Beyond the Selected Completely At Random Assumption for Learning from Positive and Unlabeled Data

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Abstract

Most positive and unlabeled data is subject to selection biases. The labeled examples can, for example, be selected from the positive set because they are easier to obtain or more obviously positive. This paper investigates how learning can be enabled in this setting. We propose and theoretically analyze an empirical-risk-based method for incorporating the labeling mechanism. Additionally, we investigate under which assumptions learning is possible when the labeling mechanism is not fully understood and propose a practical method to enable this. Our empirical analysis supports the theoretical results and shows that taking into account the possibility of a selection bias, even when the labeling mechanism is unknown, improves the trained classifiers.

Introduction

Positive and unlabeled learning focuses on the setting where the training data contains some labeled positive examples and unlabeled examples, which could belong to either the positive or negative class. This contrasts to supervised learning, where a learner has a fully labeled training set and to semi-supervised learning, where a learner (usually) observes some labeled examples from each class. PU data naturally arises in many applications. Electronic medical records (EMR) list diseases that a patient has been diagnosed with, however, many diseases are undiagnosed. Therefore, the absence of a diagnoses does not imply that a patient does not have the disease. Similarly, automatically constructed knowledge bases (KBs) are incomplete, and hence any absent tuple may be either true (i.e., belong in the knowledge base) or false (Zupanc and Davis 2018).

Elkan and Noto (2008) formalized one of the most commonly made assumptions in PU learning, which is that the observed positive examples were selected completely at random from the set of all positive examples. This assumption means that the probability of observing the label of a positive example is constant (i.e., the same for all positive examples). This assumption facilitates and simplifies both theoretical analysis and algorithmic design. Indeed, how to analyze and learn from PU data has been extensively explored in the literature (Denis 1998; Lee and Liu 2003; Liu et al. 2003; Liu et al. 2005; Denis, Gilleron, and Letouzey 2005; Zhang and Lee 2005; Mordelet and Vert 2014; Claesen et al. 2015).

Unfortunately, the “selected completely at random” assumption is often violated in real-world data sets. For example, a patient’s EMR will only contain a diagnosis if she visits a doctor, which will be influenced by factors such as the severity of the symptoms and her socio-economic status. The problem of biases in the observed labels has been recognized in the recommender systems literature (Schnabel et al. 2016; Marlin and Zemel 2009). However, that task differs from PU learning in that it (1) focuses on multi-class predictions (e.g., five star ratings), and more crucially (2) that the labels for some examples from each class are observed. Still, within the context of PU learning, there has been little (or no) work that focuses on coping with biases in the observed positive labels.

The contribution of this paper is to take a step towards filling that gap by proposing and analyzing a new, less restrictive assumption for PU learning: the Selected At Random (SAR) assumption. Instead of assuming a constant probability for all positive examples to be labeled, it assumes that the probability is a function of a subset of an example's attributes. To help analyze this new setting, we leverage the idea of a propensity score, which is term originating from the causal inference literature (Imbens and Rubin 2015). Intuitively, the propensity score can be thought of as an instance-specific probability that an example was selected to be labeled. We show theoretically how using propensity scores in a SAR setting provides benefits. Then, we discuss a practical approach for learning the propensity scores from the data and using them to learn a model. Empirically, we show that for SAR PU data, our approach results in improved performance over making the standard selected completely at random assumption.

Preliminaries

The goal of learning from positive and unlabeled (PU) data is to train a binary classifier that distinguishes between positive and negative examples, while only having access to a subset of the positive examples. The dataset is thus a set of triples \((x, y, s)\) with \(x\) a vector of the attributes, \(y\) the class and \(s\) a binary variable representing whether the tuple was selected to be labeled. The class \(y\) is always missing, but information about it can be derived from the value of \(s\). If
$s = 1$, then the example belongs to the positive class as $\Pr(y = 1|s = 1) = 1$, but when $s = 0$, the instance can belong to either class.

In PU learning, it is common to make the Selected Completely At Random (SCAR) assumption, which assumes that the observed positive examples are a random subset of the complete set of positive examples. Selecting a positive example is therefore independent of the example’s attributes $\Pr(s = 1|y = 1, x) = \Pr(s = 1|y = 1)$. The probability for selecting a positive example to be labeled is known as the label frequency $c = \Pr(s = 1|y = 1)$. A neat advantage of the SCAR assumption is that, using the label frequency, a model that predicts the probability of an example being labeled can be transformed to the classifier:

$$\Pr(y = 1|x) = \Pr(s = 1|x)/c.$$  

Knowing the label frequency is equivalent to knowing the class prior $\alpha = \Pr(y = 1)$ because the one can be calculated from the other: $c = \Pr(s = 1)/\alpha$. Under the SCAR assumption, PU learning is therefore reduced to estimating the class prior or label frequency and training a model to predict the observed labels.

Estimating the label frequency is an ill-defined problem because it is not identifiable: the absence of a label can be explained by either a small prior probability for the positive class or a low label frequency (Scott 2015). In order for the class prior to be identifiable, additional assumption are necessary. Different assumptions have been proposed, but they are all based on attributing as many missing classes as possible to the lower label frequency as opposed to a lower positive class probability. The following assumptions are listed from strong to strictly weaker. Elkan and Noto (2008) and du Plessis and Sugiyama (2014) make the strongest assumption: that the classes are non-overlapping, which makes the class prior and the labeled distribution match the unlabeled one as closely as possible. Scott (2015), du Plessis, Niu, and Sugiyama (2015) and Bekker and Davis (2018) make the assumption that there exists a positive subdomain of the instance space, but the classes can overlap elsewhere. Ramaswamy, Scott, and Tewari (2016) assumes that a function exists which only selects positive instances. Finally, Blanchard, Lee, and Scott (2010) and Jain, White, and Radivojac (2016) make the irreducibility assumption which states that the negative distribution cannot be a mixture that contains the positive distribution.

