BOWL: Bayesian Optimization for Weight Learning in Probabilistic Soft Logic

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Abstract

Probabilistic soft logic (PSL) is a statistical relational learning framework that represents complex relational models with weighted first-order logical rules. The weights of the rules in PSL indicate their importance in the model and influence the effectiveness of the model on a given task. Existing weight learning approaches often attempt to learn a set of weights that maximizes some function of data likelihood. However, this does not always translate to optimal performance on a desired domain metric, such as accuracy or F1 score. In this paper, we introduce a new weight learning approach called Bayesian optimization for weight learning (BOWL) based on Gaussian process regression that directly optimizes weights on a chosen domain performance metric. The key to the success of our approach is a novel projection that captures the semantic distance between the possible weight configurations. Our experimental results show that our proposed approach outperforms likelihood-based approaches and yields up to a 10% improvement across a variety of performance metrics. Further, we performed experiments to measure the scalability and robustness of our approach on various real-world datasets.

1 Introduction

Statistical relational learning (SRL) frameworks (Richardson and Domingos 2006; De Raedt and Kersting 2011; Getoor and Taskar 2007) combine the power of graphical models with probabilistic programming to produce accurate models on complex relational data. Probabilistic soft logic (PSL) (Bach et al. 2017) is a recently developed SRL framework that makes use of weighted first-order logical rules to generate a special kind of Markov random field (MRF) called a hinge-loss Markov random field (HL-MRF). Some of the key distinguishing properties of PSL are, unlike other SRL frameworks, random variables take continuous values between 0 and 1 and the potential functions are defined as hinge losses (further details are given in Section 2.1). These properties enable MAP inference in PSL to be cast as a convex optimization problem which makes inference in PSL scalable. PSL has achieved state-of-the-art results in various domains such as recommender systems (Kouki et al. 2017), bioinformatics (Sridhar, Fakhraei, and Getoor 2016), natural language processing (Deng and Wiebe 2015), product search (Srinivasan et al. 2019), and social network analysis (Farnadi et al. 2017).

Learning the weights of the rules is one of the key challenges for templated rule languages such as PSL, since the weighted rules interact in complex ways and cannot be optimized independently. Because of their templated nature, the weights, i.e., the parameters of the model, are used in multiple places in the instantiated graphical model, and the context varies depending on the other rules that have been instantiated. In addition, the corresponding probability distribution is not easy to compute; specifically, computing the normalization constant is often intractable.

Typically, the weights of the rules are learned through maximizing some form of likelihood function (Bach et al. 2013; Lowd and Domingos 2007; Singla and Domingos 2005; Kok and Domingos 2005; Chou et al. 2016; Sarkhel et al. 2016; Das et al. 2016; Farabi, Sarkhel, and Venugopal 2018). This is a well-motivated approach if the downstream objective makes use of the probability density function directly. However, the objective is to often improve an external domain metric such as accuracy, F1 for classification, or ROC for ranking. Several approaches address this issue by augmenting the metric into a loss function and solving a max-margin problem (Huynh and Mooney 2009; 2010; Bach et al. 2013). However, this does not directly optimize the desired metric but instead optimizes a surrogate loss. Such approaches do not easily extend to new metrics as they require deriving new losses, which may be non-convex and hard to optimize.

In this paper, we introduce a Bayesian optimization framework for finding the best weight configuration in PSL. The key advantage of our approach is that it directly optimizes the chosen domain performance metric and, unlike other approaches, does not require re-derivation of the loss function for each metric. Our proposed approach, Bayesian optimization for weight learning (BOWL), is based on Gaussian process regression (GPR) (Rasmussen and Williams 2005) in a Bayesian optimization (BO) (Mockus 1977) framework. BO is an effective approach for optimization of black-box functions (Lizotte et al. 2007; Martinez-Cantin et al. 2009; Srinivas et al. 2012; Brochu, Brochu, and de Freitas 2010) and GPR is a non-parametric Bayesian approach that is often used to approximate arbitrary functions. GPRs have been used
can be defined as:

\[ \phi(x, y) = \begin{cases} \ell_i(x, y), & \text{if } d_i = 1 \text{ (i.e., linear)} \\ \ell_i(x, y)^2, & \text{if } d_i = 2 \text{ (i.e., quadratic)} \end{cases} \]

where \( \ell_i \) is a linear function and \( d_i \in \{1, 2\} \) provides a choice of two different loss functions. For weights \( w \in \{w_1, w_2, \ldots, w_k\} \) a hinge-loss energy function can be defined as:

\[ E(y|x) = \sum_{i=1}^{k} w_i \phi_i(x, y) \quad \text{s.t., } 0 \leq y \leq 1; \, 0 \leq x \leq 1 \quad (1) \]

and the HL-MRF is defined as:

\[ P(y|x, w) = \frac{1}{Z(y)} \exp(-E(y|x)) \quad (2) \]

where \( Z(y) = \int_y \exp(-E(y|x)) \).

