

# Discriminative Machine Learning for Maximal Representative Subsampling

Bachelor's Thesis submitted

to

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# ABSTRACT

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To allow statistical inference in social sciences, survey participants must be selected at random from the target population. When samples are drawn from parts of the population that are close to hand, subgroups might be over-represented. This leads to statistical analyses under sampling bias, which in turn may produce similarly biased outcomes. The present thesis uses machine learning to reduce this selection bias in a psychological survey using auxiliary information from comparable studies that are known to be representative. Discriminative algorithms are trained to directly characterize the divergence between representative and non-representative samples.



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# 1 INTRODUCTION

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Psychological resilience is generally regarded as positive adaptation to past and ongoing exposure to potential negative effects of stressors. Accordingly, adaptation to stressful or adverse situation is a dynamic process with predictors that can differ between population groups. Within the discipline of developmental psychology, Tiescher and colleagues have provided prospective studies investigating the concept of resilience and its complex underlying mechanisms. As part of a doctoral dissertation, their studies aimed to validate the following research questions:

- Does resilience have a positive effect on the willingness to participate in politics, specifically in election?
- Does the confrontation with positive or negative statements on politics for people with lower resilience have stronger effects on the willingness to participate in politics?

The research group did its poll by selecting people from Mainz, while trying to generalize to the entire German population. The survey data (GBS,  $n=587$ ) tends to over-represent groups of higher income and higher education, since participants are primarily selected from an academic environment.

Therefore, the validity of assertions about the population beyond the original observation range is affected, even if statements are made conditional upon the available data. The basic premise for standard statistical conclusions, that the training and test set are drawn independently and identically (i.i.d.) from the same probability distribution, does not hold any more. This setting is also known as covariate-shift (Shimodaira 2000). Data sets are rarely generated under ideal conditions with bias pervasive in almost all empirical studies. The oftentimes underestimated analytic errors produce misleading descriptions of populations and ultimately yield false inferences (Aurelien, West, Sakshaug, 2016).

To get a complete picture of the subject, the research group consulted the department Data Archives for the Social Sciences. Their data archive service (GESIS) holds representative data of comparable studies in politics and psychology. The acquired sample (GESIS,  $n=4000$ ) encompasses the German speaking population with permanent residence in Germany.

This thesis is a practical application to reduce the sampling bias by selecting a maximal representative subsample (MRS) of GBS survey respondents with reference probability distri-

butions from GESIS. The effects of positive and negative treatments on political participation are then analysed in the resulting MRS and compared to the initial GBS data [Fig. 1.1].

To evaluate the research questions to a certain required level of significance, it is inevitable to keep the exclusion of instances at a minimum. Pruning the GBS data in any way, narrows the data variance and thus the reach of subsequent studies. This is especially harmful since the initial GBS survey data is already small.

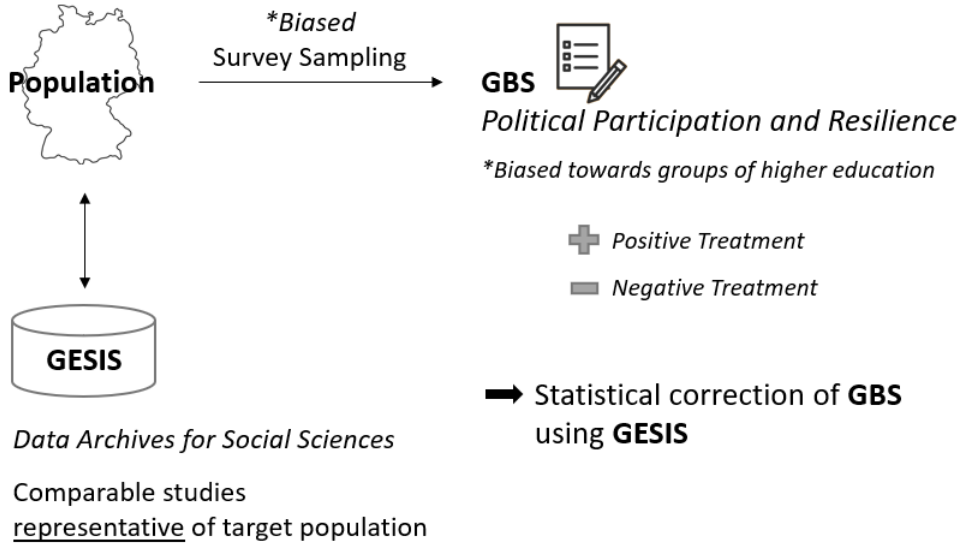


Figure 1.1: Multivariate auxiliary information GESIS linked to GBS so that expected bias can be detected and corrected for. In addition, GBS contains an attribute for positive or negative treatment of survey participants for further analysis.

In the MRS procedure, discriminative learners will look for decision boundaries to distinguish the negative class GBS from the positive class GESIS. First, both data sets are combined by adding an attribute indicating the source of origin. This label is predicted so that instances can be ranked according to their predicted probability. GBS participants that can be distinguished are removed from the result set. The remaining instances in GBS define the MRS and are expected to be more closely aligned with the target probability distribution. The area under the receiver operating characteristic curve (AUROC) is used as single number evaluation metric to measure the degree of sampling bias. The MRS is characterized by an AUROC of roughly 0.5.

The fraction of misclassified GBS instances is kept as proxy measure for the subsequent method positive-unlabeled learning (Denis et al. 2005). Positive-unlabeled learning is a semi-



supervised technique that does not make the simplifying assumption of GBS being positive or negative. GBS is in actual fact unlabeled, i.e. subgroups of the target population might be over-represented or actually representative. Apparently, subsampling does not help in the case of under-represented subgroups.

These procedures can only work when most of the observations come from a feature space which is not specific to one of the surveys. Thus, attributes must be matched correctly.

## 1.1 Related Work

The influence of sampling bias could be alleviated by weighting the instances according to their importance (Shimodaira 2000). Statistical adjustment might also be reached by developing survey weights for calibration estimators [5]. However, these techniques require density estimation which is known to be a hard problem especially in high-dimensional cases (Haerdle et al. 2004). Directly estimating the importance without estimating the density ratios would be more promising: Discriminative machine learning for maximal representative subsampling.

## 1.2 Outline

The remainder of this thesis is organized as follows. Sec. 2 starts with an initial data analysis step and focuses more narrowly on checking assumptions required for model fitting and hypothesis testing, i.e. handling missing values and making transformations of variables. Sec. 3 defines key terminology and definitions and discusses discriminative learning and positive-unlabeled learning. The resulting maximal representative subset of GBS is presented in Sec. 4 and compared to GBS regarding political participation and resilience. Sec. 5 concludes.



## 2 INITIAL DATA ANALYSIS

In order to diagnose to what extent an algorithm suffers from sampling bias, it will be useful to have another dataset. Initial data analysis is conducted independently of the problem statements to understand what properties of the data differ between GBS and GESIS for matching attributes. A brief characterization of the data currently employed in the studies is given in this chapter. The GitHub repository further specifies the list of transformations that are sequentially applied to each group of features in order to prepare the inputs for survey comparisons. Preprocessing steps and methods used to evaluate outcomes are documented as well. Scaling methods that apply to both data sets, e.g: centering and scaling of skewed continuous features for SVMs, are not mentioned but can be deduced from code easily. If an attribute is removed at some point, it will only be mentioned in the relevant section.

CODE	GBS+00027	GESIS 288506501
Gruppe	NEGATIV	
Geschlecht	männlich	Männlich
Geburtsjahr	1949-01-15	1946
Geburtsland	Deutschland	Deutschland
Nationalitaet	1	Deutschland
Familienstand	Verheiratet und lebe mit meinem/r Ehepartner/-...	Verheiratet/ Eing. LP zus. lebend
Hoechstes Bildungsabschluss	Realschulabschluss (Mittlere Reife)	Fachhochschulreife, Fachoberschule
Berufliche Ausbildung	Ausbildung an einer Fach-, Meister-, Techniker...	Fachhochschulabschluss
Erwerbstätigkeit	1	Nicht erwerbstätig
Berufsgruppe	Beamter/Beamtin, Richter/-in, Berufssoldat/-in	Missing by filter
Personen im Haushalt	2	3
Nettoeinkommen Selbst	2 250\t bis unter\t2 500 Euro	2600 bis unter 3200
Nettoeinkommen Haushalt	4 500\t bis unter\t5 000 Euro	4000 bis unter 5000
Schlechter Schlaf	3	Manchmal
Leben genießen	3	Meistens
Zu Nichts aufraffen	3	Nie
Alles anstrengend	2	Fast nie
Wahlteilnahme	NaN	Ja
Wahlabsicht	5	Ja, ich würde wählen.
Desinteresse Politiker	4	3
Zufriedenheit Leben	3	9
Aktiv	3	Erheblich
Verärgert	4	Ein bisschen
Wach	4	Erheblich
Nervös	3	Gar nicht
Ängstlich	4	Gar nicht
Zurueckhaltend	eher zutreffend (4)	3 Weder noch
leicht Vertrauen	eher zutreffend (4)	3 Weder noch
Faulheit	trifft eher nicht zu (2)	1 Trifft überhaupt nicht zu
Entspannt	eher zutreffend (4)	3 Weder noch
wenig kuenstlerisches Interesse	eher zutreffend (4)	4 Eher zutreffend
Gesellig	weder noch (3)	4 Eher zutreffend
Andere kritisieren	weder noch (3)	3 Weder noch
Gruendlich	eher zutreffend (4)	4 Eher zutreffend
Nervoes	trifft eher nicht zu (2)	3 Weder noch
Phantasievoll	weder noch (3)	4 Eher zutreffend

Figure 2.1: GBS - GESIS attribute and value comparison. Not all attributes are used in every learning task. See GitHub documentation for more information.