### Labeling Mechanisms for PU Learning

The mechanism behind selecting positive examples to be labeled is called the labeling mechanism. To date, PU learning has largely focused on the SCAR setting. However, clearly labels are not missing completely at random in most real-world problems. For example, the data included in automatically constructed KBs is biased several ways. One is that it is learned from Web data, and only certain types of information appear on the Web (e.g., it is easier to find text about high-level professional sports teams than low-level ones). Two, the algorithms used to extract information from the Web employ heuristics to ensure that only information that is likely to be accurate (e.g., by using redundancy) is included in the KB. Similarly, biases arise when people decide to like items online, bookmark webpages, or subscribe to mail lists. Therefore we believe it is important to consider and study other labeling mechanisms.

When Elkan and Noto (2008) first formalized the SCAR assumption, they noted the similarity of the PU setting to the general problem of learning in the presence of missing data. Specifically, they noted that the SCAR assumption is somewhat analogous with the missing data mechanism called **Missing Completely At Random (MCAR)** (Rubin 1976). Apart from MCAR, the two other classes of missing data mechanisms are **Missing At Random (MAR)** and **Missing Not Random (MNAR)**. To complete this analogy, we propose the following corresponding classes of PU labeling mechanisms:

**SCAR** **Selected Completely At Random**: The labeling mechanism does not depend on the attributes of the example, nor on the probability of the example being positive, i.e., each positive example has the same probability to be labeled.

**SAR** **Selected At Random**: The labeling mechanism depends on the values of the attributes of the example, but given the attribute values it does not depend on the probability of the example being positive.

**SNAR** **Selected Not At Random**: All other cases: The labeling mechanism depends on the real probability of this example being positive, even given the attribute values.

There is one very important difference between PU labeling mechanisms and missingness mechanisms in that the labeling always depends on the class value: only positive examples can be selected to be labeled. According to the missingness taxonomy, all PU labeling mechanisms are therefore MNAR. SNAR is a peculiar class because it depends on the real class probability, while the class needs to be positive by definition. The class probability refers to the probability of an identical instance to this one being positive. Consider, for example, the problem of classifying pages as interesting. If a page is moderately interesting to you, some days you might say like it while other days that you do not. The labeling mechanism in this case could depend on how much you like them and therefore on the instance’s class probability.

### Learning with SAR Labeling Mechanisms

In this paper, we focus on SAR labeling mechanisms, where the key question is how can we enable learning from SAR PU data? Our key insight is that the labeling mechanism is also related to the notion of a propensity score from causal inference (Imbens and Rubin 2015). In causal inference, the propensity score is an instance-specific probability, based on a set of an example’s attributes, that is assigned to the treatment or control group. We use an analogous idea and define the propensity score as the labeling probability for positive examples:

**Definition 1** (Propensity Score). The **propensity score**, denoted $e(x)$, for $x$ is the label assignment probability for positive instances with $X = x$,

$$e(x) = \Pr(s = 1|y = 1, x)$$
A crucial difference with the propensity score from causal inference is that our score is conditioned on the class being positive.

We propose a new method for incorporating the propensity score when learning in a PU setting, by using the propensity scores to reweight the data. In causal inference, inverse-propensity-scoring is a standard method where the examples are weighted with the inverse of their propensity score [Little and Rubin 2002; Imbens and Rubin 2015; Schnabel et al. 2016]. This cannot be applied when working with positive and unlabeled data because we have zero probability for labeling negative examples. But we can do a different kind of weighting. The insight is that for each labeled example \( (x_i, s = 1) \) that has a propensity score \( e_i \), there are expected to be \( \frac{1}{e_i} \) positive examples, of which \( \frac{1}{e_i} - 1 \) did not get selected to be labeled. This insight can be used in algorithms that use counts, to estimate the correct count from the observed positives and their respective propensity scores. In general, this can be formulated as learning with negative weights: every labeled example gets a weight \( \frac{1}{e_i} \) and for every labeled example a negative example is added to the dataset that gets a negative weight \( 1 - \frac{1}{e_i} \).

We now provide a theoretical analysis of the propensity-weighted method, to characterize its appropriateness. We consider two cases: (1) when we know the true propensity scores and (2) when we must estimate them from data. All the proofs are deferred to the appendix.

Case 1: True Propensity Scores Known

Standard evaluation measures, such as Mean Absolute Error (MAE), Mean Square Error (MSE) and log loss, can be formulated as follows:

\[
R(\hat{y}|y) = \frac{1}{n} \sum_{i=1}^{n} y_i \delta_1(\hat{y}_i) + (1 - y_i) \delta_0(\hat{y}_i),
\]

with \( n \) the size of \( y \) and \( \hat{y} \) and \( \delta_0(\hat{y}) \) represents the cost for predicting \( \hat{y} \) when the class is \( y \), for example:

- MAE: \( \delta_0(\hat{y}) = |y - \hat{y}| \),
- MSE: \( \delta_0(\hat{y}) = (y - \hat{y})^2 \),
- Log Loss: \( \delta_1(\hat{y}) = -\ln \hat{y} \), \( \delta_0(\hat{y}) = -\ln(1 - \hat{y}) \).