A PSL model defines a HL-MRF using a set of weighted first-order logical rules. PSL instantiates the hinge-loss energy function by grounding logical rules with data \( D \). This process specifies the dependencies between variables and evidence in hinge-loss potentials \( \phi_i \). PSL uses continuous random variables in \([0, 1]\) and defines potentials using convex functions that are relaxations of Boolean logical connectives. For example, \( a \rightarrow b \) corresponds to the hinge potential \( \max(a - b, 0) \), and \( a \land b \) corresponds to \( \max(a + b - 1, 0) \) (see Bach et. al. for full details).

To better understand HL-MRFs, PSL and the process of grounding, consider a simple collective labeling problem:

**Example 1.** Assume we have a set of users \( U \) and a label which can be either true or false associated with each user. Labels are observed for some users \( (U_o) \) and unobserved for the rest \( (U_u) \). The task is to infer labels for \( U_u \). The input data includes a social network of the supplied users \( U \), \( \text{Friend}(U, V) \). Suppose we also have a local predictor that makes label predictions for users, \( \text{LocalPredictor}(U) \). Below is a simple PSL model for collectively inferring labels:

\[ w_1 : \text{LocalPredictor}(U) \rightarrow \text{Label}(U) \]
\[ w_2 : \text{Label}(U) \land \text{Friend}(U, V) \rightarrow \text{Label}(V) \]

where \( w_1 \) and \( w_2 \) are non-negative weights for the rules. The above model is then grounded with users \( U \) to generate an HL-MRF. Each ground rule (such as \( w_1 : \text{LocalPredictor}(\text{"Bob"}) \rightarrow \text{Label}(\text{"Bob"}) \)) generates a hinge-loss potential \( \phi_i \). Further, each ground predicate generated by grounding users \( U_u \) with the predicate Label produces the unobserved random variables \( y \) and rest of the ground predicates generate observed random variables \( x \). Fig. 1 shows the resulting graphical model when instantiated over a small social network of 100 individuals.

Inference in PSL is performed by finding a maximum a posteriori estimate (MAP) of the random variables \( y \) given evidence \( x \). This is performed by maximizing the density function or minimizing the energy function in Equation 1. MAP inference is expressed as:

\[ \arg\max_y P(y|x) = \arg\min_y E(y|x) \quad (3) \]

A key advantage of using PSL is that the inference objective is convex. This enables the use of efficient convex optimization procedures, such as alternating direction method of multipliers (ADMM) (Boyd et al. 2011). Hence, given known weights, inference in PSL can be performed at scale enabling predictions on large real-world datasets. Unfortunately, the task of learning the rule weights from training data is not as efficient, although, as we will see, having tractable MAP inference is still helpful.

There are three primary approaches used to perform weight learning in PSL as discussed in (Bach et al. 2013):

**Maximum Likelihood Estimation (MLE)** An approach for weight learning in PSL that maximizes the log-likelihood function with respect to the weights of the rules based on the training data. Since all the potentials generated by a rule share the same weight, Equation 1 can be written as...
Large-Margin Estimation (LME) A different approach to weight learning that focuses on maximizing the MAP state rather than producing accurate probabilistic models. This approach uses the intuition that the ground-truth state $y$ should have energy lower than any alternate state $\tilde{y}$ by a large margin defined by a loss function $L$. The objective function to find the optimal set of weights is given by:

$$w^* = \arg\min_w \frac{1}{2}||w||^2 + C\xi \quad (7)$$

subject to $w^T(\Phi(\tilde{y}, x) - \Phi(y, x)) \leq -L(y, \tilde{y}) + \xi$

where $L$ is a loss function such as the L1 distance between $y$ and $\tilde{y}$, and $\xi$ is a slack variable. Equation 7 is then solved by performing a large-margin estimation based on a cutting-plane approach for structural support vector machines (Joachims, Finley, and Yu 2009).

