Unifying Knowledge Base Completion with PU Learning to Mitigate the Observation Bias

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Abstract

Methods for Knowledge Base Completion (KBC) reason about a knowledge base (KB) in order to derive new facts that should be included in the KB. This is challenging for two reasons. First, KBs only contain positive examples. This complicates model evaluation which needs both positive and negative examples. Second, those facts that were selected to be included in the knowledge base, are most likely not an i.i.d. sample of the true facts, due to the way knowledge bases are constructed. In this paper, we focus on rule-based approaches, which traditionally address the first challenge by making assumptions that enable identifying negative examples, which in turn makes it possible to compute a rule’s confidence or precision. However, they largely ignore the second challenge, which means that their estimates of a rule’s confidence can be biased. This paper approaches rule-based KBC through the lens of PU learning, which can cope with both challenges. We make three contributions. (1) We provide a unifying view that formalizes the relationship between multiple existing confidence measures based on (i) what assumption they make about and (ii) how their accuracy depends on the selection mechanism. (2) We introduce two new confidence measures that can mitigate known biases by using propensity scores that quantify how likely a fact is to be included the KB. (3) We show through theoretical and empirical analysis that taking the bias into account improves the confidence estimates, even when the propensity scores are not known exactly.

1 Introduction

Knowledge Bases (KBs) such as Wikidata (Vrandecic and Krötzsch 2014), YAGO (Rebele et al. 2016) and DBpedia (Auer et al. 2007) are large collections of knowledge about the world. They contain entities, such as Audrey, Belgium and BestActress1960, and facts about those entities such as ⟨Audrey, wasBornIn, Belgium⟩ and ⟨Audrey, wonOscar, BestActress1960⟩. KBs are typically constructed through crowdsourcing or automatically extracting information from the web (Rebele et al. 2016). Consequently, these KBs are incomplete as they do not contain all facts.

Knowledge Base Completion (KBC) (Nickel et al. 2015) aims to address the issue of incompleteness by reasoning over the knowledge base in order to derive new facts that should be included in the KB. This is typically achieved by learning a model from the initial incomplete KB. One common way to do this is to take a rule-based approach (Galárraga et al. 2013; Pellissier Tenon et al. 2017; Zapanc and Davis 2018). This would result in learning rules like ⟨X, wonOscar, Y⟩ → ⟨X, isMarriedTo, Z⟩ → ⟨Z, livesIn, USA⟩, meaning that partners of Oscar winners usually live in the USA. A common measure for the quality of (intermediate) models is confidence (precision), which is the fraction of correctly predicted facts.

However, learning from the incomplete KB is challenging for two important reasons. First, KBs operate under Open World semantics which means that the truth value of any triple not in the KB is unknown. These triples could be true (i.e., they belong in the KB) or false (i.e., they should be excluded from the KB). Practically, this means the data only contains positive examples, whereas most learners require both positive and negative examples. It also implies that a rule’s confidence cannot be computed without making additional assumptions. Second, the way knowledge bases are constructed makes it highly unlikely that the facts included in the observed KB are an i.i.d sample of the facts in the ideal knowledge base, aka the ground truth. Indeed, studies have shown that knowledge bases suffer from observation biases: They contain cultural biases, contain more facts about famous people and represents men and women differently (Callahan and Herring 2011; Wagner et al. 2015; Soulet et al. 2018).

If knowledge base completion is applied while ignoring the observation bias, then the newly inferred facts are likely to strengthen the bias. Yet, to the best of our knowledge, this is what all current KBC methods do.

PU learning (learning from positive and unlabeled examples) (Bekker and Davis 2020), which is concerned with learning a binary classifier while only having access to positive and unlabeled examples, is well-equipped for addressing both these challenges. First, it perfectly matches the type of data available for KBC: the positive examples are the facts in the KB whereas the unlabeled data is any potential fact that is not included in the KB. Second, recent work in PU learning (Kato, Teshima, and Honda 2018; Bekker, Robberechts, and Davis 2019; Gong et al. 2021) has explicitly modeled the selection mechanism that determines the probability of observing a positive example’s label, i.e., the observation bias.

Motivated by this, we view the KBC task as a PU Learning
problem, which enables us to explicitly consider the selection mechanism. We consider rule-based approaches to KBC and make three contributions. (1) We provide a unifying view that formalizes the relationship between multiple existing confidence measures based on (i) what assumption they make about and (ii) how their accuracy depends on the selection mechanism. (2) We introduce two new confidence measures that can mitigate known biases by using propensity scores that quantify how likely a fact is to be included the KB. (3) We show through theoretical and empirical analysis that taking the bias into account improves the confidence estimates, even when the propensity scores are not known exactly.

