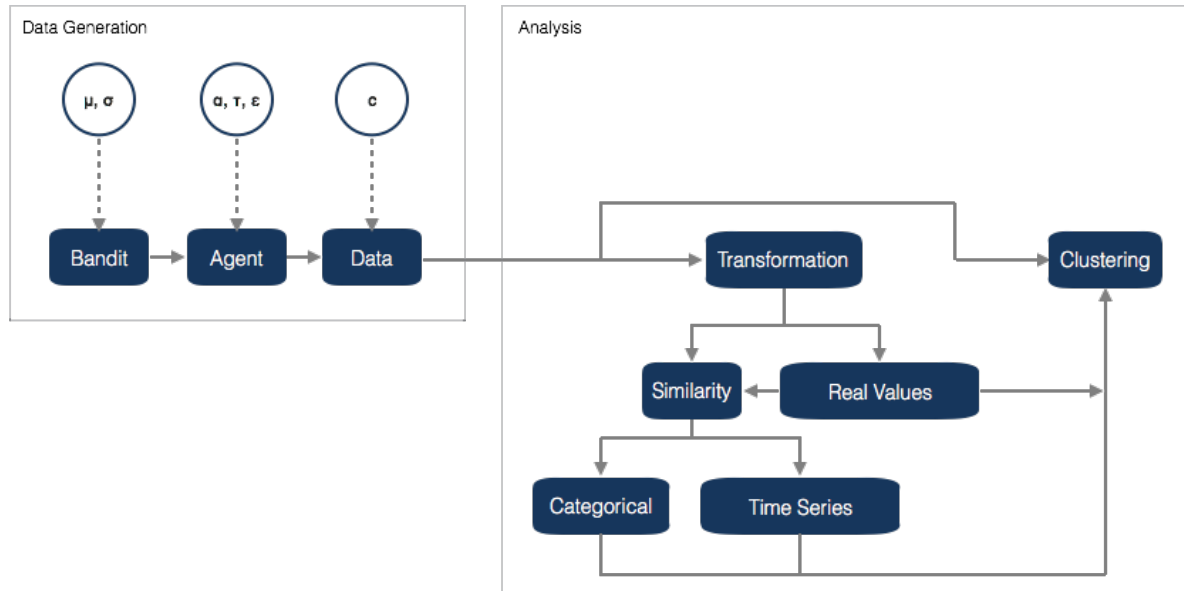


Figure 1: Flowchart experiment design

3.2 Reinforcement Learning background and multi arm bandits

In the following we provide some basics of *Reinforcement Learning* (RL) [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 particular an agents is confronted with the task of choosing sequentially from a set of choices. In comparison to *supervised learning*, where an agent is learning based on set of examples an agent in REL doesn't have any knowledge about the system apriori. Therefore, it has to learn the nature of the system by sequentially interacting with its environment and keeping tack of the obtained information. Since the agent doesn't have any apriori information about the system it has to explore new possible action and so has to deviate from the optimal action. Furthermore, it has to keep track of value of each action he did so far. So the main task of the agent is to balance exploration and exploitation. There are to basic approaches to model this trade-off; An "*Epsilon-Greedy*" selection method and Soft "*Softmax*" selection method. Before explaining both concepts we introduce the value function for a given action a . Therefore, let $Q_t(a)$ be the value function of action defined as:

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

The value function is the average over rewards.

Considering now epsilon greedy action selection method: The rule in general is to select the next action as the current current highest value function. However, to model exploration we introduce a random element to deviate from that greedy strategy. Following that the next action

$$a_{t+1} = \begin{cases} \text{random action} & , \text{ with probability } \epsilon \\ \arg \max_i Q_t(i) & , \text{ with probability } 1 - \epsilon \end{cases} \quad (2)$$

where $\epsilon \in [0, 1]$ is a parameter controlling the random behaviour of the agent.