2.2 Black-box optimization

**Black-box optimization** is a well studied technique, especially in the context of hyperparameter tuning using BO (Shahriari et al. 2016).

**Definition 2** (Black-box optimization). Given a black-box function $\gamma(\tilde{x}) : \mathbb{R}^d \rightarrow \mathbb{R}$ where $d$ is the input dimension, the task of finding the optimal value for $\gamma(\tilde{x})$ in a predefined amount of time is called black-box optimization.

The goal of black-box optimization using BO is to find the best possible value for the function $\gamma(\tilde{x})$ in a sequential setup within a predefined number of epochs. Various strategies have been proposed to choose the next point to evaluate given the previous evaluations (Srinivas et al. 2010; Kushner 1964; Mockus 1977; Thompson 1933). Each strategy is encoded through an acquisition function $\alpha$. The objective of these strategies is to minimize the number of epochs required to find the best solution. A simple black-box Bayesian approach iteratively obtains a point to explore from the acquisition function $\alpha$ using the prior distribution; then the function $\gamma$ is evaluated to obtain a new outcome at that point which is then used to update the posterior.

**Gaussian Process Regression** (GPR) is a non-parametric Bayesian approach which is effective in performing black-box optimization in a BO framework.

2.3 Gaussian Process Regression

A Gaussian process (GP) is fully characterized by its mean function $\mu_0$ and either a positive definite covariance matrix $K$ or a kernel function $k$. Consider a finite set of $s$ inputs $\tilde{X} = \tilde{x}_{1:s}$ and a random variable $y_i = \gamma(\tilde{x}_i)$ representing the function $\gamma$ evaluated at $\tilde{x}_i$ and let $\bar{y}_i$ be the noisy output of the function. In GP, we assume that $g = y_{1:s}$ is jointly Gaussian and $\bar{y}_i$ given $g$ is Gaussian. The generative model is of the form: $g|\tilde{X} \sim N(m, K)$, and $\bar{y}_i|g \sim N(g, \sigma^2 I)$, where $m_i = \mu_0(\tilde{x}_i)$, $K$ is an $(s \times s)$ positive definite matrix such that $K_{i,j} = k(\tilde{x}_i, \tilde{x}_j)$. Since the distributions are Gaussian and using the kernalization trick (Rasmussen and Williams 2005), the posterior mean and variance given a set
of observed data can be written as:

\[
\begin{align*}
\mu_s(\tilde{x}_{s+1}) &= \mu_0(\tilde{x}_{s+1}) + k(\tilde{x}_{s+1})^T(K + \sigma^2I)^{-1}(y - m) \\
\sigma_s(\tilde{x}_{s+1}) &= k(\tilde{x}_{s+1}, \tilde{x}_{s+1}) - k(\tilde{x}_{s+1})^T(K + \sigma^2I)^{-1}k(\tilde{x}_{s+1})
\end{align*}
\]

where \( k(\tilde{x}_{s+1}) \) is a kernel function applied to the inputs with observed function evaluations and the new input; i.e., it represents the covariance between observed inputs and any unobserved input. Using the above expressions, the mean and variance for any point can be computed. There is a suite of kernel functions available in the literature (Rasmussen and Williams 2005). Note that the kernel function should be chosen based on the problem domain and it is often the key to finding the best approximation of the true function.

### 3 Bayesian Optimization for Weight Learning

As mentioned earlier, commonly used approaches for rule weight learning in PSL are based on maximizing a likelihood function. In this section, we first give a motivating example that highlights the issues with likelihood-based approaches. Next, we introduce our proposed algorithm, BOWL (Bayesian Optimization for Weight Learning), which uses GPR to perform weight learning. We describe components of our approach, including the search space and acquisition function. Finally, we provide justification for our assumptions and prove the correctness of our approach.

#### 3.1 Motivating Example

Consider our simple PSL program, Example 1, applied to a toy dataset with 100 users. Fig. 2 shows the performance of the model as we vary the rule weights logarithmically from \( 10^{-6} \) to 1.0. Fig. 2 (a) shows AUROC and Fig. 2 (b) shows the log-likelihood of the model. Lighter shades (yellow) represent a high value and darker shades (dark blue) represent a low value. We observe that the AUROC is maximized when the first rule’s weight is 0.1 and the second rule’s weight is \( 10^{-6} \). However, the likelihood is not maximized at these weights. For this model and dataset, we observe that the likelihood is not well correlated with the AUROC.