2 Preliminaries

Knowledge Bases (KBs) store interlinked information about entities in the form of relations between the entities, often as RDF triple stores (WWW Consortium 2004). Using this format, the KB is a triple $(\mathcal{E}, \mathcal{P}, \mathcal{F})$, with $\mathcal{E}$ the set of entities, $\mathcal{P}$ the set of predicates and the $\mathcal{F}$ set of facts, denoted by $\langle s, p, o \rangle$ triples with subject $s \in \mathcal{E}$ and object $o \in \mathcal{E}$ and predicate $p \in \mathcal{P}$, meaning that a relation of type $p$ holds between entities $s$ and $o$. The triples in a KB are a subset of the Cartesian product $\mathcal{E} \times \mathcal{P} \times \mathcal{E}$ and each predicate and entity in $\mathcal{E}$ and $\mathcal{P}$ occurs at least once in a triple in the KB.

A knowledge base models a certain part of the world. We call a knowledge base ideal if it has a triple for each relevant fact, and incomplete if it contains only a subset of those triples. We will consistently use $I$ to refer to the ideal knowledge in some context, and $K$ to a given "known" (incomplete) knowledge base. The task of Knowledge Base Completion (KBC) is then: given a knowledge base $K$, reconstruct the ideal knowledge base $I$.

The KBC task is often approached as follows: given an incomplete knowledge base, rules are derived of the form $\text{Body}(s, o) \Rightarrow \langle s, p, o \rangle$, with the semantics that if $\text{Body}(s, o)$ (some condition on $s$ and $o$) is fulfilled in $K$, then $\langle s, p, o \rangle$ is in $I$. These rules can then be used to derive new facts (facts that are not in $K$, but are in $I$). We follow these semantics: $\text{Body}(s, o)$ is always applied to $K$, predicting $\langle s, p, o \rangle$ to be in $I$. $\text{Body}(s, o)$ is typically a conjunctive condition (Galárraga et al. 2013; Fürnkranz, Gamberger, and Lavrač 2014; Pellissier Tanon et al. 2017; Zupanc and Davis 2018; Lajus, Galárraga, and Suchanek 2020), though this is not essential for this paper.

In the remainder of this paper, we will use the following notation. In the context of a specific rule, $R$ refers to the rule itself, and $p$ refers to the (fixed) predicate of the rule’s prediction. We use the following indicator functions (which return 1 if the associated condition is true and 0 otherwise):

- $R(s, o) : \langle s, o \rangle$ fulfills the rule’s conditions $\text{Body}(s, o)$
- $y(s, o) = y(\langle s, p, o \rangle) : \langle s, p, o \rangle$ is in $I$ ("is a fact")
- $l(s, o) = l(\langle s, p, o \rangle) : \langle s, p, o \rangle$ is in $K$ ("is observed")
- $y(s) = y(\langle s, p \rangle) = \max_o y(s, o)$
- $l(s) = l(\langle s, p \rangle) = \max_o l(s, o)$

For readability, we use the short versions $y(s, o), l(s, o), y(s), l(s)$ when $p$ is implied (e.g., in the context of a single rule).

Note that $y(s)$ and $l(s)$ indicate that, for this specific $s$, at least one triple of the form $\langle s, p, \cdot \rangle$ is respectively in $I$ or in $K$.

Based on the above functions, we define the following sets:

- $R = \{ \langle s, o \rangle \mid R(s, o) = 1 \}$
- $R^+ = \{ \langle s, o \rangle \in R \mid y(s, o) = 1 \}$
- $R^1 = \{ \langle s, o \rangle \in R \mid l(s, o) = 1 \}$
- $R_s^+ = \{ \langle s, o \rangle \in R \mid y(s) = 1 \}$
- $R_s^1 = \{ \langle s, o \rangle \in R \mid l(s) = 1 \}$

That is, $R$ is the rule’s coverage containing all $\langle s, o \rangle$ triples for which the rule fires (i.e., the rule’s predictions); among those, $R^+$ and $R^1$ contain respectively the true and observed ones. $R_s^+$ and $R_s^1$ respectively restrict $R$ to triples with an $s$ for which at least one $\langle s, p, o \rangle$ is true or observed.

This paper focuses on evaluating rules of the format just described. Confidence measures are typically used to evaluate the quality of rules, during rule induction and model evaluation. The confidence of a rule is

$$\text{conf}(R) = \frac{\sum_{(s, o) \in R} y(s, o)}{|R|} = \frac{|R^+|}{|R|}.$$

This definition reflects the fact that rules are executed on $K$ but their predictions are considered correct if the predicted triple is in $I$.

When constructing a rule set from a knowledge base, a learner typically repeatedly tries to pick the highest-confidence rule from a number of options. As the learner has access to $K$ but not $I$, it cannot compute $\text{conf}(R)$, so it must estimate it. Before discussing existing and novel estimators in section 4, we first discuss how current KBC approaches deal with this.

3 Assumptions on the Selection Mechanism

If $K$ were an i.i.d. sample from the set of all triples, labeled positive or negative according to whether they are in $I$, and each triple had the same probability of being included in $K$, then simply counting how many of the predicted triples are labeled positive or negative would yield an unbiased estimator of $\text{conf}(R)$ (just like test set accuracy is an unbiased estimator for population accuracy). But $K$ contains no negative examples at all. This poses the following challenge:

How can one estimate the confidence of a rule without access to negative examples?