## 2.1 Feature Selection and Data Imputation

If not stated differently, deletion of rows is applied to every instance with missing values in GESIS to reduce the class imbalance in the later described classification problem. Missing values are sparse in GBS and can be imputed, e.g: with median substitution, with negligible effects. Mean substitution can not be used as this might lead to previously unseen values. Discriminative algorithms will then use these new values to distinguish GBS and GESIS that have been created by ill-considered data imputation. Note that the following figures represent the data after attribute and value matching described in Sec. 2.2.

Fig. A.2 lends itself to first thoughts about whether missing data elements depend on observable attributes or occur entirely at random and is also able to detect functional dependencies in GESIS. Fig. A.3 summarizes the main observations from GBS. The correlation matrix with ratio -1 to +1 in Fig. A.4 is used as another way to visualize differences in GESIS and GBS and to further simplify preprocessing decisions. Potential bugs and issues can also be detected with this graph.

## 2.2 Perspectives on Response Styles

In survey analysis, scales measuring attributes need to be reliable and valid. Therefore, GBS and GESIS almost entirely use already tested scales from the literature.

### 2.2.1 Likert-Type Scale

The Big Five is an empirically-derived model of human personality and psyche. When factor analysis is applied to personality survey data, five clusters of traits consistently emerge. The BFI-10 is a 10-item scale measuring the Big Five personality traits, two BFI items for each dimension, representing both the high and low pole of each factor [Fig X]. Likert scales are the most frequently used instruments in GBS and GESIS. They consist of statements which measure the intensity of one's estimation towards the preceding statement. Respondents are asked to rate the BFI-10 items on a level of agreement on a consistent rating scale ranging from "Strongly Agree (5)" to Strongly Disagree (1)" for all items in both survey.

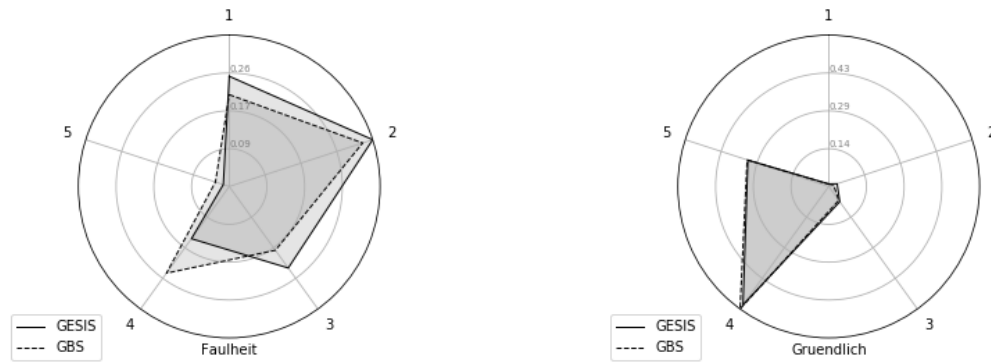


Figure 2.2: Conscientiousness is the degree of organization, self-regulation, and responsibility one exhibits. *"I see myself as someone who tends to be lazy."*(left). *"I see myself as someone who does a thorough job."*(right). The graphs are almost identical for the Likert item "Gruendlich". Respondents specify their level of disagreement for "Faulheit" more in GBS.

is still ongoing debate on whether to use a Likert scale item as categorical or numeric feature. The intervals between positions on the scale are monotonic but never so well-defined as to be numerically uniform increments. A "Strongly Agree (5)" response indicates more agreement than "Agree", but it does not show agreement that is five times stronger than "Strongly Disagree (1)".

There is an underlying measurement continuum, but This project treats the responses as if they fell on an interval scale.

Figure X. shows the response distribution of values for "Conscientiousness" of GBS and GESIS participants (see Appendix for a visualization of distribution shifts in "Agreeableness", "Openness", "Extraversion" and "Neuroticism").

Since GESIS and GBS analyse on a group level should be relatively insensitive to problems that may arise.

In all these cases each aggregate measure (perhaps the mean) is based on many individual responses (e.g.,  $n=50, 100, 1000$ , etc.). In these cases the original Likert item begins to take on properties that resemble an interval scale at the aggregate level. life satisfaction of states or countries, job satisfaction of departments,

## 2.2.2 Data Mismatch

John Tukey wrote otherwise (back in 1960) in a monograph "Data Analysis and Behavioral Science" (published in Collected Works v. III). One result he obtained is that if you're getting better than about 10percent test-retest agreement, your scale isn't narrow enough!

[1] It is confirmed that different numbers of rating bars in a subjective rating scale can have significant effects on the subjective measurement, thus the assessment of the Big Five dimensions of personality.

Raw Data	GESIS	1	2	3	4	5	6
	GBS	1	2	3	4	5	
Max Scaler	GESIS	0.83	1.7	2.5	3.3	4.2	5.0
	GBS	1	2	3	4	5	
Min-Max Scaler	GESIS	1	1.8	2.6	3.4	4.2	5
	GBS	1.0	2.25	3.5	4.75	6.0	
Cut-Off Mapping	GESIS	1	2	3	4	5	5
	GBS	1	2	3	4	5	

Table 2.1: Different value scalings of attribute "Desinteresse Politiker".

Shortcomings in attribute mappings may result in inappropriate representation and incorrect conclusions.

attribute	GBS values	GBS values count	GBS values	GBS values count
Wach	4	311	Einigermassen	1697
	3	183	Erheblich	1389
	2	66	Ein bisschen	467
	1	14	Aeusserst	367
	-1	1	Gar nicht	184
	-9	1		

Table 2.2: Caption.

Inconsistencies are discovered later with the planned learning models as

Techniques for reducing the length of scales while maintaining psychometric quality. Figure X shows an example of such as a statement.

In some cases, an additional "opt-out" option is provided for those respondents who truly cannot respond in GBS only.

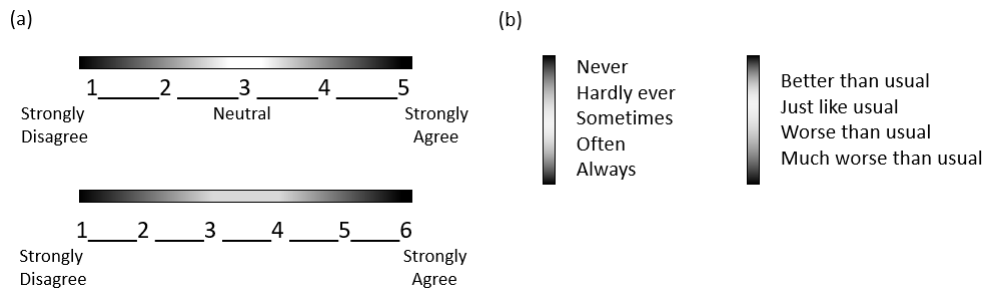


Figure 2.3: Example of a Likert item discrepancy. GBS uses an odd number of responses with a "neutral" option, such as "no opinion", "neither agree nor disagree" or some phrase to that effect. In contrast, there is an even number of responses for this item in GESIS encouraging participants to voice a positive or negative opinion.

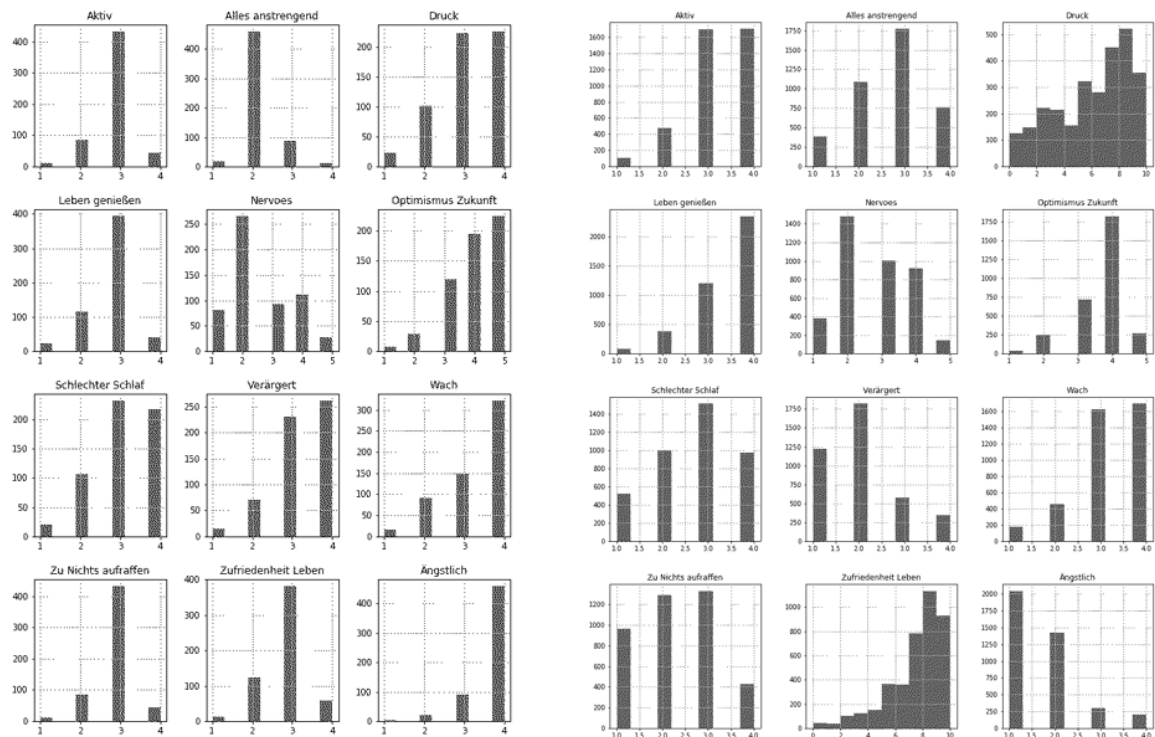


Figure 2.4: GESIS hists.