We can formulate propensity-weighted variants estimator of these cost functions as follows:

**Definition 2** (Propensity-Weighted Estimator). Given propensity the scores \( e \) and PU labels \( s \), the propensity weighted estimator of \( R(\hat{y}|y) \) is

\[
\hat{R}(\hat{y}|e, s) = \frac{1}{n} \sum_{i=1}^{n} s_i \left( \frac{1}{e_i} \delta_1(\hat{y}_i) + (1 - \frac{1}{e_i}) \delta_0(\hat{y}_i) \right) + (1 - s_i) \delta_0(\hat{y}_i),
\]

where \( y \) and \( \hat{y} \) are vectors of size \( n \) containing, respectively, the true labels and predicted labels. \( \delta_p(\hat{y}) \) is the cost for predicting \( \hat{y} \) when the true class is \( y \).

This estimator is unbiased:

\[
\mathbb{E}[\hat{R}(\hat{y}|e, s)] = \frac{1}{n} \sum_{i=1}^{n} \frac{y_i e_i}{e_i} \left( \frac{1}{e_i} \delta_1(\hat{y}_i) + (1 - \frac{1}{e_i}) \delta_0(\hat{y}_i) \right) + (1 - y_i e_i) \delta_0(\hat{y}_i)
\]

\[
= \frac{1}{n} \sum_{i=1}^{n} y_i \delta_1(\hat{y}_i) + (1 - y_i e_i) \delta_0(\hat{y}_i) = R(\hat{y}|y)
\]

To characterize how much the estimator can deviate from the expected value, we provide the following bound:

**Proposition 1** (Propensity-Weighted Estimator Bound). For any predicted classes \( \hat{y} \) and real classes \( y \) of size \( n \), with probability \( 1 - \eta \), the propensity-weighted estimator \( \hat{R}(\hat{y}|s, e) \) does not differ from the true evaluation measure \( R(\hat{y}|y) \) more than

\[
|\hat{R}(\hat{y}|e, s) - R(\hat{y}|y)| \leq \sqrt{\frac{\delta_{\max}^2 \ln \frac{2}{\eta}}{2n}},
\]

with \( \delta_{\max} \) the maximum absolute value of cost function \( \delta_\eta \).

The propensity-weighted estimator can be used as the risk for Expected Risk Minimization (ERM), which searches for a model in the hypothesis space \( \mathcal{H} \) by minimizing the risk:

\[
\hat{y}_R = \arg\min_{\hat{y} \in \mathcal{H}} \hat{R}(\hat{y}|e, s)
\]

The following proposition characterizes how much the estimated risk for hypothesis \( \hat{y}_R \) can deviate from its true risk.

**Proposition 2** (Propensity-Weighted ERM Generalization Error Bound). For a finite hypothesis space \( \mathcal{H} \), the difference between the propensity-weighted risk of the empirical risk minimizer \( \hat{y}_R \) and its true risk is bounded, with probability \( 1 - \eta \), by:

\[
R(\hat{y}_R|y) \leq \hat{R}(\hat{y}_R|e, s) + \sqrt{\frac{\delta_{\max}^2 \ln \frac{|\mathcal{H}|}{\eta}}{2n}}
\]

Case 2: Propensity Scores Estimated from Data

Often the exact propensity score is unknown, but we have an estimate \( \hat{e} \) of it. In this case, the bias of the propensity-weighted estimator is:

**Proposition 3** (Propensity-Weighted Estimator Bias).

\[
\text{bias}(\hat{R}(\hat{y}|e, s)) = \frac{1}{n} \sum_{i=1}^{n} \frac{y_i (1 - \frac{1}{e_i})}{e_i} (\delta_1(\hat{y}_i) - \delta_0(\hat{y}_i))
\]

From the bias, it follows that the propensity scores only need to be accurate for positive examples. An incorrect propensity score has a larger impact when the predicted classes have more extreme values (i.e., tend towards zero or one). Underestimated propensity scores are expected to result in a model with a higher bias. Lower propensity scores result in learning models that estimate the positive class to be more prevalent than it is, which results in a larger \((\delta_1(\hat{y}_i) - \delta_0(\hat{y}_i))\) for positive examples.
Side Note on Sub-Optimality of Expected Loss  Another method that one might be inclined to use when incorporating the propensity score is to minimize the expected loss\footnote{Derivation in appendix}.

\[
\hat{y}^* = \arg\min_{y \in \mathbb{R}} \frac{1}{n} \sum_{i=1}^{n} \left( s_i \left( 1 - s_i \left( \frac{y_i - e_i}{1 - y_i e_i} \right) \right) \delta_1(y_i) \\
+ (1 - s_i) \frac{1 - y_i}{1 - y_i e_i} \delta_0(y_i) \right)
\]

This is, however, not expected to give an unbiased estimate of \( f \), but will prefer classifiers which predict class probabilities closer to 0 or 1. To see this, take for example the simple case of a constant propensity score \( \forall i: e_i = 0.5 \), no distinction between examples \( \forall i,j: x_i = x_j \) and 30 out of 100 examples have a positive label. The unbiased estimate for \( f \) would be 0.6, however, depending on the loss function it can minimize to 0.0 (MSE) or 1.0 (log loss).

Learning under the SAR Assumption

If the propensity scores for all examples are known (i.e., the exact labeling mechanism is known), they can be directly incorporated into the learning algorithm. However, it is more likely that they are unknown. Therefore, this section investigates how to permit learning in the SAR setting when the exact propensity scores are unknown. We discuss two such settings. The first is interesting from a theoretical perspective and the second from a practical perspective.