In the softmax action selection method compute for each action a probability (also called *Boltzmann Distribution*). The probability for action a is computed by:

$$P(a_t|X) = \frac{e^{\frac{Q_t(a)}{\tau}}}{\sum_i^K e^{\frac{Q_t(i)}{\tau}}} \quad (3)$$

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

$$a_{t+1} \sim p_a \quad (4)$$

After selecting an action the agent is updating its believe of the chosen action. Formally the update rule is defined

$$Q(a)_{k+1} = Q(a)_k + \alpha [R(a)_k - Q(a)_k], \quad (5)$$

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

3.3 Unsupervised learning methods, data handling and similarity

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 about distance and similarity measures to respect the nature of our data and algorithms.¹ 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. Let X be a discrete random variable with probability p , then the entropy is defined as [MacKay, 2005, page 32]:

$$H(X) := - \sum_{i=1}^N p_i \log_2 p_i \quad (6)$$

Entropy gives measure on how random a random variable behaves. Withing the entropy framework we consider to types of entropies. For each time step we compute the entropy using the choices done so far. We call this *cumulative entropy*. Furthermore, we might want to observe more clearly how individuals adapt their behavior over time.

¹A formal definition of the distance and similarity can be found in the appendix

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 aimed to discriminate individuals by their level of randomness in their behavior.

A second approach is based on the experimental setting. We know within our simulation and our simulation and real data framework the 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. Table 1 shows an overview of the algorithms and their corresponding distance/similarity requirement. A technical description for all of them is provided in the appendix.

Algorithm	Input	Datatype
Spectral Clustering	Similarity	-
Affinity Propagation	Similarity	-
K-Means Clustering	L_2 Distance	-
Ward Clustering	Data Matrix	-
PCA + Ward Clustering	Data Matrix	-

Table 1: Overview clustering algorithms

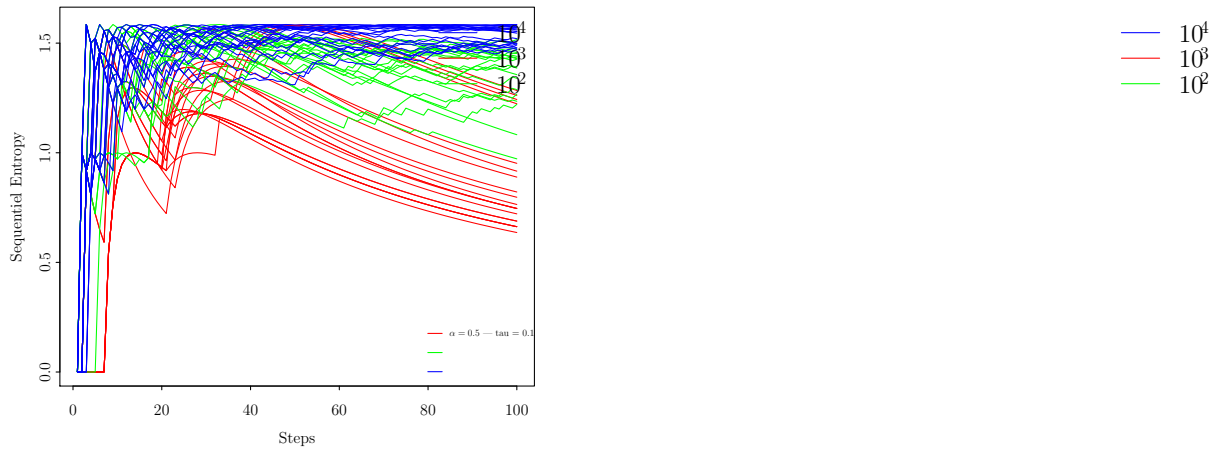
According to our different data types and for our different algorithms we apply the following distance and similarity concepts.²

²Note that distance and similarity can be converted according to equation (7) in the appendix

Similarity/Distance	Data type
Cosine Similarity	Categorical
Levenstein Distance	Categorical
Lin Similarity	Categorical
Edit Distance on Real Sequence	Time series
Dynamic Time Warp	Time series
RBF Kernel	Real Data

Table 2: Overview similarity and distance measures

3.4 Simulation results

**Figure 2:** ACF and PACF of MCSI

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.³

³For 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]

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

Specification	μ	σ	CL Size	SD	Decision	α	τ	N	ALG	TRNS	MI	NMI	AMI	CS	HS	VMS
1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

Table 3: 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 five different data sets. As mentioned in the introduction the Iowa gambling task is popular way to monitor decision and learning process. We were provided with data from various sources and with various types of bad behavior (namely people with criminal background, mental illness, drug habits). The first four data sets we approach are based on that test setting. The last data set is gathered in a multi arm bandit context.