3.1 Typical Assumptions in KBC

In general, evaluating models without access to negative examples remains an open problem (Speranskaya, Schmitt, and Roth 2020; Pezeshkpour, Tian, and Singh 2020). A common approach in KBC is to make assumptions that allow deriving negative examples. Two prominent assumptions are:

The closed-world assumption (CWA) (naively) assumes that all facts not included in $K$ are false. Hence, if a rule derives a fact not in $K$, that corresponds to a false positive.

The partial-completeness assumption (PCA) (a.k.a. local closed-world assumption) assumes that if a $\langle s, p, o \rangle$ triple
Assumptions in PU Learning about the selection probabilities range from Selected Completely At Random (SCAR), where each positive example has the constant probability $e(·) = c$ to be selected, to Selected At Random (SAR), where the propensity score is a function of the example’s features (Bekker, Robberechts, and Davis 2019).

Based on this, we propose the following taxonomy for assumptions about KBC selection probabilities:

- **Closed World Assumption (CWA):** All facts are observed: $e(⟨s, p, o⟩) = 1$.
- **SCAR** All facts have the same probability to be selected: $e(⟨s, p, o⟩) = c$.
- **SCAR-per-predicate (SCARp):** All facts about the same predicate $p$ have the same probability to be selected: $e(⟨s, p, o⟩) = c_p$.
- **SCAR-per-rule (SCARR):** All facts predicted by a rule $R$ have the same probability to be selected: $R(s, o) = 1 ⟹ e(⟨s, p, o⟩) = c_R$.

**SAR:** The probability that a fact gets selected, depends on its characteristics in the incomplete KB $K$.\(^1\)

Note that this categorization is largely orthogonal to any dependence structures in the selection mechanism. In particular, all five levels are compatible with PCA, though additional restrictions may apply (e.g., SCAR-per-rule under PCA implies that rules with different $c_R$ cannot cover the same subject $s$). Only SAR, the least strict assumption, can in general represent common observation biases such as higher propensity scores for famous entities, and certain predicates having different propensity scores for women and men (Callahan and Herring 2011; Wagner et al. 2015). SCAR-per-rule can include such biases, but only if each rule covers one group exclusively (famous or plebeian, man or woman).

Note that all except the SAR assumption consider the observed facts covered by a certain rule to be unbiased. The next section will show that this assumption is made implicitly by all existing confidence measures.

### 4 Confidence Estimators

We now return to the problem of estimating the confidence of a rule $R$, $\text{conf}(R)$. First, we discuss and analyze estimators that have been used in the KBC field. Second, we will introduce new estimators that account for possible observation bias.

#### 4.1 Existing Confidence Estimators

**CWA-based estimator** Under the closed-world assumption, a prediction is considered correct if it is known to be correct (i.e., the predicted triple is observed in $K$), and incorrect otherwise. The confidence calculated as such is usually referred to as the standard confidence (Galárraga et al. 2013), but for clarity, we call it the CWA-based estimator.

$$\text{CWA}(R) = \frac{\sum_{(s, o) \in R} \text{Pr}(l(s, o))}{|R|} = \frac{|R^1|}{|R|} = \frac{\text{conf}(R)}{|R|}$$

\(^1\)More realistically, the probability depends on its true (possibly unobserved) characteristics. However, in the KBC task, only the characteristic that are observable are relevant.
The three biases can cancel each other out, making it hard to predict how PCA(R) will perform, when the problem is not well understood. We explain the three biases using an example rule that predicts which people won an Oscar, e.g., \((\text{Audrey}, \text{wonOscar}, \text{BestActress1954})\). Under PCA, \(K\) is assumed to contain either all or none of the Oscars that each person has won.

\(\text{CWA}(R)\) generally underestimates \(\text{conf}(R)\) because \(K \subseteq I\) and therefore \(|R|^I \leq |R^+|\), yielding \(\text{CWA}(R) \leq \text{conf}(R)\).

Now consider different possible realizations of \(K\) given some \(I\). Because the probability for a fact to be included in \(K\) is \(\Pr(l(s,o) = 1) = c(s,o)\), the expected value for \(\text{CWA}(R)\) over all \(K\) is

\[
\mathbb{E}_{s \sim \text{conf}(R)} \left[ \text{CWA}(R) \right] = \frac{\text{conf}(R)}{|R^+|} \sum_{(s,o) \in R^+} c(s,o).
\]

Under SCAR-per-predicate, with a constant \(c(s,o) = c_p\) per predicate \(p\), it has the same constant multiplicative bias \(c_p\) for all rules for a predicate \(p\), meaning that the ranking of rules is still expected to be correct. To better analyze the problem for the setting where only the relative ranking of rules matter, we introduce an inverse \(c_p\)-weighted version of the CWA-based estimator \(\text{ICW}(R) = \frac{1}{c_p} \text{CWA}(R)\), which is indeed unbiased under SCAR-per-predicate: \(\mathbb{E}_{s \sim c_p} \left[ \text{ICW}(R) \right] = \text{conf}(R)\).