## 3 FEASIBILITY OF LEARNING

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No practical amount of data can distinguish between two distributions, thus instances of GBS can not be proven to come from GESIS. However, machine learning allows to infer the conditional probability of '*GBS participant is representative*' given the survey data within a probabilistic framework.

This leads to a binary classification task with GESIS as positive class and GBS as negative class, i.e. representative and non-representative sample respectively. Discriminative learners will look for decision boundaries to distinguish the different views of GBS from GESIS in each of the four reference studies. False negatives are then more closely aligned with the target probability distribution. The process of classification is repeated until the learner starts fitting noise more than is warranted. To avoid overfitting, the learning objective needs to be refined as contingency tables lack proper interpretability. An importance weighted adaption of cross-validation serves as model selection criterion. Given the imbalanced nature and size of GBS, learning is restrained to simpler algorithms with lesser degrees of freedom. The fraction of false positives in the result set of this procedure is kept as proxy measure for the subsequent method positive-unlabeled learning (PU learning). The development of classification models in this setting is often referred to as positive-unlabeled learning (Denis et al. 2005).

### 3.1 Terminology and Definitions

A well-defined learning problem involves a number of design choices, including selecting the type of training experience, the target function to be learned, a representation for this target function, and an algorithm to learn from the source of training experience [2]. In modelling a political participation process, a computer program is designed to approximate the likelihood of a person going to vote on election day. Ideally, for every instance with unknown political interest and willingness to participate, there is enough data of people of similar demographics, socioeconomics and psychological traits to generalize from. This chapter defines key terminology and distinctions when learning from biased data. Basic design issues and approaches to supervised learning are covered, while conceptual elements of interest are introduced with regards to overfitting. The role of noise in the bias-variance

decomposition will be analyzed and further broken down. sources of error.

### 3.1.1 Sampling Bias

Sampling bias is often referred to as selection bias or sample selection bias. I will stick to the more descriptive term sampling bias. It underlines the fact that the bias arises in how the data was sampled. Also, the use of the term becomes less ambiguous, because there exists another notion of selection bias in the context of model selection. This type of bias is usually referred to as bad generalization, where the performance of the selected hypothesis is overly optimistic. [input: convenience sampling]

It is usually difficult to draw a simple random sample from the population, due to cost and practical considerations such as no comprehensive sampling frame available

Although one could employ a census to measure the entire population, it is more common to take a sample of the population. A properly designed probability sample (see probability sampling) can be used to make estimates for not only the sample itself, but also for the underlying population from which it was selected. A probability sample is one in which each element of the (underlying) population has a known and non-zero chance of being selected. That is, every person has a chance to be included in the study and have his or her characteristics, opinions, etc., become part of the data. It should be noted that everyone does not have to have an equal chance of being selected just a known non-zero chance of being selected. Probability samples have several desirable characteristics. They enable us to put a margin of error or confidence interval on our estimates essentially a measure of how accurate the estimate is compared to the same estimate calculated on the full population. Probability samples make it possible to not only compare the sample to the population, but also to compare a sample from one population to a sample from another population,

### 3.1.2 Representative Sample

Some examples include sex, age, education level, socioeconomic status or marital status. Information collections with biased tendencies can't generate a representative sample.

Variables considered in the study must accurately reflect the populations characteristics.

Consider *attribute: income* of a subset of GBS participants. Statistical significance tests, e.g. Kolmogorov-Smirnov, Chi-Squared

Given a subset of GBS, similarity scores can be defined to evaluate the distance to reference distributions from GESIS. Kolmogorov-Smirnov tests or Chi-Squared assess the like-

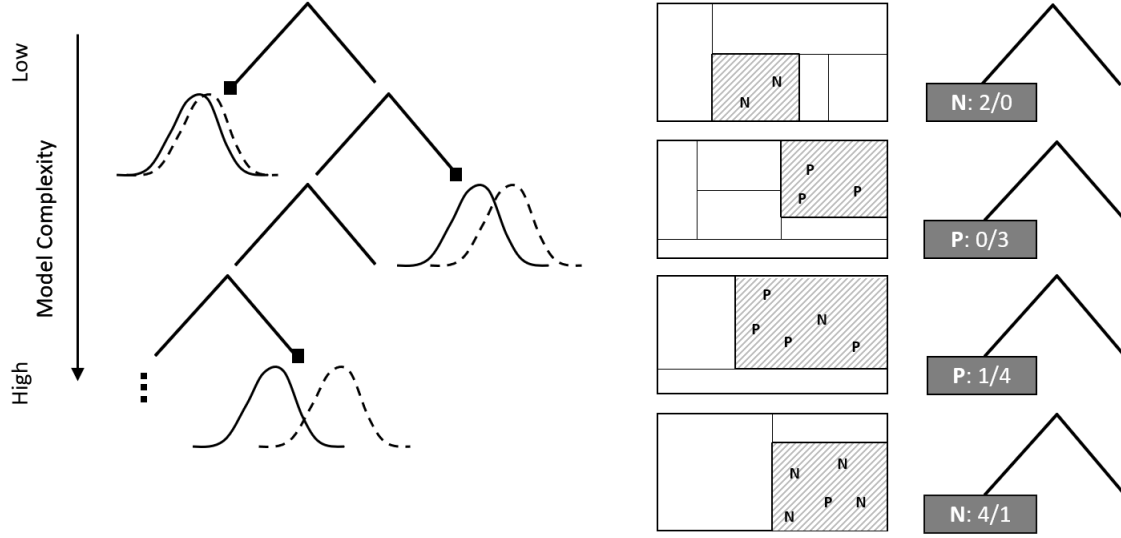


Figure 3.1: .

likelihood of an attribute of GBS There are  $2^{|GBS|} = 2^{587}$  subsets of GBS. Evaluating every possible combination of GBS participants and its score is computationally intractable.

A well-dened learning problem where large polls (Umfragedaten) may contain valuable implicit regularities, requires a well-specied task, performance metric and source of training experience [2]. The MRS problem is now stated as a binary classification task with GESIS as positive class and GBS as negative class. Consider designing a computer program to learn to distinguish between . Using prior knowledge together with past experience to guide learning, a machine learning algorithm is fed with data from games that have been played by chess grandmasters. From this information, the program will learn to apply certain functions to specic board states and make decisions about which move to play next.

Consider a randomly chosen survey participant, i.e. an instance of GBS or GESIS. If the poll indicates the or

Descriptive statistics can be used to

No practical amount of data can distinguish between two distributions, thus instances of GBS can not be proven to come from GESIS. However, discriminative learning allows to infer the conditional probability of '*instance of GBS/GESIS*' given the survey data within a probabilistic framework:

GBS is in actual fact unlabeled, i.e. subgroups of the target population might be over-represented or under-represented.

PU learning is a semi-supervised technique that does not make the simplifying assumption

of GBS instances being negative. Instead, a one-class classifier is trained on GESIS only. [...] This can result in even better assessment.

### 3.1.3 The Problem of Overfitting

The model in supervised learning usually refers to the mathematical structure of how to make predictions  $y_i$  given  $x_i$ . The most common model is a linear regression model, where the prediction is given by a linear combination of weighted input features. The parameters, the weights of these features, are the undetermined part that need to be learned from data. Depending on the task, the prediction value can have different interpretations, i.e. regression or classification. The categorical outcome, "did vote" or "did not vote", makes political participation a binary classification problem [7]. In machine learning, the terms hypothesis and model are often used interchangeably. This paper uses the following convention [3] as the terminology to describe ideas and concepts is not standardized:

- The phrase single hypothesis refers to a single probability distribution or function. An example is the polynomial  $2x^2 + 3x + 1$ .
- The word model refers to a set of probability distributions or family of functions with the same functional form. An example is the set of all quadratic functions.
- As a generic term, hypothesis refers to both single hypotheses and models.

With the definitions above, it is a hypothesis selection problem if both the degree of a polynomial and the corresponding parameters are of interest. The phrase single hypothesis refers to a single probability distribution or function. A machine learning model, the composite hypothesis, refers to a family of probability distributions or functions with the same functional form. An example is the set of all second-degree polynomials [9].