Reducing SAR to SCAR

Learning the propensity scores from positive and unlabeled data requires making additional assumptions: if any arbitrary instance can have any propensity score, then it is impossible to know if an instance did not get labeled because of the low propensity score or low class probability. Therefore, the propensity score needs to depend on fewer attributes than final classifier \cite{imbens2015}. A simple way to accomplish this is to assume that the propensity function only depends on a subset of the attributes: the propensity attributes \( x_e \in x \):

\[
\Pr(s = 1 | y = 1, x) = \Pr(s = 1 | y = 1, x_e)
\]

Often, this is not an unrealistic assumption. It is trivially true if the labeling mechanism does not access all attributes (e.g., because some were collected later). It may also arise if a labeler cannot interpret some attributes (e.g., raw sensor values) or only uses the attributes that are known to be highly correlated with the class.

To see why this can be a sufficient assumption for learning in a SAR setting, consider the case where the propensity attributes \( x_e \) have a finite number of configurations, which is true if these attributes are all discrete. In this case, it is possible to partition the data into strata, with one strata for each configuration of \( x_e \). Within a strata, the propensity score is a constant (i.e., all positive examples have the same propensity score) and can thus be determined using standard SCAR PU learning techniques. Note that, as discussed in the preliminaries, the SAR assumption alone is not enough to enable learning from PU data, and hence one of the additional assumptions \cite{blanchard2010, scott2015, du2015, ramaswamy2016, bekker2018} must be made.

Reducing SAR to SCAR is suboptimal in practice as it does not work if \( x_e \) contains a continuous variable. Even for the discrete case, the number of configurations grows exponential as the size of \( x_e \) increases. Furthermore, information is lost by partitioning the data. Some smoothness of the classifier over the propensity attributes is expected, but this is not encouraged when learning different classifiers for each configuration. Similarly the propensity score itself is expected to be a smooth function over the propensity variables.

EM for Propensity Estimation

In practice, due to the problems with reducing the SAR to the SCAR case, it is best to jointly search for a classifier and lower dimensional propensity score function that best explain the observed data. This approach also offers the advantage that it relaxes the additional assumptions: if they hold in the majority of the propensity attributes’ configurations, the models’ smoothness helps to overcome potential issues arising in the configurations where the assumptions are violated. This subsection presents a simple expectation-maximization method for simultaneously training the classification and the propensity score model. It aims to maximize the expected log likelihood of the combination of models.

**Expectation** Given the expected classification model \( \hat{f} \) and propensity score model \( \hat{e} \), the expected probability of the positive class \( \hat{y}_i \) of instance \( x_i \) with label \( s_i \) is:

\[
\hat{y}_i = \Pr(y_i = 1 | s_i, x_i, \hat{f}, \hat{e}) = s_i + (1 - s_i) \frac{\hat{f}(x_i) (1 - \hat{e}(x_i))}{1 - \hat{f}(x_i) \hat{e}(x_i)}.
\]

**Maximization** Given the expected probabilities of the positive class \( \hat{y}_i \), the models \( f \) and \( e \) are trained to optimize the expected log likelihood:

\[
\max_{f,e} \sum_{i=1}^{n} \mathbb{E}_{y_i|x_i, s_i, \hat{f}, \hat{e}} \ln \Pr(x_i, s_i, y_i | f, e)
\]

\[
= \max_{f} \sum_{i=1}^{n} \left[ \hat{y}_i \ln \hat{f}(x_i) + (1 - \hat{y}_i) \ln(1 - \hat{f}(x_i)) \right]
\]

\[
= \max_{e} \sum_{i=1}^{n} \hat{y}_i \left[ s_i \cdot \ln \hat{e}(x_i) + (1 - s_i) \cdot \ln(1 - \hat{e}(x_i)) \right]
\]

From the maximization formula, it can be seen that to optimize the log likelihood, the models both need to optimize

\( \hat{f} \)

\( \hat{e} \)
the log loss of a weighted dataset. The classification model \( f \) receives each example twice, once as positive, weighted by the expected probability of it being positive \( y_i \), and once as negative, weighted by the expected probability of it being negative \( 1 - y_i \). The propensity score model \( e \) receives each example once, positive if the observed label is positive and negative otherwise, weighted by the expected probability of it being positive \( y_i \).

This method is expected to work best if the classes are separable, because the log loss of the classifier is being minimized. In fact, if the classes are not separable, then the trained classification model is not expected to be the optimal one for the trained propensity model (see previous section). In that case, it is advisable to retrain the classifier with the obtained propensity score, using the propensity-weighted risk estimation method.

The classification model is initialized by fitting a balanced model which considers the unlabeled examples as negative. This is a good starting point because the true class prior is likely to be closer to 0.5 than to the ratio of labeled examples. The propensity score model is initialized by using the classification model to estimate the probabilities of each unlabeled example being positive.

Classic EM converges when the log likelihood stops improving. However, the likelihood could stop improving before the propensity score model has converged. Convergence is therefore formulated as convergence of both the log likelihood and the propensity model. We measure the change in the propensity score model by the average slope of the minimum square error line through the propensity score prediction of the last \( n \) iterations.