**PCA-based estimator** To solve the above-mentioned underestimation problem, the PCA-based estimator only considers the subset of predictions \(R_s^I\) assumed to have a known truth value under the PCA assumption. That is, the PCA-based estimator only considers predictions \(R_s^I\) for which the subject appears in an observed fact in \(K\) \((l(s) = 1)\). For all triples in \(R_s^I\), if the specific triple is observed \((l(s,o) = 1)\) then the prediction is considered correct, if it is not observed \((l(s,o) = 0)\) then the prediction is considered incorrect (Galárraga et al. 2013):

\[
\text{PCA}(R) = \frac{\sum_{(s,o) \in R} l(s,o)}{\sum_{(s,o) \in R} l(s)} = \frac{|R_s^I|}{|R_s^I|}.
\]

While the PCA-based estimator is a commonly-used confidence estimator, we are, to the best of our knowledge, the first to study under which conditions it is expected to perform well. The PCA-based estimator can suffer from biases induced by three factors, which are mathematically derived and interpreted in Appendix A:\footnote{The appendices can be found at: https://github.com/ML-KULeuven/KBC-as-PU-Learning}

\[
\mathbb{E}_{s \sim \text{conf}(R)} \left[ \text{PCA}(R) \right] \approx \frac{\mathbb{E}_{s \sim \text{conf}(R)} \left[ \frac{|R_s^I|}{|R_s^I|} \right]}{\mathbb{E}_{s \sim \text{conf}(R)} \left[ \frac{|R_s^I|}{|R_s^I|} \right]}
\]

\[
= \text{conf}(R) \cdot \text{bias}_{g(s)}(R) \cdot \text{bias}_{y(s)}(R) \cdot \text{bias}_{c(s)}(R)
\]

\[
\approx \text{conf}(R) \frac{\sum_{(s,o) \in R} c(s,o)}{\sum_{(s,o) \in R} c(s)} \frac{|R_s^I|}{|R_s^I|} \frac{1}{|R^+_s|} \sum_{(s,o) \in R_s^+} c(s)
\]

The three biases can cancel each other out, making it hard to predict how \(\text{PCA}(R)\) will perform, when the problem is not well understood. We explain the three biases using an example rule that predicts which people won an Oscar, e.g., \((\text{Audrey}, \text{wonOscar}, \text{BestActress1954})\). Under PCA, \(K\) is assumed to contain either all or none of the Oscars that each person has won.

To illustrate when \(\text{bias}_{g(s)}\) arises, consider a KB that only contains facts denoting four of Audrey Hepburn’s six Oscars meaning the PCA assumption is violated for the \((\text{Audrey}, \text{wonOscar})\) pair. Suppose a rule is learned that correctly derives all six of Audrey Hepburn’s Oscars (Figure 2). Making the PCA assumption results in the two Oscar wins not in the KB being incorrectly denoted as false positives, yielding an underestimation of the rule’s confidence just like in the CWA case. More formally, this bias arises whenever a rule fires for a \((s,p)\) pair for which the PCA assumption is violated and the rule derives a \((s,p,o)\) s.t. \(l((s,p,o)) = 0\) and \(y((s,p,o)) = 1\) (an unobserved fact). This bias never arises for functional predicates (where each subject appears in at most 1 fact) because the PCA trivially holds for such predicates.

To illustrate when \(\text{bias}_{y(s)} = 0\) arises, consider a rule that predicts that Alan Rickman won an Oscar, which is a false positive since he has never won an Oscar. However, because there is no fact \((\text{AlanRickman}, \text{wonOscar}, \_)\) in \(K\), since no such facts exist, the PCA estimator disregards the prediction in its confidence. In this case the PCA estimator overestimates the rule’s confidence. More generally, such an overestimate occurs whenever a rule predicts a triple \((s,p,o)\) where \(\forall o : y((s,p,o)) = 0\) (\(s\) occurs in no facts). In these cases, these false positive predictions \(R \setminus R_s^+\) are ignored by the PCA.

The third bias factor \(\text{bias}_{c(s)}\) is the mean \(e(s)\) over all correct predictions \(R_s^+\) made by the rule divided by the mean \(e(s)\) over all its predictions \(R^+_s\) (restricting \(s\) to those \(s\) where \(y(s) = 1\)) (Figure 3). This bias is \(> 1\) when correct predictions tend to have higher \(e(s)\), or, put differently, when there are more correct predictions for high-propensity subjects. Vice versa, this bias is \(< 1\) when there are fewer correct predictions for high-propensity subjects. In our Oscars example, when a rule happens to give more accurate predictions for high-propensity Oscar winners than for low-propensity ones, the confidence of this rule is overestimated.

In our experiments in Section 5, Q3 illustrates how \(\text{PCA}(R)\) can vary due to this bias when \(e(s)\) varies for different subjects.