![Figure 2: Heat map for accuracy and log-likelihood for the toy dataset with 100 users.](image)

(a) AUROC  
(b) log-likelihood

#### 3.2 Problem definition

Consider a PSL model with \( r \) template rules where each rule \( i \in \{1 \ldots r\} \) is associated with a weight \( w_i \in [0, 1] \). Grounding all the rules with data \( D \) yields a set of \( m \) observed random variables \( x = \{x_1, \ldots, x_m\} \), \( n \) unobserved random variables \( y = \{y_1, \ldots, y_n\} \), and \( r \) potentials \( \phi = \{\phi_1, \phi_2, \ldots, \phi_r\} \). The unobserved random variables \( y \) are inferred by optimizing Equation 3. Further, all unknown random variables are associated with corresponding ground truth \( y^* = \{y_1^*, \ldots, y_n^*\} \) used to compute evaluation metrics. Let \( w = \{w_1, \ldots, w_r\} \) be the vector representing the set of rule weights, i.e., the weight configuration. Next, let \( \omega(y, y^*) : (y, y^*) \rightarrow \mathbb{R} \) be a problem-specific performance metric (e.g., accuracy, AUROC, or F-measure) and let \( \gamma(w) : w \rightarrow \omega(y, y^*) \) be the same function \( \omega \) parameterized by \( w \) that maps weights to the metric. Then the objective of weight learning can be expressed as finding the set of weights that maximize \( \gamma \), which represents the true metric function \( \omega \), i.e., \( \arg\max_w \gamma(w) \).

The objective of GPR is to find an approximate function \( g \approx \gamma \) by sampling \( t \) weight configurations from a set of possible weight configurations \( W \).

#### 3.3 BOWL

A high-level sketch for BOWL is as follows: first, a weight configuration \( w \in W \) is chosen using an acquisition function \( \alpha \). Next, inference is performed using the current weight configuration \( w \), and \( \gamma(w) \) is computed. Then, \( GPR \) is updated with \( w \) and \( \gamma(w) \). Finally, after \( t \) iterations the weight configuration that resulted in highest value for \( \gamma \) is returned.

There are two primary components of BOWL that need to be defined: the kernel function used in GPR and the acquisition function \( \alpha \). These two components will determine the effectiveness of BOWL. Note that we restrict the weights to be \( w_i \in [0, 1] \), whereas weights in PSL take values \( w_i \in \mathbb{R}^+ \). Later, in Section 4, we show that this restriction does not limit the capabilities of the model.

#### 3.4 BOWL-OS

In order to use GPR and choose a kernel function, we must make an assumption about the function \( \gamma \). Here, we assume that the function \( \gamma \) is smooth. This assumption is true if the problem is well-defined and the metric function \( \omega \) being optimized is a smooth function, such as mean square error (MSE). For now, we make this assumption (justified further in Section 4), and choose the squared exponential kernel as the kernel for the GP:

\[
k(w_i, w_j) = \tilde{\sigma} \cdot \exp\left(\frac{\delta^2}{2\tilde{\sigma}^2}\right)
\]

where \( \tilde{\sigma} \) is the amplitude, \( \rho \) is the characteristic length-scale, and \( \delta \) is the distance between any two weight configurations. \( \rho \) and \( \sigma \) are the kernel hyperparameters. The scaling factor \( \rho \) affects the smoothness of the approximation (a large value implies a smoother approximation) and the number of iterations required to explore the space. We choose \( \rho \) such that a reasonable exploration of the space is possible in \( t \) iterations. The value of \( \tilde{\sigma} \) is chosen based on the range of the metric being learned.
The distance function $\delta$ is crucial in determining the co-
variance between two weight configurations. Ideally, if the
distance between two weight configurations is zero then the
output of the function $\gamma$ should be the same. And, as the
distance between the two weight configurations increases,
the correlation between the output of the $\gamma$ function should
go to zero. We refer to the weights in the $[0,1]^r$ space as the
original space (OS), and define the distance function $\delta$ as follows:

$$\delta_{i,j} = ||w_i - w_j||_2^2$$  \hspace{1cm} (9)

We refer to the GPR which uses the above distance function
as BOWL-OS.