In the simulation setting we initially define participants with a certain set of parameters. There exists techniques to estimate to those parameters from actual data.

4.1 Recover cognitive parameters

4.2 Prison data and approach

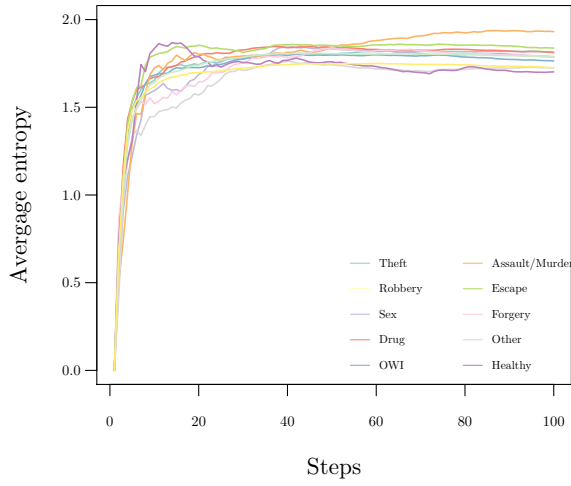
With acknowledgment to [HERE WE ADD THE GUY] we were provided with experimental data from [Yechiam et al., 2008]. We try to apply our methods to cluster different groups in the data. The participants had to perform the Iowa gambling task (detailed description see later on). [Steingroever et al., 2015] 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

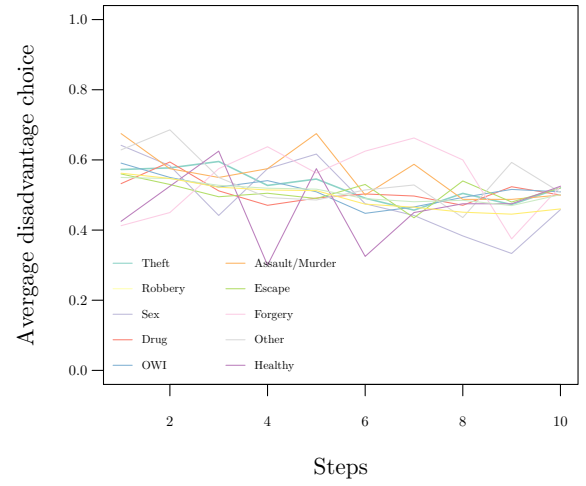
In particular we have data of 96 individuals with different criminal profile. Table 4 gives a broad summary of some demographics.

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, each deck has its own variance and a set of profits.

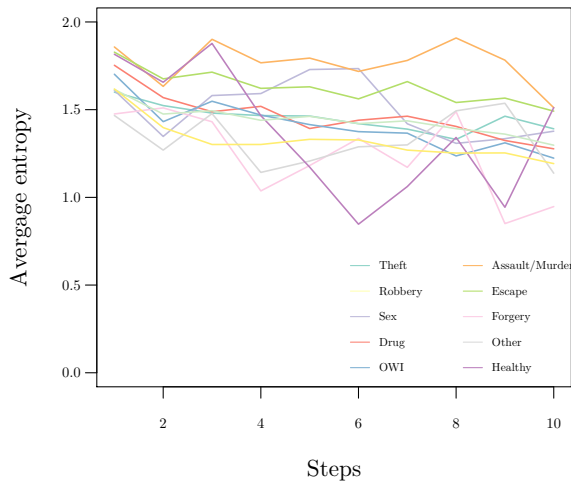
Figure 3 (a) shows the average cumulative entropy averaged across groups. We observe a random behavior independent from group affiliation. However, normal people show the least random behavior. Furthermore, Figure 3 (b) shows the average people of negative choices people chose over steps of ten periods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