**Empirical Evaluation**

The aim of this section is to answer the following questions:

**Q1** How does propensity-weighted learning perform with a provided propensity score function or label frequency? And how is the performance affected by:

**Q1a** The number of propensity attributes?

**Q1b** A biased estimate of the propensity score function?

**Q1c** Class correlation of the propensity attributes?

**Q2** Can the SAR assumption facilitate better learning from SAR PU data when the propensity score is unknown?

**Q2a** Can the propensity score function be recovered?

**Q2b** Does the number of propensity attributes and their correlation with the class affect the performance?

**Data**

We use eight real-world datasets that are summarized in Table 1. For 20 News Groups we distinguish between computer (pos) and recreational (neg) documents. After removing their headers, footers, quotes, and English stopwords, the documents were transformed to 200 word occurrence attributes using the Scikit-Learn count vectorizer. For Cover Type, we distinguish the Lodgepole Pine (pos) from all other cover type (neg). The Diabetes data was preprocessed in a similar manner to [Strack et al., 2014](http://archive.ics.uci.edu/ml/). Additionally we dropped attributes with the same value in 95% of the examples, and replaced uncommon attribute values by “other”. The positive class is patients being readmitted within 30 days. Image Segmentation was used to distinguish between nature (sky, grass or foliage) and other scenes (brickface, cement, window, path). Adult, Breast Cancer, Mushroom, and Splice were used as is. All the datasets were further preprocessed to have exclusively continuous attributes, scaled between -1 and 1. Multivalued attributes were binarized.

**Methodology and Approaches**

**Constructing Datasets.** The datasets were randomly partitioned into train (80%) and test (20%) sets five times. For each of the five train-test splits, we transformed the data into positive and unlabeled datasets in a number of ways. First, the number of attributes used to derive the propensity score was varied from one to four. Only attributes that had a standard deviation of at least 0.6 were considered. The attributes were selected in one of two ways: (1) at random, which was then repeated for three different combinations of attributes or (2) based on the largest correlation with the class.

For a given set of selected attributes, positive examples were selected to be labeled according to the following propensity score:

\[
e(x_e) = \prod_{i=1}^{k} \left( \text{sc}(x_e(i), p^-, p^+) \right)^{\frac{x_e(i)-\min x_e(i)}{\max x_e(i)-\min x_e(i)}}
\]

This gives propensity scores between \( p^- \) and \( p^+ \), with all propensity attributes attributing equally to it. In our experiments the propensity scores were between 0.2 and 0.8. For each set of selected propensity attributes, we generated five labelings.

**Settings and Approaches.** We consider two settings. Within in each setting we consider three approaches:

Table 1: Datasets

| Dataset         | # Instances | # Attrib | Pr(\( y = 1 \)) |
|-----------------|-------------|----------|-----------------|
| 20 Newsgroups   | 3,979       | 200      | 0.55            |
| Adult           | 48,842      | 14       | 0.24            |
| Breast Cancer   | 683         | 9        | 0.35            |
| Cover Type      | 581,012     | 54       | 0.49            |
| Diabetes        | 99,492      | 127      | 0.11            |
| Image Segm.     | 2,310       | 18       | 0.43            |
| Mushroom        | 8,124       | 111      | 0.48            |
| Splice          | 3,175       | 60       | 0.52            |
Figure 1: Propensity-weighted learning performs well for any number of propensity attributes.

assuming the data is SAR and using propensity score weighting (denoted SAR), assuming the data is SCAR and using class prior weighting (denoted SCAR), and assuming all unlabeled examples belong to the negative class (denoted (Naive)). We also show the performance given fully supervised data (denoted Sup.). We always use logistic regression as the base classifier. Setting 1 assumes that the true propensity scores (SAR) or the true class prior (SCAR) are provided. Setting 2 assumes that these must be estimated from data. Here, our EM method was to estimate the the propensity score under SAR assumptions. To estimate the class prior, two state-of-the-art methods for learning under SCAR assumptions were used with standard settings: KM2 from Ramaswamy, Scott, and Tewari (2016) and TičE from Bekker and Davis (2018).

Question 1b investigates the effect of over- and underestimated propensity score estimates. The correct propensity score or label frequency was altered with a bias ∈ {1.1, 1.3, 1.5}, multiplying the score with it for an overestimated or dividing for a negative one.

Unless the correlation of propensity attributes with the class is explicitly studied, propensity models with random attributes are used for the experiments.

Evaluation Metric. The Mean Square Error (MSE) is used to report performance. We evaluate two things: (1) classification performance, and (2) the propensity model performance. When evaluating the propensity models, we compared the predicted propensity score from our model to the true propensity scores.

Results with Provided Propensity Scores

A1 & A1a. Either incorporating the propensity score or using the class prior leads to better classification performance than naively assuming all unlabeled examples are negative (Fig. 1). When the PU data is generated by a SAR labeling mechanism where the propensity scores depends on the attribute values, training a model using the propensity scores results in superior performance compared to making

the SCAR assumption. This is true even though the SCAR learner knows the correct label frequency.

A1b. Using an under- or overestimated propensity score clearly affects the performance, however in most cases the biased propensity scores, and even often biased label frequencies, outperform treating the unlabeled examples as negative. Interestingly, an overestimate hurts the performance less. This is in agreement with proposition 3 (Fig. 2).

A1c. The correlation, either positive or negative, of the propensity attributes with the class has a big influence on the difficulty of the problem, as can be understood from the performance of the naive approach. It has a smaller influence when the label frequency was used and is almost unnoticeable when using the propensity scores (Fig. 3).