"Overfitting is the disease. Noise is the cause. Learning is led astray by fitting the noise more than the actual signal"[6]. To avoid overfitting you might deliberately exclude certain factors, increase sample size, stop the analysis early, or simply pick less complex algorithms. Regularization puts a break where additional iterations of algorithms start to harm the performance. Validation is another way to see what will actually happen out-of-sample

By definition, statistical inference is taking the results of applying some sort of construct or model to specific data and then speculating that it would continue to perform well beyond the original observation range. Given a set of training samples  $(x_i, y_i)$  and a single hypothesis

$h$  that "fits the data well":  $y_i = h(x_i)$  for most  $i$ . The equation is characterized by a trade-off between goodness-of-fit and complexity of the hypothesis:

- if  $h$  is too simple,  $y_i = h(x_i)$  may not hold for many values of  $i$ ;
- if  $h$  is too complex, it fits the data very well but will not generalize well on unseen data.

PU learning is a semi-supervised technique that does not make the simplifying assumption of GBS instances being negative. Instead, a one-class classifier is trained on GESIS only. [...] This can result in even better assessment. [Read Literature] - Importance weighted cross validation and pu learning with proper assessment.

For further, more technical reading, references to background papers are provided in [38].

Overtfitting stands out as one of the biggest challenges for machine learning. It is not exclusive to machine learning but rather a fundamental problem across science and is at the very heart of the dangers of statistical inference. By definition, statistical inference is taking the results of applying some sort of construct or model to specific data and then speculating that it would continue to perform well beyond the original observation range.

State-of-the-art techniques in positive-unlabeled learning tackle this problem by treating the unlabeled sample as negatives and training a classifier to distinguish between labeled (positive) and unlabeled examples. Surprisingly, for a variety of performance criteria, non-traditional classifiers achieve similar performance under traditional evaluation as optimal traditional classifiers (Blanchard et al. 2010; Menon et al. 2015).

## 3.2 Discriminative Learning

	TP Rate	FP Rate	Precision	Recall	F-Measure	ROC Area	PRC Area	Class
	0.000	0.000	?	0.000	?	0.500	0.130	GBS
	1.000	1.000	0.870	1.000	0.931	0.500	0.870	GESIS
W. Avg.	0.870	0.870	?	0.870	?	?	0.500	0.774

Table 3.1: Some descriptive statistics of location and dispersion for 2100 observed swap rates for the period from February 15, 1999 to March 2, 2007. Swap rates measured as 3.12 (instead of 0.0312). See Table ?? in the appendix for more details.

### 3.3 Learning from Positive and Unlabeled Data

Breiman [9] introduced bagging as a technique to construct strong ensembles by combining a set of base models. Breiman [10] stated that the essential problem in combining classifiers is growing a suitably diverse ensemble of base classifiers which can be done in various ways [12]. In bagging, the ensemble models use majority voting to aggregate decisions of base models which are trained on bootstrap resamples of the training set. From a Bayesian point of view, bagging can be interpreted as a Monte Carlo integration over an approximated posterior distribution [40].

In his landmark paper, Breiman [9] noted that base model instability is an important factor in the success of bagging which led to the use of inherently unstable methods like decision trees in early bagging approaches [19, 11]. The main mechanism of bagging is often said to be variance reduction [4, 10]. In more recent work, Grandvalet [24] explained that base model instability is not related to the intrinsic variability of a predictor but rather to the presence of influential instances in a data set for a given predictor (so-called leverage points). The effect of bagging is explained as equalizing the influence of all training instances, which is beneficial when highly influential instances are harmful for the predictors accuracy.

We have shown the effect of resampling contaminated sets and provided some basic insight into the mechanics of bagging. We will now link these two elements to justify bagging approaches in the context of contaminated training sets. Its usefulness can be considered by both the variance reduction argument of Bauer and Kohavi [4] and equalizing the influence of training points as described by Grandvalet [24]. Variance reduction. Resampling a contaminated set yields different levels of contamination in the resamples as explained in Section 3.1. Varying the contamination between base model training sets induces variability between base models without increasing bias. This observation enables us to create a diverse set of base models by resampling both P and U. The variance reduction of bagging is an excellent mechanism to exploit the variability of base models based on resampling [4, 10]. In the context of RESVM, a tradeoff takes place between increased variability (by training on smaller resamples, see Figure 1) and base models with increased stability (larger training sets for the SVM models). (<https://arxiv.org/pdf/1402.3144.pdf>)

---

**Input:**  $P$ : set of positive instances (GESIS)

$U$ : set of unlabeled instances (GBS)

$n_{models}$ : number of base models in ensemble

$n_P$ : size of bootstrap sample of  $P$

$n_U$ : size of bootstrap sample of  $U$

**Result:** Scoring function  $f : U \rightarrow \mathbb{R}$

---

Initialize:  $f(x) \leftarrow 0$  and  $c(x) \leftarrow 0$

**for**  $t = 1$  to  $n_{models}$  **do**

    Draw a bootstrap sample  $P_t$  of size  $n_P$ .

    Draw a bootstrap sample  $U_t$  of size  $n_U$ .

    Train classifier  $f_t$  to discriminate  $P_t$  against  $U_t$ .

    For any  $x \in U \setminus U_t$ , update:

$$f(x) \leftarrow f(x) + f_t(x),$$

$$c(x) \leftarrow c(x) + 1$$

**end**

Return

$$s(x) = f(x)/c(x)$$

**Algorithm 1:** PU training procedure

### 3.3.1 Recovering Model Performance

methods to estimate true classification performance.

be recovered with the knowledge of class priors

results in biased empirical estimates of the classifier performance now can be corrected with the knowledge of class priors using the One-Class SVM and its ability to capture the shape of the data set, hence performing better when the data is strongly non-Gaussian, i.e. with two well-separated clusters;

The ROC curve provides in-sight into trade-offs between the classifiers accuracies on positive versus negative examples over a range of decision thresholds. (pr-rec) curve, a plot of precision as a function of recall. The precision-recall evaluation, including summary statistics

derived from the pr-rc curve, may be preferred to ROC curves when classes are heavily skewed (Davis and Goad-rich 2006). Although model learning and performance evaluation in a supervised setting are well understood (Hastie et al. 2001), the availability of unlabeled data gives additional options and also presents new challenges. A typical semi-supervised scenario involves the availability of positive, negative and (large quantities of) unlabeled data. Here, the unlabeled data can be used to improve training (Blum and Mitchell 1998) or unbiased the labeled data (Cortes et al. 2008); e.g., to estimate class proportions that are necessary to calibrate the model and accurately estimate precision when class balances (but not class-conditional distributions) in labeled data are not representative (Saerens et al. 2002). This is often the case when it is more expensive or difficult to label examples of one class than the examples of the other.

The intuition for these results comes from the fact that in many practical situations, the posterior distributions in traditional and non-traditional setting provide the same optimal ranking of data points on a given test sample (Jain et al. 2016; Jain, White, and Radivojac 2016).

Such performance estimation often involves computing the fraction(s) of correctly and incorrectly classified examples from both classes; however, in absence of labeled negatives, the fractions computed under the non-traditional evaluation are incorrect, resulting in biased estimates. Figure 1 illustrates the effect of this bias by showing the traditional and non-traditional ROC curves on a handmade data set. Because some of the unlabeled examples in the training set are in fact positive, the area under the ROC curve estimated when the unlabeled examples were considered negative (non-traditional setting) underestimates the true performance for positive versus negative classification (traditional setting). This paper formalizes and evaluates performance estimation of a non-traditional classifier in the traditional setting when the only available training data are (possibly noisy) positive examples and unlabeled data.

Though the efficacy of non-traditional classifiers has been thoroughly studied (Peng et al. 2003; Elkan and Noto 2008; Ward et al. 2009; Menon et al. 2015), estimating their true performance has been much less explored.

the widely-accepted evaluation approaches using ROC or pr-rc curves are insensitive to the variation of raw prediction scores unless they affect the ranking.

Let  $f$  be the true distribution over the input space  $X$  from which unlabeled data is drawn. With distributions  $f_1$  and  $f_0$  of the positive and negative examples, respectively, it follows



that

$$f(x) = \alpha f_1(x) + (1 - \alpha) f_0(x)$$

with positive class prior  $\alpha \in [0, 1], x \in X$ .

Consider the binary classification problem from input  $x \in X$  (BFI-10 and BRS data) to output  $y \in Y$  (representative: '1', not representative: '0'). The learning objective is to discriminate between  $X_p$  drawn according to  $f_1$  and  $X_u$  drawn according to  $f$  and recover its performance estimate in the traditional setting, i.e. evaluating the decision boundary between positive and negative data.

The two main criteria considered in this work are the area under the ROC curve (AUC) and the F-Measure. The ROC curve plots the true positive rate (recall) of a classifier as a function of its false positive rate (Fawcett 2006) over a range of decision thresholds. Furthermore, AUC has a meaningful probabilistic interpretation that is used to the ability of the classifier to separate classes and is often used to rank classifiers (Hanley and McNeil 1982). Another important performance criterion generally used in information retrieval relies on the precision-recall

The most extensively studied and widely used performance evaluation in binary classification involves estimating the Receiver Operating Characteristic (ROC) curve

Recall  $\gamma$ , FPR  $\eta$  and Precision  $\rho$  are defined as:

$$\gamma = P[\hat{Y} = 1 | Y = 1]$$

$$\eta = P[\hat{Y} = 1 | Y = 0]$$

$$\rho = P[Y = 1 | \hat{Y} = 1]$$

where  $\hat{Y}$  is an estimate of the true class label  $Y$ .