4.2 Observation Bias Aware Confidence Estimators

In this section we propose two novel confidence estimators that can counteract observation biases by explicitly taking the selection mechanism into account. The difference between the estimators is whether or not they make the PCA assumption. The proposed estimators need propensity scores as input, therefore we additionally analyze their bias when using imperfect propensity scores and show that rough estimates are
The Inverse Propensity Weighted estimator (IPW) aims to debias CWA(C) by weighting the observed triples with inverse propensity score estimates \( \hat{e}(s, o) \):

\[
\text{IPW}(C) = \frac{1}{|C|} \sum_{(s, o) \in C} \frac{l(s, o)}{\hat{e}(s, o)}
\]

From its expected value over all possible \( K \), it is clear that the estimator is unbiased when \( \hat{e}(s, o) = e(s, o) \):

\[
\mathbb{E}_{sel \sim \epsilon}[\text{IPW}(C)] = \text{conf}(C) \frac{1}{|C|} \sum_{(s, o) \in C} \frac{e(s, o)}{\hat{e}(s, o)}
\]

Similarly, the Inverse Propensity Weighted PCA-based estimator (IPW-PCA) aims to debias PCA(C):

\[
\text{IPW-PCA}(C) = \frac{\sum_{(s, o) \in C} l(s, o) e(s, o)}{\sum_{(s, o) \in C} \hat{e}(s, o)}
\]

The first-order Taylor approximation of its expected value is:

\[
\mathbb{E}_{sel \sim \epsilon}[\text{IPW-PCA}(C)] 
\approx \text{conf}(C) \cdot \text{bias}_{\text{IPW-PCA}}(C) \cdot \text{bias}_{\text{PCA}(C)}
\]

\[
\approx \text{conf}(C) \cdot \frac{\sum_{(s, o) \in C} l(s, o) e(s, o)}{\sum_{(s, o) \in C} \hat{e}(s, o)} \cdot \frac{\sum_{(s, o) \in C} l(s, o) e(s, o)}{\sum_{(s, o) \in C} \hat{e}(s, o)} \cdot \frac{\sum_{(s, o) \in C} l(s, o) e(s, o)}{\sum_{(s, o) \in C} \hat{e}(s, o)}
\]

Here, 2 of the 3 bias factors are inverse propensity weighted versions of the corresponding PCA(C) biases. Note that when \( \hat{e}(s) = e(s) \), the bias \( \text{IPW-PCA}(C) \) related to the selection mechanism completely disappears.

Most often, the exact propensity scores \( e(s, o) \) cannot be used for \( \hat{e}(s, o) \), as they are unknown. When the propensity scores are not known exactly, using reasonable estimates for \( \hat{e}(s, o) \) can still result in a better confidence estimator than not using any \( \hat{e}(s, o) \) and making a SCAR assumption.

To investigate how accurate the propensity score estimates \( \hat{e}(\cdot) \) should be, we compare confidence estimators when the PCA does or does not hold, respectively: IPW-PCA(C) and PCA(C) vs CWA(C).³

³To allow for rule comparison, we considered the calibrated version ICW(C) = \( \frac{1}{\epsilon \text{conf}(C)} \) CWA(C).

In Appendix B, we show that an individual triple \( (s, o) \) has a smaller error contribution in the IPW(PCA) estimator than in the CWA(PCA) estimators when its propensity score estimate \( \hat{e}(s, o) \) satisfies:

\[
\begin{align*}
\textsf{true direction} & : c \leq \hat{e}(s, o) \leq e(s, o) \iff e(s, o) - c \geq e(s, o) - \hat{e}(s, o), \\
\textsf{wrong direction} & : c \geq \hat{e}(s, o) \geq e(s, o) \iff e(s, o) - c \leq e(s, o) - \hat{e}(s, o),
\end{align*}
\]

As shown, reasonable estimates \( \hat{e} \) can be used in the IPW(PCA) estimators that do not need be calibrated; only their relative values matter. In practice, these relative \( \hat{e} \) could be derived from domain knowledge, e.g., from research on KB bias (Callahan and Herring 2011; Wagner et al. 2015), or estimated through incompleteness estimation (Razniewski, Suchanek, and Nutt 2016; Galárraga et al. 2017). For example, in a movie-recommendation setting, Saito et al. (2020) use a movie’s popularity as its propensity score.
of rules serves as the testbed for our confidence estimators (thus, the same rules are used over all $K$ and estimators). See Appendix E for the rule list.

The applied selection mechanisms differ in two ways. First, they either explicitly uphold the PCA (by selecting subjects $s$ in Q3) or not (by selecting triples in Q1, Q2). For functional $p$, the PCA always holds by definition. Second, the mechanisms differ in which assumptions hold for the propensity scores: CWA, SCAR$_p$, or SAR. Under SCAR$_p$, $c_p$ is varied. Two SAR mechanisms are considered: 1) SAR$_{group}$ where the subjects of the triples are divided into two groups $S_q$, $S_{¬q}$ (e.g., actors and non-actors), each with a constant propensity score $c_q$, $c_{¬q}$, and 2) SAR$_{pop}$ where a triple’s propensity score is a logistic function of the number of facts in which the subject occurs, thus reflecting the subject’s popularity:

$$\#(s,p) = \{\{(s,q’,s) \in I\} \cup \{\{s,q,s\} \in I\}, q \neq p\},$$

$$e((s,p,o)) = \max \left[ \frac{2}{1 + e^{-k \#(s,p)} - 1}, c_{\min} \right]$$

More popular $s$ have a higher $e$. The scaling factor $k$ determines how often $s$ must occur for a given $e((s,p,o))$. Choosing $c_{\min} > 0$ allows unpopular $s$ to be selected.