Results with Learned Propensity Scores

A2. When the labeling mechanism is unknown, but the propensity attributes are, learning both the propensity score and the classification model from the data almost always outperforms learning under the SCAR assumption or the naive method. For the diabetes dataset, the naive method seems outperforms all others. The dataset is very imbalanced and MSE is not the most appropriate measure in this case. The F1 scores for Diabetes are 0.15 (Sup.), 0.24 (SAR), 0.20 (KM2), 0.20 (TičE) and 0.09 (Naive), showing that actually SAR is here to the best method (Table 2).
A2a. Learning under SAR assumptions always results in a better model than under SCAR assumptions (Table 3).

A2b. When increasing the number of propensity attributes, the MSE of the propensity model improves for most settings, both SAR and SCAR. Like noted before, this is because the more variables, the better the variations in the label frequency can be explained as noise. The MSE of the SAR classification model is mostly unaffected by the number of attributes (Fig. 4). The correlation of the propensity attributes with the class does not have a large effect on the performance when learning under SAR assumptions (Fig. 5).

Related Work

PU learning is also a special case of semi-supervised learning (Chapelle, Scholkopf, and Zien 2009). Furthermore, it is also related to one-class learning (Khan and Madden 2014). As previously noted, almost all PU learning work that we are aware of focuses on the setting with the observed positive examples are selected completely at random from the set of all positive examples. The work of Schnabel et al. (2016) on dealing with biases in the observed ratings for recommender systems is also closely related to ours. They also make use of propensity scores to cope with the biases. However, there is a crucial difference in that their approach has access to labels for all classes. This is important in practice as that means that the propensity score for each example is non-zero. In contrast, in PU learning, the propensity score for any negative example is zero: You never observe these labels.

Conclusions

This paper investigates learning from SAR PU data: positive and unlabeled data with non-uniform labeling mechanisms. We proposed and theoretically analyzed a empirical-risk-minimization based method for weighting PU datasets with the propensity scores to achieve unbiased learning. Furthermore, we explored which assumptions are necessary to learn from SAR PU data generated by an unknown labeling mechanism. We proposed a practical EM-based method for this setting. Empirically, we demonstrated that for SAR PU data our proposed propensity weighted method offers superior performance over making the SCAR. This is true for both given and learned propensity scores.
References

[2018] Bekker, J., and Davis, J. 2018. Estimating the class prior in positive and unlabeled data through decision tree induction. In Proceedings of the 32th AAAI Conference on Artificial Intelligence.

[2010] Blanchard, G.; Lee, G.; and Scott, C. 2010. Semi-supervised novelty detection. Journal of Machine Learning Research 11:2973–3009.

[2009] Chapelle, O.; Scholkopf, B.; and Zien, A. 2009. Semi-supervised learning. IEEE Transactions on Neural Networks 20(3):542–542.

[2015] Claesen, M.; De Smet, F.; Suykens, J. A. K.; and De Moor, B. 2015. A robust ensemble approach to learn from positive and unlabeled data using svm base models. Neurocomputing 160:73–84.

[2005] Denis, F.; Gilleron, R.; and Letouzey, F. 2005. Learning from positive and unlabeled examples. Theoretical Computer Science 348(1):70–83.

[1998] Denis, F. 1998. Pace learning from positive statistical queries. In ALT.

[2014] du Plessis, M. C., and Sugiyama, M. 2014. Class prior estimation from positive and unlabeled data. IEICE Transactions 97-D:1358–1362.

[2015] du Plessis, M. C.; Niu, G.; and Sugiyama, M. 2015. Class-prior estimation for learning from positive and unlabeled data. Machine Learning 106:463–492.

[2005] Elkan, C., and Noto, K. 2008. Learning classifiers from only positive and unlabeled data. In KDD.

[1963] Hoeffding, W. 1963. Probability inequalities for sums of bounded random variables. Journal of the American statistical association 58(301):13–30.

[2015] Imbens, G. W., and Rubin, D. B. 2015. Causal inference in statistics, social, and biomedical sciences. Cambridge University Press.

[2016] Jain, S.; White, M.; and Radivojac, P. 2016. Estimating the class prior and posterior from noisy positives and unlabeled data. In NIPS.

[2014] Khan, S., and Madden, M. 2014. One-class classification: taxonomy of study and review of techniques. The Knowledge Engineering Review.

[2003] Lee, W. S., and Liu, B. 2003. Learning with positive and unlabeled examples using weighted logistic regression. In ICML, 448–455.

[2002] Little, R., and Rubin, D. 2002. Statistical analysis with missing data. John Wiley & Sons.

[2003] Liu, B.; Dai, Y.; Li, X.-L.; Lee, W.; and Yu, P. 2003. Building text classifiers using positive and unlabeled examples. In ICDM, 179–186.

[2005] Liu, Z.; Shi, W.; Li, D.; and Qin, Q. 2005. Partially supervised classification—based on weighted unlabeled samples support vector machine. In ADMA, 118–129.

[2009] Marlin, B. M., and Zemel, R. S. 2009. Collaborative prediction and ranking with non-random missing data. In Proceedings of the 2009 ACM Conference on Recommender Systems, 5–12.

[2014] Mordelet, F., and Vert, J.-P. 2014. A bagging svm to learn from positive and unlabeled examples. Pattern Recognition Letters 201–209.

[2016] Ramaswamy, H.; Scott, C.; and Tewari, A. 2016. Mixture proportion estimation via kernel embedding of distributions. In ICML.

[1976] Rubin, D. 1976. Inference and missing data. Biometrika.

[2016] Schnabel, T.; A.Swaminathan; A.Singh; Chandak, N.; and Joachims, T. 2016. Recommendations as treatments: Debiasing learning and evaluation. In ICML.