TPR  $\gamma$  can be estimated directly, because  $X_p$  was sampled from  $f_1$ , while this does not hold true for  $\eta$  given the absence of samples from  $f_0$ .

$$\gamma = \mathbb{E}[f_1[h(x)]] = \frac{1}{|X_p|} \sum_{x \in X_p} h(x)$$

$$\hat{\gamma}^{pu} = \mathbb{E}[f[h(x)]] = \frac{1}{|X|} \sum_{x \in X} h(x)$$

The area under precision-recall curves  $AUPR$  can be expressed using the approximated

value for the fraction of positives  $\alpha$  in  $X_u$

$$\rho = \frac{\alpha\gamma}{\hat{\eta}^{pu}}$$

The area under ROC curves  $AUROC^{pu}$  so far could only be estimated for the positive versus unlabeled classification by plotting  $\gamma$  and  $\hat{\eta}^{pu}$ . To calculate  $AUC$  from  $AUC^{pu}$ , S. Jain et al. (2015) express  $\eta$  in terms of  $\hat{\eta}^{pu}$  and  $\alpha$  and provide a full derivation from the probabilistic definition of the AUC with

$$\eta = \frac{\hat{\eta}^{pu} - \alpha\gamma}{1 - \alpha}$$

so that

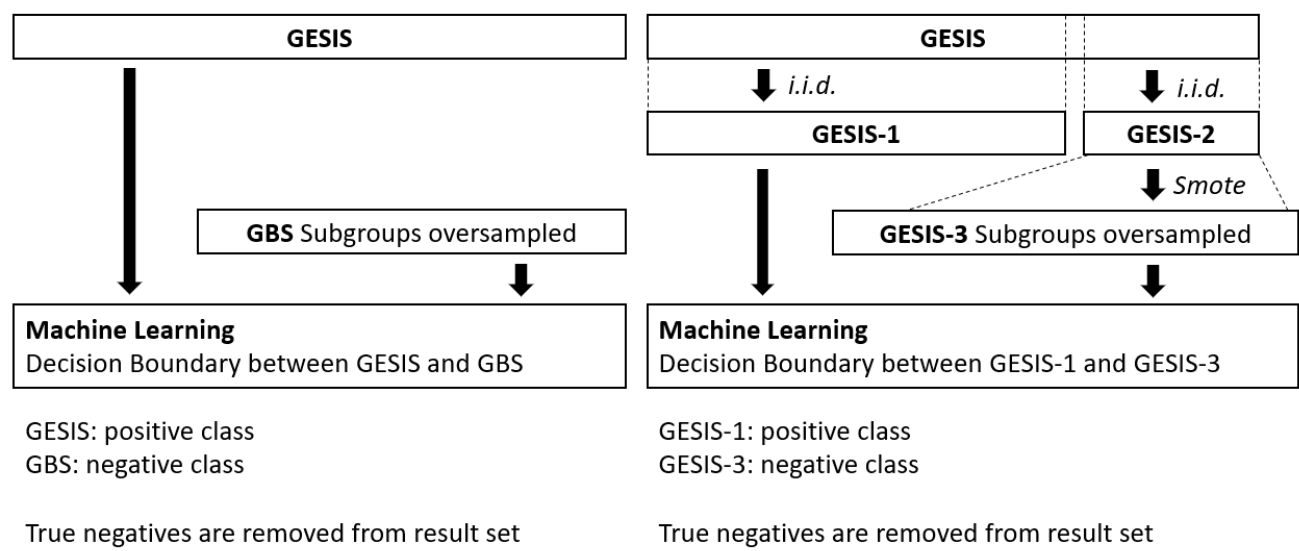
$$AUC = \frac{AUC^{pu} - \frac{\alpha}{2}}{1 - \alpha}$$

proving

$$AUC > AUC^{pu} \iff AUC^{pu} > \frac{1}{2}$$

### 3.4 Artificial Data Synthesis

Try to avoid giving the synthesized data properties that makes it possible for a learning algorithm to distinguish synthesized from non-synthesized example such as if all the synthesized data comes from one of 20 car designs, or all the synthesized audio comes from only 1 hour of car noise. This advice can be hard to follow.





## 4 RESULTS

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### 4.1 Maximal Representative Subsample

There is almost always not enough data available to partition it into separate training and test sets without losing significant modelling or testing capability. In these cases, a fair way to properly estimate model prediction performance is to use cross-validation as a powerful general technique[5].

The overly optimistic resubstitution error, is not a good indicator of model performance. To evaluate the actual performance of a model, the given data samples need to be split. The proper procedure uses three sets: training data, validation data, and test data [2]. The holdout method is the most common approach to get a reliable performance estimation: A certain amount of data is reserved for testing while the remainder is used for the actual training. Because the method is very fast, it is useful to use when the algorithm is slow to train and the dataset is large. Training and test sets might not be representative of the same underlying distribution, e.g. class hardly represented in the test set.

The holdout estimate can be made more reliable by repeating the process with different subsamples. The error rates on the different iterations are averaged to yield an overall error rate. To further reduce the variance of the error estimate, each class is sampled with approximately equal proportions in both datasets, a technique called stratification. Figure X shows the results on the GFI-10 data.

#### 4.1.1 Fraction of Positives

Estimating Positive Class Prior with One-Class SVMs. In a simple random sample, one can assume that observations are independent from each other. The complex sample design of GBS however

, e.g. multi-stage samples from different survey periods, Complex sample design, such as multi-stage samples of schools, classes and students, students from one classroom are likely to be more correlated than those from another classroom.

we need to compensate for complex survey designs with features including, but not limited to, unequal likelihoods of selection, differences in response rates across key subgroups, and

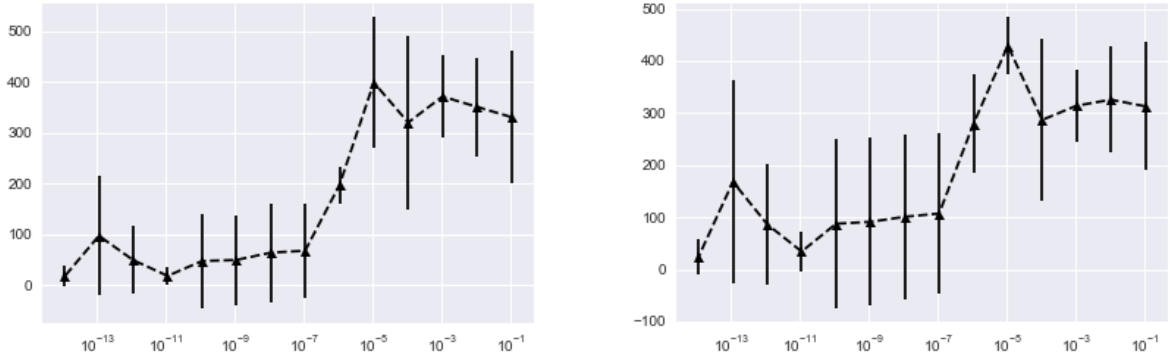


Figure 4.1: Tuning parameter  $nu$  that controls the trade-off between the fraction of non-representative samples and the number of support vectors in one-class SVM. More than 0.73 of GBS (right) are classified as representative with high confidence (low sdt) for the optimal value  $nu = 10^{-5}$ .

deviations from distributions on critical variables found in the target population from external sources, such as a national Census

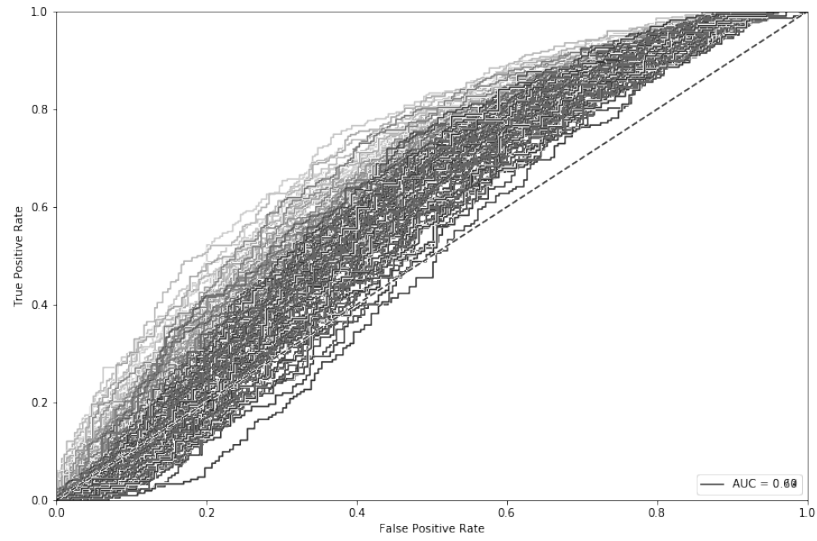
### 4.1.2 ROC and puROC Evaluation

most commonly through the development of survey weights for statistical adjustment. If complex sample designs are implemented in data collection but the analysis assumes simple random sampling, the variances of the survey estimates can be underestimated and the confidence interval and test statistics are likely to be biased (Heeringa, West, Berglund, 2010).