When a rule’s coverage $R$ changes by applying the rule to different $K$, not only the estimators but also the rule’s actual confidence $conf(R)$ can change. In order to keep $conf$ constant, the chosen selection mechanisms should not affect $R$. Therefore, 1) only non-recessive rules are considered, and 2) each selection mechanism is applied to a single $p \in \mathcal{P}$ at a time; the facts of $\mathcal{P} \setminus \{p\}$ are completely included in $K$ (cf. CWA). This way, we can vary $e(\cdot)$ for $p$ while keeping the confidence $conf(R)$ constant.

As evaluation metric, the Brier score $\mathbb{E}_R[conf(R) - conf(R)]^2$ is chosen (with $conf$ any estimator); this is a standard way of evaluating probability estimates.

For Q1 and Q2, we compare ICW($R$)$^4$ and IPW($R$) to CWA($R$) and PCA($R$). For Q3, we compare IPW-PCA($R$) to PCA($R$), as the former modifies the latter to consider propensity scores.

Propensity scores are required to calculate IPW-PCA($R$). We use correct propensity scores $e(\cdot)$ for the idealized scenarios in Q1 and Q3 and noisy versions $e$ for Q2.

More details about the exact setup can be found in Appendix C. Our source code is publicly available.\(^5\)

5.2 Results

Q1) Does using the ground truth propensity scores lead to a better confidence estimate? Table 1 shows the Brier scores for the estimators under SCAR$_p$, SAR$_{group}$ and SAR$_{pop}$. Only the leftmost IPW($R$) column is relevant for Q1, i.e., the column with superscript Q1. The table shows that using correct propensity scores under SCAR$_p$ and SAR results in a much better $conf$ estimate: the Brier score for IPW($R$) is often orders of magnitude lower than for the other estimators. (See also Tables 3, 4 and 5 in Appendix D.)

\(^4\) For $c_p$, the average $e(\cdot)$ over all $p$-triples in $K$ is used. Note that under SCAR$_p$, ICW($R$) = IPW($R$).

\(^5\)https://github.com/ML-KULeuven/KBC-as-PU-Learning

Figure 5: For a single rule under SCAR$_p$ (left), dividing CWA($R$) by $c_p$ is (trivially) as good as ICW($R$) = IPW($R$) $\approx$ $conf(R)$ for all $c_p$. Under SAR$_{group}$ (right), dividing CWA($R$) by $c_p$ fails to account for the bias for most $c_{¬q}$. Correct propensity scores are used, and $c_q = 0.5$ for SAR$_{group}$. $conf(R)$ is hidden by IPW($R$).

Figure 5 zooms in on a single rule. It shows how, under SCAR$_p$, both IPW($R$) and ICW($R$) almost perfectly compensate for CWA($R$)’s underestimation. However, under SAR$_{group}$, ICW($R$) does not recover $conf(R)$ for most $c_{¬q}$, while IPW($R$) still does.

This illustrates how bad CWA($R$) can be by ignoring the observation bias. If a learner merely ranks rules predicting the same predicate $p$ under the simple SCAR$_p$, all CWA($R$) are biased with the same constant $c_p$. Under this simple setting, CWA($R$) works as well as ICW($R$) (and hence IPW($R$)). However, CWA($R$) fails under more complex settings (e.g., SAR$_{group}$), where using propensity scores allows IPW($R$) to be clearly superior to CWA($R$).

Figure 5 (left) shows PCA($R$) and IPW-PCA($R$) for a single rule under SCAR$_p$, for both $p$ (person, diedin, place) and its inverse $p^{-1}$ (place, heredied, person). Here, the PCA holds for $p$ (a person dies in at most 1 place), but not for $p^{-1}$ (only a fraction $c_p$ of all the people who died somewhere are in $K$). Therefore, PCA$_{p^{-1}}(R)$ remains constant for most $c_p$, differing from $conf(R)$ with a constant factor $bias_{p^{-1}}(R) = |\mathbb{R}|/|\mathbb{R}^+_p|$. In contrast, $bias_{p^{-1}}(R)$ causes PCA$_{p^{-1}}(R)$ to vary with $c_p$.

The three factors that can cause PCA($R$) to be biased interact; if they are unknown in advance, it is difficult to say how well PCA($R$) will perform. For example in Figure 6 (left), PCA$_{p^{-1}}(R)$ is equal to $conf(R)$ at approximately $c_p = 0.7$ due to an ‘accidental’ combination of these dimensions. However, if the PCA holds and $|\mathbb{R}|/|\mathbb{R}^+_p|$ is close to 1, PCA($R$) will be close to $conf(R)$ for all $c_p$, as shown with PCA$_{p^{-1}}(R)$. Figure 6 (right) illustrates PCA($R$) under SAR. The difference between PCA$_{p^{-1}}(R)$ and $conf(R)$ is equal to $|\mathbb{R}|/|\mathbb{R}^+_p|$ for the SCAR point ($c_q = c_{¬q}$), but changes when varying the relative number of triples in $S_q$ and $S_{¬q}$ in $K$ (see also the results for Q3).