[2015] Scott, C. 2015. A rate of convergence for mixture proportion estimation, with application to learning from noisy labels. In AISTATS.

[2014] Strack, B.; DeShazo, J.; Gennings, C.; Olmo, J.; Ventura, S.; Cios, K.; and Clore, J. 2014. Impact of hba1c measurement on hospital readmission rates: analysis of 70,000 clinical database patient records. BioMed research international.

[2005] Zhang, D., and Lee, W. 2005. A simple probabilistic approach to learning from positive and unlabeled examples. In UKCI, 83–87.

[2018] Zupanc, K., and Davis, J. 2018. Estimating rule quality for knowledge base completion with the relationship between coverage assumption. In Proceedings of the Web Conference.
Proof of Proposition [1]

Proposition 1 (Propensity-Weighted Estimator Bound). For any predicted classes $\hat{y}$ and real classes $y$ of size $n$, with probability $1 - \eta$, the propensity-weighted estimator $\hat{R}(\hat{y}|e, s)$ does not differ from the real evaluation measure $R(y)$ more than

$$|\hat{R}(\hat{y}|e, s) - R(y)| \leq \sqrt{\frac{\delta_{\max}^2 \ln \frac{2}{\eta}}{2n}},$$

with $\delta_{\max}$ the maximum absolute value of cost function $\delta_y$.

Proof. All the examples are selected to be labeled independently from each other. Therefore, the weighted costs of the examples are independent random variables. As a result, the Hoeffding inequality can be applied [Hoeffding 1963]:

$$\Pr(|\hat{R}(\hat{y}|e, s) - E[\hat{R}(\hat{y}|e, s)]| \geq \epsilon) \leq 2 \exp \left(-\frac{2n\epsilon^2}{\delta_{\max}^2}\right)$$

$$\leftrightarrow \Pr(|\hat{R}(\hat{y}|e, s) - R(y)| \geq \epsilon) \leq 2 \exp \left(-\frac{2n\epsilon^2}{\delta_{\max}^2}\right)$$

By setting defining the right-hand side of the inequality to $\eta$, the bound $\epsilon$ can be calculated in terms of $\eta$:

$$\eta = 2 \exp \left(-\frac{2n\epsilon^2}{\delta_{\max}^2}\right)$$

$$\epsilon = \sqrt{\frac{\delta_{\max}^2 \ln \frac{2}{\eta}}{2n}}.$$

Proof of Proposition [2]

Proposition 2 (Propensity-Weighted ERM Generalization Error Bound). For a finite hypothesis space $\mathcal{H}$, the difference between the propensity-weighted risk of the empirical risk minimizer $\hat{y}_R$ and its true risk is bounded, with probability $1 - \eta$, by:

$$R(\hat{y}_R|y) \leq \hat{R}(\hat{y}_R|e, s) + \sqrt{\frac{\delta_{\max}^2 \ln |\mathcal{H}|}{2n}}$$

Proof. For a finite hypothesis space $\mathcal{H}$, the propensity-weighted estimator $\hat{R}(\hat{y}|e, s)$ and real classes $y$ are independent random variables. As a result, the Hoeffding inequality can be applied:

$$\Pr\left(|\hat{R}(\hat{y}|e, s) - R(\hat{y}|y)\right) \geq \epsilon \right) \leq \Pr\left(|\hat{R}(\hat{y}|e, s) - R(y)| \geq \epsilon \right)$$

$$\leq \Pr\left(|\hat{R}(\hat{y}|e, s) - R(y)\right) \geq \epsilon \right) \leq \Pr\left(|\hat{R}(\hat{y}|e, s) - R(y)\right) \geq \epsilon \right)$$

$$\leq \sum_{i=1}^{|\mathcal{H}|} \Pr\left(|\hat{R}(\hat{y}|e, s) - R(y)| \geq \epsilon \right)$$

$$\leq |\mathcal{H}| \cdot \exp \left(-\frac{2n\epsilon^2}{\delta_{\max}^2}\right) = \eta$$

$$\epsilon = \sqrt{\frac{\delta_{\max}^2 \ln \frac{|\mathcal{H}|}{\eta}}{2n}}.$$

Proof of Proposition [3]

Proposition 3 (Propensity-Weighted Estimator Bias).

$$\text{bias}(\hat{R}(\hat{y}|e, s)) = \frac{1}{n} \sum_{i=1}^n y_i \left(1 - \frac{e_i}{e_i}ight) (\delta_1(\hat{y}_i) - \delta_0(\hat{y}_i))$$

Proof.

$$\text{bias}(\hat{R}(\hat{y}|e, s)) = \text{bias}(\hat{R}(\hat{y}|e, s))$$

$$= \frac{1}{n} \sum_{i=1}^n y_i e_i \left(\frac{1}{e_i} \delta_1(\hat{y}_i) + (1 - \frac{1}{e_i}) \delta_0(\hat{y}_i)\right)$$

$$= \frac{1}{n} \sum_{i=1}^n y_i e_i \delta_1(\hat{y}_i) + (1 - y_i e_i) \delta_0(\hat{y}_i)$$

$$= \frac{1}{n} \sum_{i=1}^n y_i \left(1 - \frac{e_i}{e_i}ight) (\delta_1(\hat{y}_i) - \delta_0(\hat{y}_i)).$$
Expected Loss Derivation