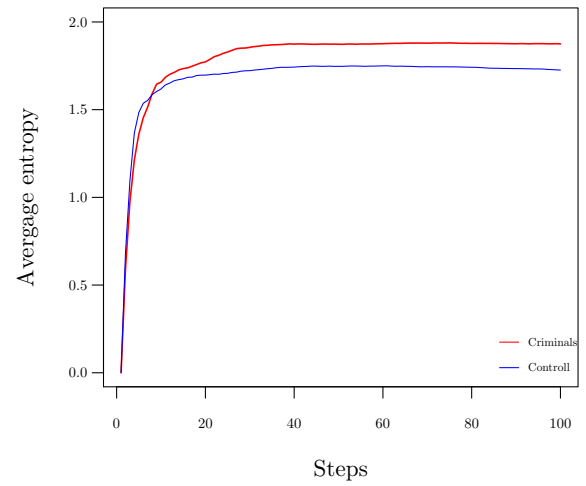
(a) Average Entropy across groups



(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)
Probabiton	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 4: Summary prison data (means with standard deviation in parenthesis)

Yechiam et al. found three clusters by using the attention to recent outcomes (ARO) and attention to gains (AG) parameters from the Expectancy Valance model. The most distinct group were the Robbery convicts with the only negative attention to gains mean at -0.36 and the highest attention to recent outcomes mean 0.57. The second cluster is made of assault and murder convicts with ARO of 0.26 and AG of 0.1. The third cluster is formed of all the remaining prisoner groups with ARO means between 0 and -0.1 and AG between 0.1 and 0.2.

4.2.2 Prison data results

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

Following the clusters given by the EV model, we tried pairwise clustering between robbers and other prisoner groups and assault offenders and other prisoner groups.

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.⁴ The average age 33.04 with standard

⁴One did not wish to answer

deviation 11.75. Furthermore, the participants overall have a stronger higher education background where 261 participants have college degree 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).⁵ In the study there were considered 14 participants 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 5 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 5: 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 1 gives a summary of demographic profile.

⁵The Huntington Disease is an illness of the central nervous system. There 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 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]

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 6: Demographic summary of cocaine abusers (means with standard deviations in parenthesis)

4.6 Cocaine Abusers data results

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 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. 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]:

$$S(\mathbf{x}_i, \mathbf{x}_j) = \frac{1}{1 + d(\mathbf{x}_i, \mathbf{x}_j)} \quad \Leftrightarrow \quad d(\mathbf{x}_i, \mathbf{x}_j) = \frac{1}{S(\mathbf{x}_i, \mathbf{x}_j)} - 1 \quad (7)$$

.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 7. Let \mathbf{x}, \mathbf{y} be two time series over N-periods. Then the L_2 distance between two time series is define as:

$$d_E(\mathbf{x}, \mathbf{y}) := \sqrt{\left(\sum_{i=1}^N (x_i - y_i)^2 \right)} \quad (8)$$

.0.2 Similarity measures for categorical data

Referring to equation 8 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.

In [Borah 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.

$$d_O(\mathbf{x}, \mathbf{y}) := \begin{cases} 1 & , \text{if } \mathbf{x} = \mathbf{y} \\ \frac{n_k^2}{n_k^2 + 2} & \text{otherwise} \end{cases} \quad (9)$$

Furthermore, we consider *lin* similarity

$$d_{lin}(\mathbf{x}, \mathbf{y}) := \begin{cases} 2 \log \hat{p}_k(X_k) & , \text{if } \mathbf{x} = \mathbf{y} \\ 2 \log (\hat{p}_k(x_k) + \hat{p}_k(y_k)) & \text{otherwise} \end{cases} \quad (10)$$

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	Σ
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 7: 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