This illustrates how complex the behavior of the PCA($R$) is. Its disadvantage is its dependence on different interacting biases. In contrast, using propensity scores allows IPW($R$) to be close to $conf(R)$ in all settings.

Q2) Can noisy propensity scores be used to improve confidence estimates? The rightmost IPW columns in Table 1 (with superscript Q2) show Brier scores for IPW($R$) with respectively 0.1 and −0.1 added as noise to the correct propen-
sity scores for SCAR, and SAR\textsubscript{group}. For SAR\textsubscript{pop}, the noisy propensity scores are obtained by increasing/decreasing \(k\) by 10\%. The results show that IPW\((R)\) is generally the best estimator for conf\((R)\) if the noise is not too large. The exact differences between IPW\((R)\), CWA\((R)\) and PCA\((R)\) depend on 1) the specific selection mechanism affecting CWA\((R)\) and PCA\((R)\) as seen in Q1, and 2) the noisy propensity scores affecting IPW\((R)\).

(Q3) When the PCA holds, PCA\((R)\) becomes a better estimate as bias\textsubscript{perc}(R) = 1. Are there then still situations in which PCA\((R)\) can be improved by using propensity scores? Here, we compare IPW-PCA\((R)\) and PCA\((R)\) under SAR\textsubscript{group} and explicitly uphold the PCA for non-functional \(p\) by selecting subjects, e.g., if a person is a citizen of multiple countries, then either all or none of its triples are selected. We consider rules with predictions in both subject groups \(S_q\) and \(S_{\neg q}\), with neither group dominating in size: \(0.3 \leq |(R \cap S_q)|/|R| \leq 0.7\). We only include rules for which the group-local confidence (the confidence considering only the predictions in a group) differs by at least 0.1. The total confidence is the weighted mean of the group-local confidences where the weights are the fraction of predictions per group. By varying \(c_{\neg q}\) for a fixed \(c_q\), bias\textsubscript{perc}(R) is varied (while bias\textsubscript{perc}(s)\(=0\)) \(\text{R} = | \text{R}|/|\text{R}_k^{-}\) remains constant): the relative number of subjects (and thus triples) in \(K\) belonging to each group varies, and is different from \(I\) for \(c_q \neq c_{\neg q}\). Consequently, the total PCA\((R)\) moves towards the group-local PCA\((R)\) of the overrepresented group (Figure 7). However, IPW-PCA\((R)\) remains relatively constant. Table 2 shows the Brier scores for this specific scenario. The results highlight how well PCA\((R)\) works under PCA without needing propensity scores: although IPW-PCA\((R)\) is mostly better, its improvement is rather small.

In conclusion, CWA\((R)\) and PCA\((R)\) fail to account for general observation biases in contrast to IPW\((R)\) and IPW-PCA\((R)\), which make them explicit through propensity scores.

6 Related Work

Several confidence measures for KBC have been introduced to address the problem of dealing with the lack of negative examples (Galárraga et al. 2013; Pellissier Tanon et al. 2017; Zupanc and Davis 2018), but none of them handle general observation biases. The confidence measures from Zupanc and Davis and Pellissier Tanon et al. were omitted from the discussion, because, the former consists of an ad-hoc pipeline, and the latter consistently underestimates the confidence (see Appendix F). Other confidences were introduced with different goals: xconf (Zhou, Sadeghian, and Wang 2019) to limit computation effort and smooth confidence to cope with rules with low support (Mellicke et al. 2019).

Estimating propensity scores is closely related to estimating where the KB is more and less complete. The limited work on this topic combines several simple completeness oracles such as popularity, cardinality and change over time (Razniewski, Suchanek, and Nutt 2016; Galárraga et al. 2017). Soulet et al. (2018) estimate representativeness as deviation from an i.i.d. sample, but do not estimate which bias is causing the deviation nor propose a method for mitigating the bias at learning time.

Most of the work in PU Learning has been conducted under the SCAR assumption, where the labeled examples are an i.i.d. sample from the true positive examples (Elkan and Noto 2008). This is clearly violated by KBs. The more general SAR assumption allows for non-i.i.d. selection mechanisms, but needs additional assumptions to enable learning. Only a handful of such assumptions have been proposed (Kato, Teshima, and Honda 2018; Bekker, Robberechts, and Davis 2019; Gong et al. 2021). While none of these assumptions are sufficient for the KBC setting, the notion of explicitly modeling the selection mechanism inspired this paper.