3.5 Correlated Configurations

In PSL, the rule weights correspond to their relative impor-
tance, and multiple weight configurations with the same rel-
ative importance result in the same solution for $y$. This in
turn produces the same value for the $\gamma$ function. This means
that if we are not careful, the behavior of the function $\gamma$ may
not correlate with the distance function defined in Equation 9, i.e.,
two weight configurations $w_1$ and $w_2$ might be far apart,
$\delta_{1,2} \gg 0$, but perfectly correlate, $\gamma(w_1) = \gamma(w_2)$. This
leads to inefficient exploration of the space and will likely
result in a poor approximation of the function. To illus-
trate this issue consider the following example:

Example 2. Consider a model with two rules $w = \{w_1, w_2\}$. Let us assume three possible weight configurations for this problem: $w_1 = \{0.1, 0.1\}$, $w_2 = \{1.0, 1.0\}$, and $w_3 = \{0.1, 0.0001\}$. Assuming that the number of groundings for both rules are the same, the weights of the rules in $w_1$ and $w_2$ indicate that both rules are equally import-
ant, while in $w_3$ the first rule is 1000 times more im-
portant than the second rule. This results in the function $\gamma$
producing the same output for $w_1$ and $w_2$, and potentially
a different value for $w_3$. Based on this, the weight configu-
ration $w_3$ should be significantly different from the weight
configurations $w_1$ and $w_2$, while $w_1$ and $w_2$ should be sim-
ilar. Unfortunately, the distances measured using Equation 9,
$\delta_{1,2} = 1.27$, $\delta_{1,3} = 0.09$, and $\delta_{2,3} = 1.34$, do not be-
have in this manner. The distance $\delta_{1,2}$ is much larger than
distance $\delta_{1,3}$. Therefore, BOWL-OS would infer that the
function value of $\gamma(w_1)$ is more correlated with $\gamma(w_3)$ than
$\gamma(w_2)$. However, as argued above, we want the opposite
behavior. This discrepancy can lead to a poor approximation
of the function $\gamma$.

3.6 BOWL-SS

To match the actual correlation between the weight config-
figurations and their corresponding distance, we define a new
configuration space, the scaled space (SS). The SS is a pro-
jection of weights onto a relative space. We use the ratio of
weights between the rules to define the relative importance of
weights in the configuration. This projection results in
distances that correspond to the actual correlation between
the weight configurations in PSL. Formally, we define SS
and the distance measured in SS as:

**Definition 3.** Given a set of weights $w = \{w_1, \ldots, w_r\} \in (0,1]^r$, the SS $E$ is a projection defined on $w$ such that $E(w) \in \mathbb{R}^{(r-1)}$ is given by:

$$E(w) = \{\forall_{i=2}^{r}(ln(w_i) - ln(w_1))\}$$  \hspace{1cm} (10)

and the distance $\Delta$ between weights is defined as:

$$\Delta_{i,j} = ||E(w_i) - E(w_j)||_2$$  \hspace{1cm} (11)

In SS, $E$, a distance of $\Delta_{i,j} = 0$, implies that the two
weight configurations yield the same solution for the random
variables $y$ at the time of inference.

**Theorem 1.** Given two weight configurations $w_1$ and $w_2$, if $E(w_1) = E(w_2)$ (i.e., $\Delta_{1,2} = 0$) then the solution ob-
tained for $y$ by minimizing Equation 1 with both the weight
configurations are the same.

**Proof.** Let $w_1 = \{w_{1,1}, \ldots, w_{1,r}\}$, $w_2 = \{w_{2,1}, \ldots, w_{2,r}\}$ and $E(w_1) = E(w_2)$. As the two weight configurations are the same in SS, the equality can be written as:

$$ln(w_1) - ln(w_{1,1}) = ln(w_2) - ln(w_{2,1})$$

$$w_1 = \frac{w_{1,1}}{w_{2,1}}\cdot w_2$$

Since $w_{1,1} \in (0,1]$ and $w_{2,1} \in (0,1]$ are constants, the re-
sulting optimization problems are equivalent:

$$\arg\min_y E(y|x, w_1) = \arg\min_{y} \frac{w_{1,1}}{w_{2,1}} \cdot E(y|x, w_2)$$

$$= \arg\min_{y} E(y|x, w_2)$$

Therefore, if the distance between two weight configurations
is 0 in SS, then the solutions of their corresponding PSL
program by optimizing Equation 3 are the same.

Theorem 1 proves the soundness of the scaled space. Note
that in SS we use the weight of the first rule to compute the
projection. This choice is arbitrary and can be switched to
any rule without affecting the space.