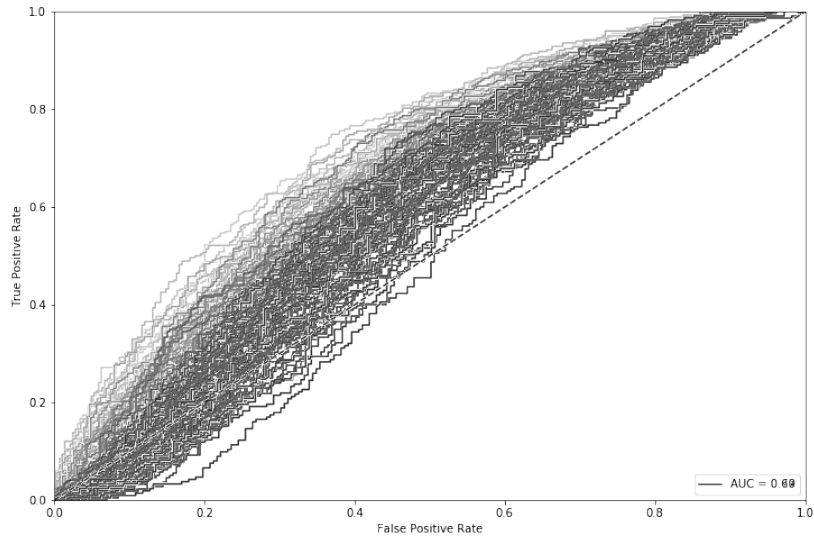
In a recent meta-analysis of 150 sampled research papers analyzing several surveys with complex sampling designs, it is found that analytic errors caused by ignorance or incorrect use of the complex sample design features were frequent. Such analytic errors define an important component of the larger total survey error framework, produce misleading descriptions of populations and ultimately yield misleading inferences (Aurelien, West, Sakshaug, 2016). It is thus of critical importance to incorporate the complex survey design features in statistical analysis.

## 4.2 Political Participation and Resilience

XGBoost is an open-source software library for predictive modelling, created by Tianqi Chen in 2014 [1]. The name XGBoost stands for "Extreme Gradient Boosting" and implements



(a) Feature importance GBS (n=579) in classification of political participation "Wahlteilnahme".



(b) Feature importance GBS MRS (n=280) in classification of political participation "Wahlteilnahme".

Figure 4.2: (a) Numerical solutions for the small-time system with a constant-curvature body shape showing the scaled leading-order vertical.

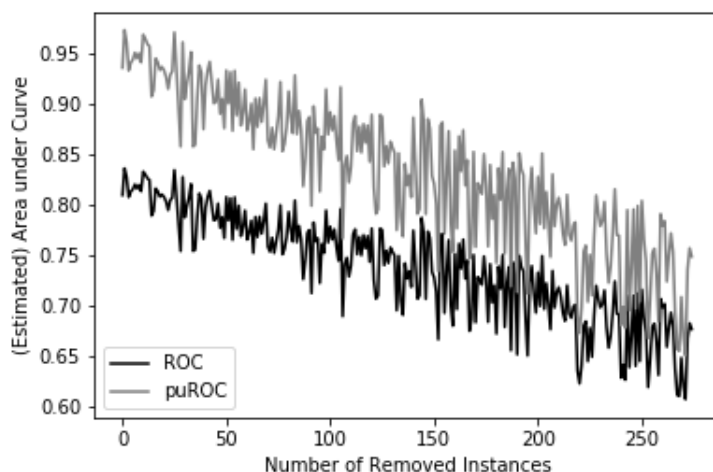
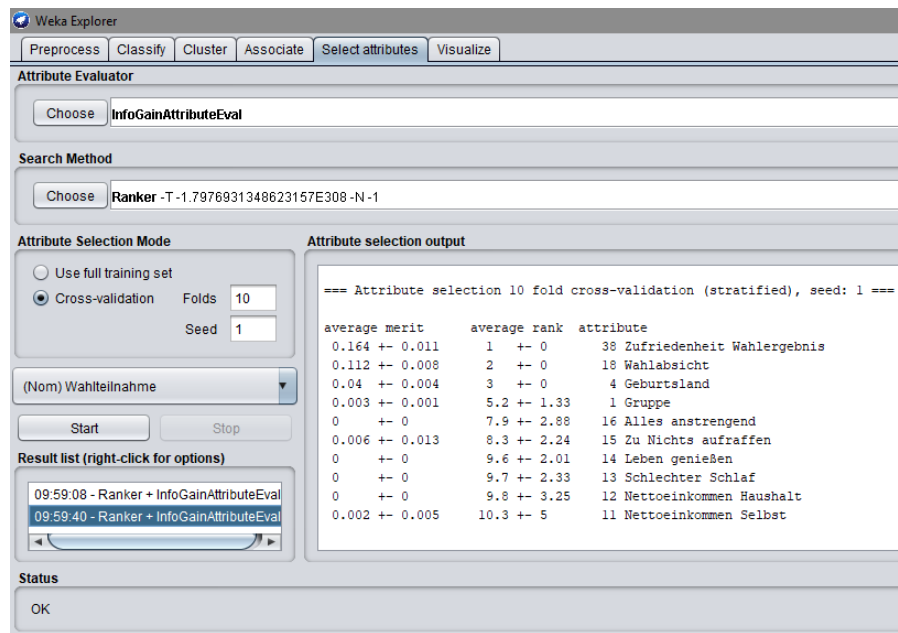


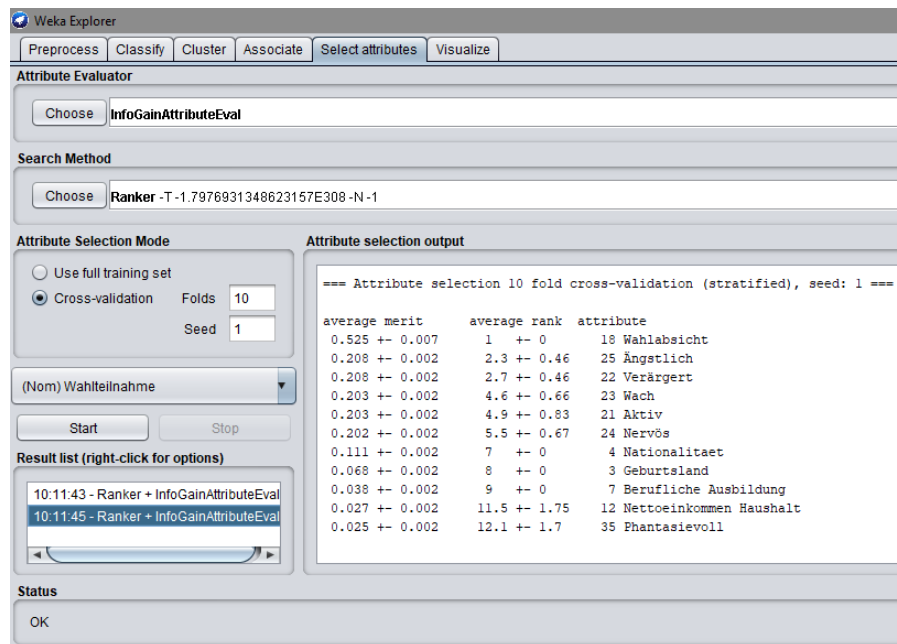
Figure 4.3: .

"Gradient Boosting" as proposed in Greedy Function Approximation: A Gradient Boosting Machine by Friedman, while the term "extreme" refers to the engineering goal to maximize the resources used by the algorithm to achieve high accuracy, computational efficiency and scalability. What started off as a terminal application for a research project, has become a scalable end-to-end tree boosting system that has integrations with scikit-learn in Python, the caret package in R, as well as big data frameworks like Apache Spark and Hadoop. Since its introduction, XGBoost has been used in more than half of the winning solutions in Kaggle competitions, after it gained much popularity and attention in the community by winning the Higgs boson machine learning challenge.





(a) Feature importance GBS (n=579) in classification of political participation "Wahlteilnahme".



(b) Feature importance GBS MRS (n=280) in classification of political participation "Wahlteilnahme".

Figure 4.4: (a) Numerical solutions for the small-time system with a constant-curvature body shape showing the scaled leading-order vertical.



## 5 CONCLUSION

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Imbalanced setting where the minority class GBS is the unlabeled class of interest but handled as negative. evaluation in the absence of actual negatives is further enhanced by class imbalance. puF-Measure instead of (or in addition to) puROC could reduce the effects of class imbalance. inclusion of f1-measure would be interesting. finally, the label "representative" is actually a property of a sample and not its single instances. survey mismatch from gbs to gesis renders most attributes useless regarding entropy. forces valu comparisons essentially introduce non existent pattern. one class classification suffers from high variance in estimating the fraction of actually representative gbs data. assessment of binary classifiers in pu settings does not lead to more accurate roc curve estimations as the fraction of positives cannot be estimated. overrepresentative underrep. rep and nonrep. trthroughout the thesis are not properly defined.

at the analysis stage or the manuscript writing stage, this leads to time-consuming and cost-inefficient rechecking of data, redoing analyses, and rewriting of the manuscript. The following is a list of issues that IDA may detect that show the possible importance of such detection:

This combination of class imbalance with non-stationary environments poses significant and interesting practical problems for classification

Numerical summaries of distributions A distribution can be summarized with various descriptive statistics. The mean and median capture the center of a distribution (central tendency) while the variance describes the distribution spread or variability (see online book material). Mean: the average of a number of values. It is calculated by adding up the values and dividing by the number of the values (how many the values there are).