Recommender systems solve a problem similar to KBC, but with only 1 predicate type (|\(P| = 1\). Similar to our approach, Saito et al. (2020) and Gupta et al. (2021) adapt the PU learning loss function from Bekker, Robberechts, and Davis (2019). Amongst others, our paper differs from these works in 1) our unifying view on how KBs are constructed (including the taxonomy of assumptions) that allows analyzing the conditions under which evaluation metrics can be evaluated, 2) our analysis of the commonly used CWA and PCA estimators and 3) our newly proposed IPW(-PCA)
We investigated rule evaluation, specifically confidence estimates. Yet, this is exactly what existing methods do. We have proposed two new confidence estimators that can mitigate known biases by using propensity scores that quantify how likely a fact is to be included in the KB. We have shown that these estimators are unbiased with respect to the observation bias. Our experiments showed that the Brier score of our IPW($R$) measure is often orders of magnitude lower than those of the other estimators when observation biases are present. Our metric even outperforms the others when it has inexact values for the propensity scores.

| SCAR$_p$ | $c_p = 0.3$ | 47 | 292.5 | 192.7 | 4.6 | 4.6 | 154.2 | 40.9 |
| SCAR$_p$ | $c_p = 0.7$ | 47 | 53.8 | 173.3 | 1.1 | 1.1 | 18.1 | 10.0 |
| SAR$_{group}$ | $c_q = 0.5$, $c_{-q} = 0.3$ | 33 | 189.5 | 155.6 | 8.1 | 3.4 | 50.3 | 14.0 |
| SAR$_{group}$ | $c_q = 0.5$, $c_{-q} = 0.7$ | 33 | 83.8 | 155.1 | 4.0 | 1.8 | 6.9 | 4.6 |
| SAR$_{pop}$ | $k = 0.01$ | 47 | 458.6 | 264.2 | 168.5 | 62.8 | 81.8 | 56.6 |
| SAR$_{pop}$ | $k = 0.1$ | 47 | 172.3 | 182.7 | 51.0 | 3.5 | 7.4 | 6.2 |

Table 1: Results for Q1 and Q2 (see superscript). $[\text{conf} - \text{conf}]^2 \cdot 10^4$ under SCAR$_p$, SAR$_{group}$ and SAR$_{pop}$. Results are averaged over $p$, the rules and (for SAR$_{group}$) $q$. The 3 IPW confidence columns: 1 with correct $\hat{e} = e$ (left) and 2 with noisy $\hat{e} \neq e$ (middle and right). For SCAR$_p$, noisy $\hat{c}_p = c_p \pm 0.1$. For SAR$_{group}$, noisy $\hat{c}_{-q} = c_{-q} \pm 0.1$. For SAR$_{pop}$, the noisy $\hat{e}$ are obtained by using $\hat{k} = k \pm 0.1k$.

| $p$ | # R | $c_{-q} = 0.3$ | PCA | IPW-PCA | IPW-PCA-Δ | IPW-PCA+Δ |
| --- | --- | --- | --- | --- | --- | --- |
| dealswith | 1 | 22.4 | 16.9 | 13.5 | 19.9 | 9.1 | 12.4 | 10.7 | 14.0 |
| diedin | 1 | 3.9 | 1.6 | 3.7 | 2.0 | 1.4 | 0.5 | 0.7 | 0.7 |
| happenededin | 1 | 6.6 | 1.7 | 4.0 | 3.3 | 2.3 | 0.7 | 1.0 | 1.1 |
| iscitizenof | 2 | 13.1 | 14.5 | 20.0 | 13.2 | 11.0 | 9.9 | 10.2 | 10.0 |
| isleaderof | 1 | 58.1 | 55.5 | 58.0 | 56.6 | 74.1 | 72.0 | 72.7 | 71.6 |
| ispoliticianof | 3 | 8.0 | 9.3 | 16.9 | 7.8 | 9.2 | 8.3 | 8.4 | 8.5 |
| livesin | 1 | 7.0 | 6.8 | 8.5 | 6.7 | 4.7 | 4.0 | 4.1 | 4.1 |
| participatedin | 1 | 16.0 | 11.6 | 8.1 | 14.1 | 10.9 | 13.2 | 12.1 | 14.2 |

Table 2: Results for Q3. $[\text{conf} - |R|/|R^+| \cdot \text{conf}]^2 \cdot 10^4$ for SAR$_{group}$ with PCA upheld (avg. over $q$ and rules predicting $p$). $c_{-q} \in \{0.3, 0.7\}$ with $c_q = 0.5$ Bold is best per $c_{-q}$ and $p$. Three IPW-PCA($R$) columns for $\hat{c}_{-q} = c_{-q} + \Delta$, $\Delta \in \{0, \pm 0.1\}$. Rules are included if $0.3 \leq (|R| \cap S_q) / |R| \leq 0.7$ and the difference in group-local $|R|/|R^+| \cdot \text{conf}(R)$ is at least 0.1.

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7 Conclusion

Biases are mostly studied in the fairness literature (Mehrabii et al. 2019; Barocas, Hardt, and Narayanan 2019), with the aim to learn bias-free models. This paper, in contrast, does not enforce certain ideals, but rather aims to increase model quality by being conscious of observation biases. This is a recent perspective in fairness literature (Blum and Stangl 2020).
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