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

$$ARI(u, v) = \frac{2(N_{00}N_{11} - N_{01}N_{10})}{(N_{00} + N_{01})(N_{01} + N_{11}) + (N_{00} + N_{10})(N_{10} + N_{11})} \quad (12)$$

$$H(u) = - \sum_{i=1}^R \frac{a_i}{N} \log \frac{a_i}{N} \quad (13)$$

$$H(v) = - \sum_{i=1}^C \frac{b_i}{N} \log \frac{a_i}{N} \quad (14)$$

$$H(u, v) = - \sum_{i=1}^R \sum_{j=1}^C \frac{n_{i,j}}{N} \log \frac{n_{i,j}}{N} \quad (15)$$

$$H(u|v) = - \sum_{i=1}^R \sum_{j=1}^C \frac{n_{i,j}}{N} \log \frac{n_{i,j}/N}{b_j/N} \quad (16)$$

$$H(v|u) = - \sum_{i=1}^C \sum_{j=1}^R \frac{n_{i,j}}{N} \log \frac{n_{i,j}/N}{b_j/N} \quad (17)$$

$$I(u, v) = \sum_{i=1}^R \sum_{j=1}^C \frac{n_{i,j}}{N} \log \frac{n_{i,j}/N}{a_i b_j / N} \quad (18)$$

$$(19)$$

Normalized Info Score:

This is one example of a normalized version

$$NMI_{max}(u, v) = \frac{I(u, v)}{\max(H(u), H(v))} \quad (20)$$

$$\begin{aligned} AMI_{max}(u, v) &= \frac{NMI_{max}(u, v) - \mathbb{E}[NMI_{max}(u, v)]}{1 - \mathbb{E}[NMI_{max}(u, v)]} \\ &= \frac{I(u, v) - \mathbb{E}[I(u, v)]}{\max(H(u), H(v)) - \mathbb{E}[I(u, v)]} \end{aligned} \quad (21)$$

$$\mathbb{E}[I(u, v)] = \sum_{i=1}^R \sum_{j=1}^C \sum_{n_{i,j}=\max(a_i+b_j-N, 0)}^{\min(a_i, b_j)} \frac{n_{i,j}}{N} \log \left(\frac{N n_{i,j}}{a_i b_j} \right) \frac{a_i! b_j! (N - a_i)! (N - b_j)!}{N! n_{i,j}! (a_i - n_{i,j})! (b_j - n_{i,j})! (N - a_i - b_j + n_{i,j})!} \quad (22)$$

Homogeneity:

$$h = \begin{cases} 1 & ,\text{if } H(u, v) = 0 \\ 1 - \frac{H(u|v)}{H(u)} & \text{otherwise} \end{cases} \quad (23)$$

Completeness:

$$c = \begin{cases} 1 & ,\text{if } H(v, u) = 0 \\ 1 - \frac{H(v|u)}{H(v)} & \text{otherwise} \end{cases} \quad (24)$$

V Measure Score:

$$V_\beta = \frac{(1 + \beta)hc}{\beta h + c} \quad (25)$$

.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.

$$G = \{V, E\} \quad (26)$$

$$V = \{v_1, \dots, v_n\} \quad (27)$$

$$E = \{e_1, \dots, e_n\} \quad (28)$$

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

$$\mathbf{W} = \begin{cases} w_{i,j} & \text{,if } v_i v_j \in E \\ 0 & \text{otherwise} \end{cases} \quad (29)$$

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:

$$d_i := \sum_{j=1}^n w_{ij} = \sum_{i=1}^n w_{ij} \quad (30)$$

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

$$\mathbf{D} := \text{diag}(\mathbf{d}) \quad (31)$$

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

$$\mathbf{L} := \mathbf{D} - \mathbf{W} \quad (32)$$

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:

$$\mathbf{L}_{norm} := \mathbf{D}^{1/2} \mathbf{L} \mathbf{D}^{1/2} = \mathbf{I} - \mathbf{D}^{1/2} \mathbf{W} \mathbf{D}^{1/2} \quad (33)$$

A Affinity Propagation

[Brusco and Köhn, 2008]