Median: The "median is the number separating the higher half of a data sample, a population, or a probability distribution, from the lower half" (Reviews, 2013). For a highly skewed distribution, the median may be a more appropriate measure of central tendency than the mean. For example, the median is more widely used to characterize income, since potential outliers (e.g., those with very high incomes) have much more impact on the mean.

Variance: Variance is a measure of the extent to which a set of numbers are "spread out".

Precision: Precision is the reciprocal of the variance and is most commonly seen in Bayesian analysis (see Guideline 9).



## BIBLIOGRAPHY

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GALLANT, A. R. (1987): *Nonlinear Statistical Models*, New York: John Wiley & Sons.



## A SUPPLEMENTARY MATERIAL

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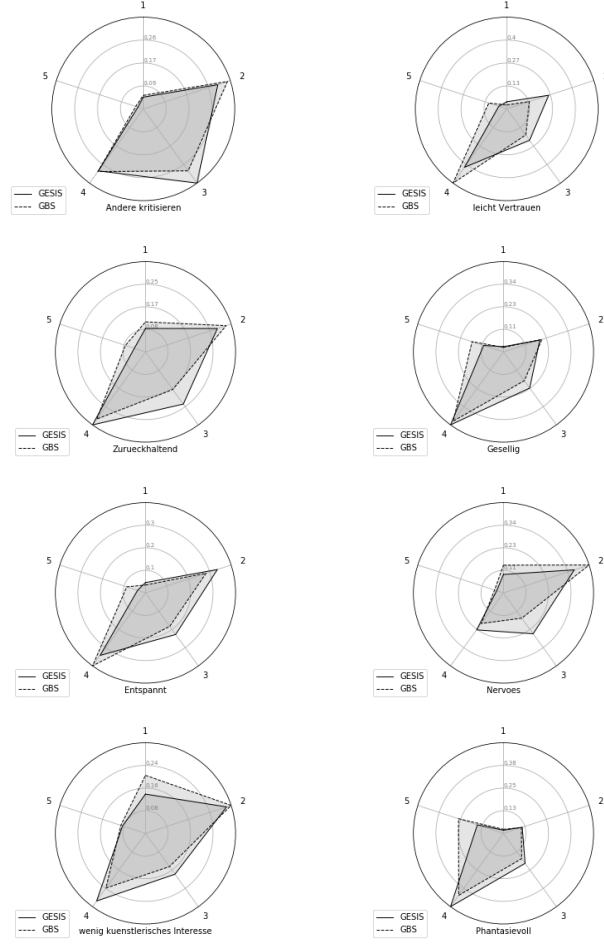


Figure A.1: Agreeableness is the measure of one's cooperation, empathy, and willingness to trust and help others. Openness estimates whether one is hesitant or eager about new objects or situations. Extraversion refers to level of sociability, seeking and enjoyment of social contact, and energy and assertiveness in social situations. Neuroticism is characterized by easily experiencing negative emotions, and a poor coping response to those emotions. The cyclic structure of the chart, i.e. "Strongly Disagree" next to Strongly Agree", provides a vivid example for the central-tendency bias across all items.

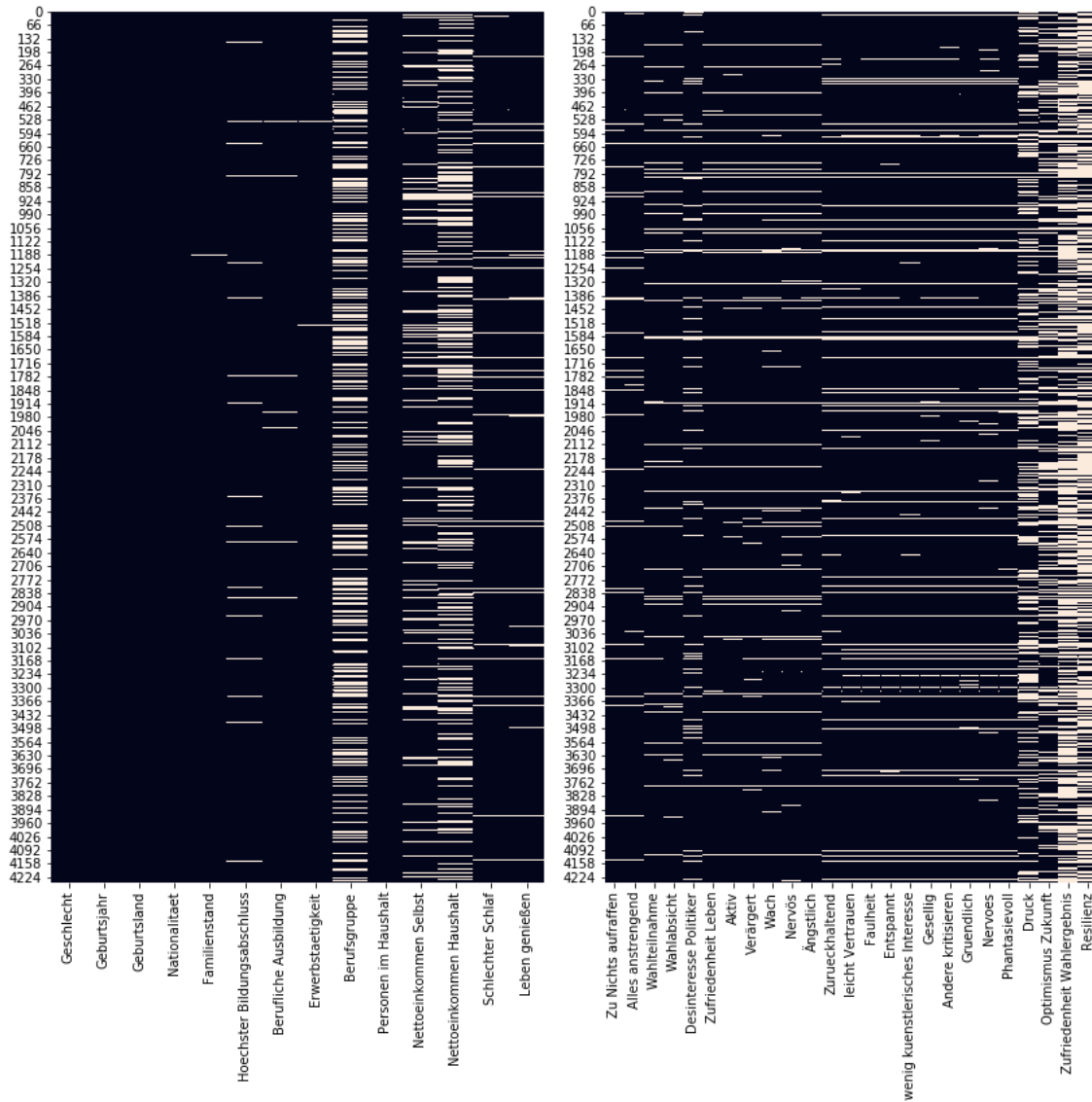


Figure A.2: Missing values in GESIS. The attribute values of a participant are always known for "Geschlecht", "Geburtsland", "Geburtsjahr", "Nationalitaet", "Familienstand", "Personen im Haushalt". In contrast, the last three columns "Druck", "Optimismus Zukunft", "Zufriedenheit Wahlergebnisse" and "Resilienz" are almost always missing and are therefore removed from the analysis. Participants with missing BFI-10 elements are removed. Sample size will only be reduced slightly as missing values often occur for the same instance. These dependencies form a line pattern in the graph. "Berufsgruppe" was surveyed as a text field so that the column clearly suffers from ambiguous value mismatch. To include "Berufsgruppe" mappings need to be redefined first. For now, "Berufsgruppe" is removed.