The expected loss is defined as

\[ E_{y|e,s,\hat{y}}[R(\hat{y}|y)] = \mathbb{E}_{y|e,s,\hat{y}} \left[ \frac{1}{n} \sum_{i=1}^{n} y_i \delta_1(\hat{y}_i) + (1 - y_i) \delta_0(\hat{y}_i) \right] \]

\[ = \frac{1}{n} \sum_{i=1}^{n} \Pr(y_i = 1|e_i, s_i, y_i) \delta_1(\hat{y}_i) \]

\[ + (1 - \Pr(y_i = 1|e_i, s_i, y_i)) \delta_0(\hat{y}_i) \]

The conditional probabilities \( \Pr(y_i = 1|e_i, s_i, y_i) \) are derived next.

\[ \Pr(y_i = 1|e_i, s_i = 1, \hat{y}_i) = 1 \]

\[ \Pr(y_i = 1|e_i, s_i = 1, \hat{y}_i) = \frac{\Pr(y_i = 1|\hat{y}_i, e_i) \Pr(s = 0|\hat{y} = 1, \hat{y}_i, e_i)}{1 - \Pr(s = 1|\hat{y}, e_i)} \]

\[ = \frac{\hat{y}_i (1 - \Pr(s = 1|\hat{y} = 1, \hat{y}_i, e_i))}{1 - \hat{y}_i e_i} \]

\[ \Pr(y_i = 1|e_i, s_i, \hat{y}_i) = s \Pr(y_i = 1|e_i, s_i = 1, \hat{y}_i) \]

\[ + (1 - s) \Pr(y_i = 1|e_i, s_i = 1, \hat{y}_i) \]

\[ = s + (1 - s) \frac{\hat{y}_i (1 - e_i)}{1 - \hat{y}_i e_i} \]

Filling in the conditional probabilities proofs that

\[ E_{y|e,s,\hat{y}}[R(\hat{y}|y)] \]

\[ = \frac{1}{n} \sum_{i=1}^{n} \left( s_i + (1 - s_i) \frac{\hat{y}_i (1 - e_i)}{1 - \hat{y}_i e_i} \right) \delta_1(\hat{y}_i) \]

\[ + (1 - s_i) \frac{1 - \hat{y}_i}{1 - \hat{y}_i e_i} \delta_0(\hat{y}_i) \]

Expectation Maximization Derivation

Expectation

\[ \Pr(y = 1|s = 1, x) = 1 \]

\[ \Pr(y = 1|s = 0, x) \]

\[ = \frac{\Pr(y = 1|x) \Pr(s = 0|y = 1, x)}{\Pr(s = 0|x)} \]

\[ = \frac{\Pr(y = 1|x) (1 - \Pr(s = 1|y = 1, x))}{1 - \Pr(s = 1|x)} \]

\[ = \frac{\Pr(y = 1|x) (1 - \Pr(s = 1|y = 1, x))}{1 - \Pr(y = 1|x) \Pr(s = 1|y = 1, x)} \]

\[ \Pr(y = 1|s, x, f, e) \]

\[ = s + (1 - s) \frac{f(x) (1 - e(x_e))}{1 - f(x)e(x_e)} \]
Maximization

\[
\max_{f,e} E_{y_i|x_i,s_i,f,e} \sum_{i=1}^{n} \ln \Pr(x_i, s_i, y_i|f, e)
\]

\[
= \max_{f,e} E_{y_i|x_i,s_i,f,e} \sum_{i=1}^{n} \ln \Pr(x_i) \Pr(y_i|x_i, f) \Pr(s_i|y_i, x_i, e) \\
= \max_{f,e} E_{y_i|x_i,s_i,f,e} \sum_{i=1}^{n} \ln \Pr(y_i|x_i, f) \Pr(s_i|y_i, x_i, e) \\
= \max_{f,e,n} \sum_{i=1}^{n} \left[ E_{y_i|x_i,s_i,f,e} \ln \Pr(y_i|x_i, f) + \ln \Pr(s_i|y_i, x_i, e) \right] \\
= \max_{f} \sum_{i=1}^{n} \left[ \hat{y}_i \ln \Pr(y_i = 1|x_i, f) \\
+ (1 - \hat{y}_i) \ln \Pr(y_i = 0|x_i, f) \right] \\
+ \max_{e} \sum_{i=1}^{n} \left[ \hat{y}_i \ln \Pr(s_i|y_i = 1, x_i, e) \\
+ (1 - \hat{y}_i) \ln \Pr(s_i|y_i = 0, x_i, e) \right] \\
= \max_{f} \sum_{i=1}^{n} \left[ \hat{y}_i \ln f(x_i) + (1 - \hat{y}_i) \ln(1 - f(x_i)) \right] \\
+ \max_{e} \sum_{i=1}^{n} \left[ \hat{y}_i [s_i \cdot \ln e(x_i) + (1 - s_i) \cdot \ln(1 - e(x_i))] \\
+ (1 - \hat{y}_i) \ln \Pr(s_i = 0|y_i = 0, x_i, e) \right] \\
= \max_{f} \sum_{i=1}^{n} \left[ \hat{y}_i \ln f(x_i) + (1 - \hat{y}_i) \ln(1 - f(x_i)) \right] \\
+ \max_{e} \sum_{i=1}^{n} \hat{y}_i [s_i \cdot \ln e(x_i) + (1 - s_i) \cdot \ln(1 - e(x_i))]
\]

To avoid a convoluted derivation, we use \( \hat{y}_i \) as a shorthand for \( \Pr(y_i = 1|s_i, x_i, \hat{f}, \hat{e}) \).