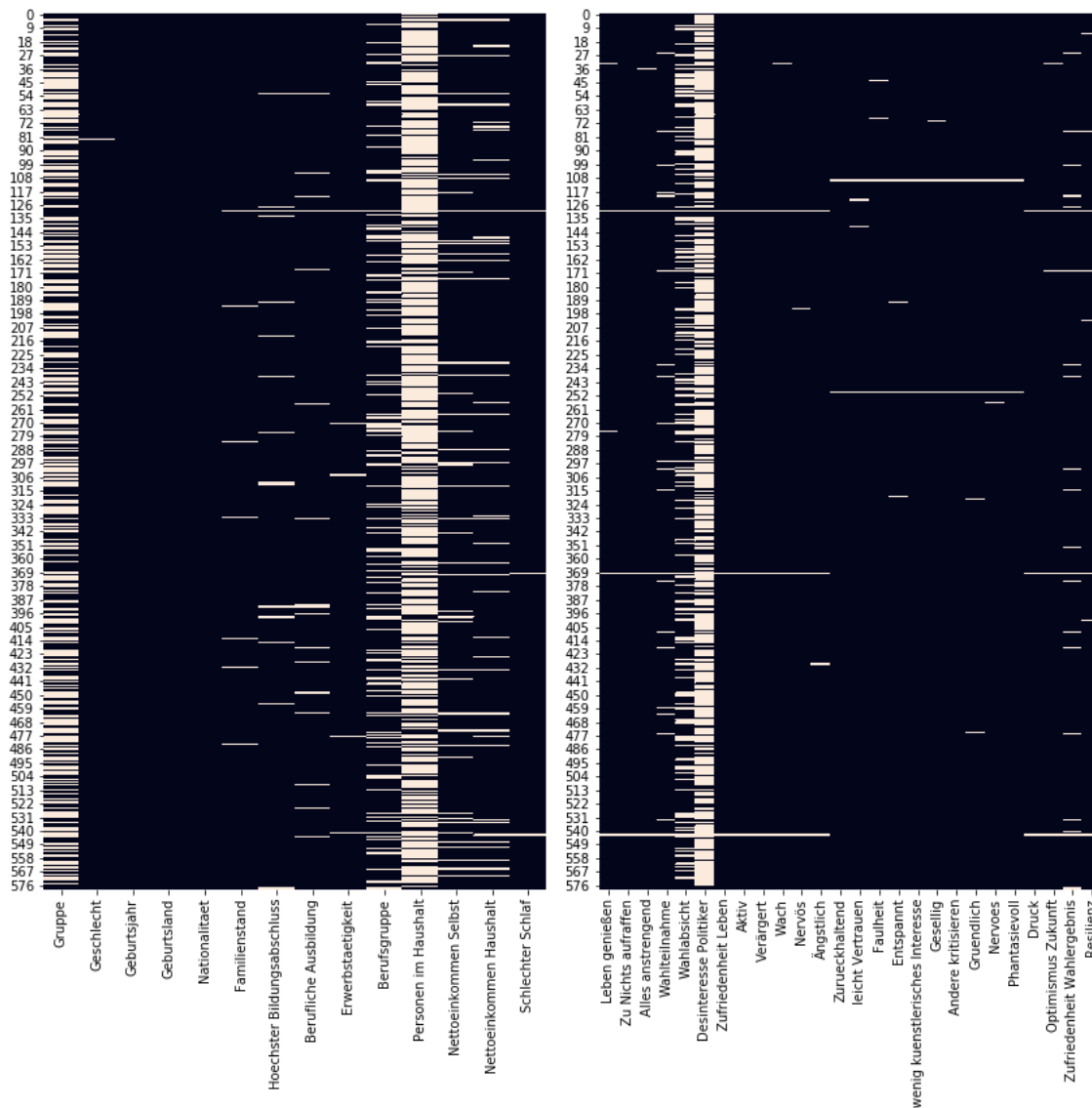


Figure A.3: Missing values in GBS. There is one more attribute in "Gruppe". Not every participant received a positive a negative psychological treatment. Therefore, "Gruppe" is more likely to be missing than not. However, the absence of a value indicates no treatment rather than a missing positive or negative. "Gruppe" is not properly represented yet. "Desinteresse Politiker" is given by multiple data sources from different excel files. Some of them being the inverse of the attribute itself. The survey design regarding this issue is unclear to me. To incorporate "Desinteresse Politiker" the attribute(s) need to be imported correctly, if possible. Another import issue is given by "Personen im Haushalt". If the actual value is greater than one, the cell will be empty. To correct this, the corresponding csv-file needs to be fixed. The text field "Berufsgruppe" suffers on both ends, GBS and GESIS, due to current oversimplification of value and potential data mismatch.

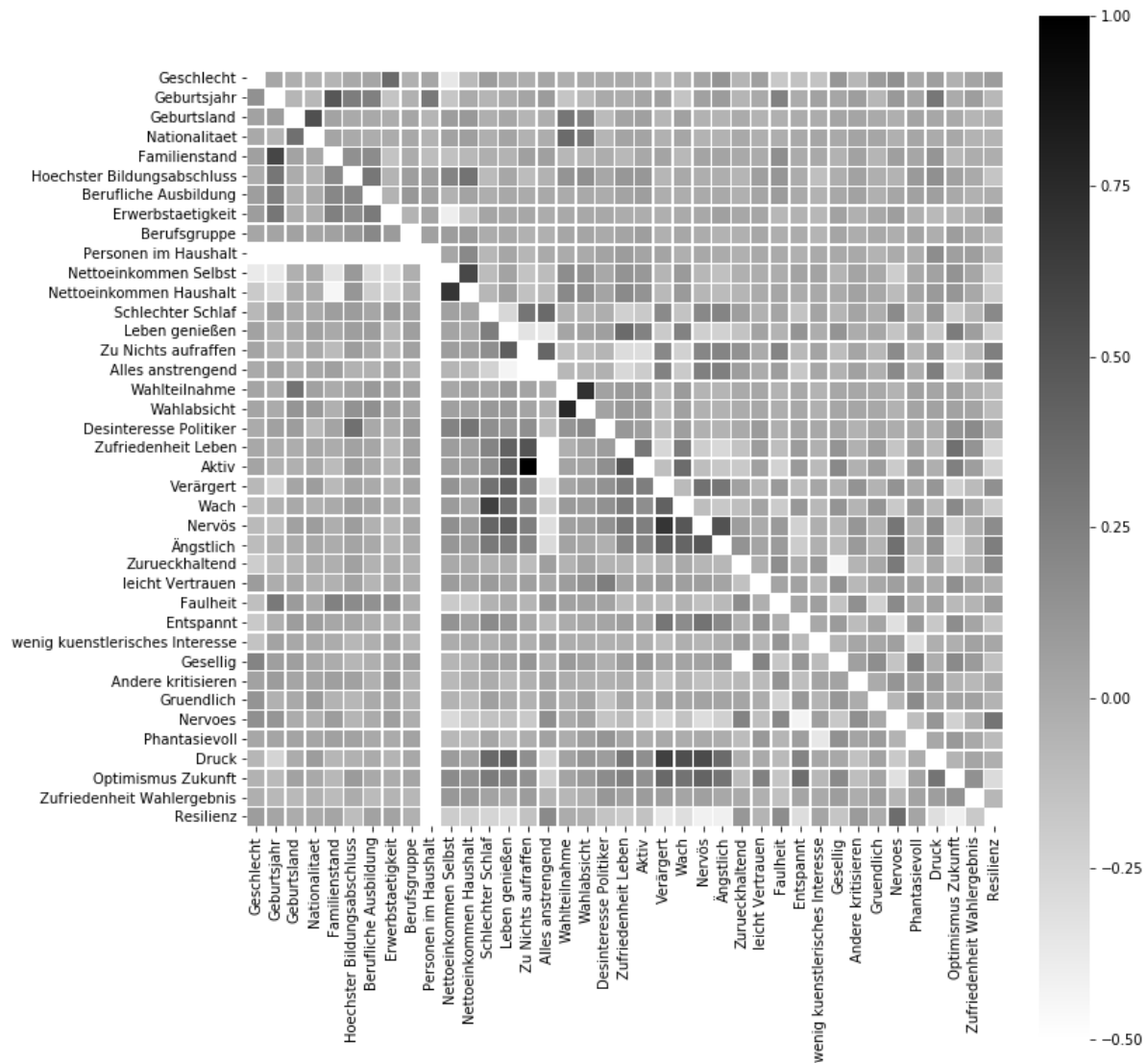












Figure A.4: The upper right triangular matrix shows GESIS correlations while GBS correlations are shown in the lower left. The main diagonal should not be confused with white squares. These trivial combinations are simply excluded and not colored black. As can be seen "Personen im Haushalt" in GBS can not be calculated, since there is only one possible value. "Nettoeinkommen Selbst" and "Nettoeinkommen Haushalt" are highly correlated but not removed or handled at all. I will keep this in mind, when facing the naive bayes assumption in the learning process. Entropy-based mutual information in "Wahlteilnahme" and "Wahlabsicht" have led to almost perfect classification performances in predicting political participation. "Wahlabsicht" is therefore removed.


## B GITHUB REPOSITORY

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 laksannathan update todo and ideas

Latest commit 88209c6 5 hours ago

 data	add more plots	a day ago
 docs	add appendix	5 hours ago
 src	switched ida and feas	9 hours ago
 tex	add appendix	5 hours ago
 .gitignore	starting to work in germany	2 days ago
 LICENSE	Initial commit	9 days ago
 README.md	add appendix	5 hours ago
 ideas.txt	update todo and ideas	5 hours ago
 todo.txt	update todo and ideas	5 hours ago

 README.md

### Discriminative Machine Learning for Maximal Representative Subsampling

This project deals with selection bias in social sciences. Discriminative learners are trained and combined to reduce the effects of bias in psychological and political studies. With positive-unlabeled learning and artificial data synthesis, performance estimation becomes more accurate in a non-traditional setting.

### Motivation

In scope of my bachelor thesis, the main goal is to apply machine learning to the fields of survey analytics.

### Installation

Python 3.6+ with Jupyter notebook and WEKA are necessary to get a development env running. If random\_state is not provided, any init will come close to analysed results.

### Project Structure

```
.
├── ...
├── data                # data sources: GESIS and GBS
│   ├── raw_input      # survey results
│   └── _proc.csv       # preprocessed (ml ready) data
├── docs                # documentation on data sources
├── src                 # source code: Python, WEKA
├── tex                 # thesis: LaTeX Code
│   ├── paper          # MRS thesis
│   └── fig             # figures, tables and plots
```

### License

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Figure B.1: The upper right triangular matrix ”erformances in predicting political participation. ”Wahlabsicht” is therefore removed.



# DECLARATION OF AUTHORSHIP

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I hereby confirm that I have authored this Bachelor's thesis independently and without use of others than the indicated sources. All passages which are literally or in general matter taken out of publications or other sources are marked as such.

Mainz, October 15, 2018

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**Laksan Nathan**