Example 2. (Continued) Consider our earlier example. The weights and the distances of our running example in the SS $E$
using Equation 10 and 11 are: $E(w_1) = \{0\}$, $E(w_2) = \{0\}$,
$E(w_3) = \{6.907\}$, $\Delta_{1,2} = 0$, $\Delta_{1,3} = 47.7$, and $\Delta_{2,3} =
47.7$.

A drawback of SS is that it does not support a weight of
zero for any rule in the model. This means that all rules
in the configuration must participate in the model. How-
ever, in practice, we mitigate this by simply assuming a very
small lower bound (e.g., $10^{-5}$, where $\varrho \in \mathbb{Z}^*$, $\varrho > 0$) and
sample weights uniformly from the log space, i.e., $w \sim
\exp(\text{Unif}([ln(10^{-5}), ln(1.0)]^r))$.

3.7 The Effect of Varied Number of Groundings

Our discussion so far has made a very important simplifying
assumption, that the number of groundings for each rule in
the model is the same. However, the number of groundings
produced by a rule has an impact on the inference of the
random variables. The weight associated with each rule is
repeated for each ground instance of that rule. This leads to the weight of each rule having varied influence on the minimization of the energy function. For instance, if a model has two equally weighted rules, but one rule produces 10 times more groundings than the other, then that rule implicitly becomes 10 times more important in the model.

We modify BOWL to accommodate the number of groundings of the rules in the model. Consider a model with \( r \) rules and let \( \beta = \{ \beta_1, \ldots, \beta_r \} \) be the number of groundings for each of the \( r \) rules. We define a grounding factor \( \kappa \) for each rule. For rule \( z \), the grounding factor \( \kappa_z = \frac{\beta_z}{\max(\beta)} \), where \( \kappa = \{ \kappa_1, \ldots, \kappa_r \} \) is the vector of grounding factors. Therefore, the true weight associated with the \( z \)th rule is \( \kappa_z \cdot w_z \) and the grounding adjusted weight configuration can be represented as an element-wise dot product between \( \kappa \) and \( w \), i.e., \( \tilde{w} = \kappa \cdot w \). The distance between two weight configurations \( \tilde{w}_i \) and \( \tilde{w}_j \) in OS can be re-written as \( ||\tilde{w}_i - \tilde{w}_j||^2 \). Similarly the distance in SS can be re-written as \( ||\kappa \cdot (\tilde{w}_i) - \kappa \cdot (\tilde{w}_j)||^2 \). However, the scaling factor \( \kappa \) does not affect the distance in SS as \( \kappa \) is constant for both weight configurations and cancels when computing the distance.

**Theorem 2.** Given two weight configurations \( w_i \) and \( w_j \), a set of grounding factors of \( \kappa \), and the grounding adjusted weight configurations \( \tilde{w}_i = \kappa \cdot w_i \) and \( \tilde{w}_j = \kappa \cdot w_j \), the distance measured between both \( (\tilde{w}_i, \tilde{w}_j) \) and \( (\tilde{w}_i, \tilde{w}_j) \) in SS are equal, i.e., \( ||\kappa \cdot (\tilde{w}_i) - \kappa \cdot (\tilde{w}_j)||^2 = ||\kappa \cdot (\tilde{w}_i) - \kappa \cdot (\tilde{w}_j)||^2 \).

**Proof.** To prove the above theorem we consider the difference between the weight configurations \( \kappa \cdot (\tilde{w}_i) - \kappa \cdot (\tilde{w}_j) \):

\[
\kappa \cdot (\tilde{w}_i) - \kappa \cdot (\tilde{w}_j) = (\ln(\kappa \cdot w_i) - \ln(\kappa \cdot w_j)) - (\ln(\kappa_1 \cdot w_{i,1}) - \ln(\kappa_1 \cdot w_{j,1})) = (\ln(w_i) - \ln(w_j)) - (\ln(w_{i,1}) - \ln(w_{j,1})) = \kappa \cdot (\tilde{w}_i) - \kappa \cdot (\tilde{w}_j)
\]

Since \( \kappa \cdot (\tilde{w}_i) - \kappa \cdot (\tilde{w}_j) = \kappa \cdot (\tilde{w}_i) - \kappa \cdot (\tilde{w}_j) \), the distances are also equal. \( \square \)

**Theorem 3.** Consider any PSL program with \( r \) rules and weights \( w = \{w_1, \ldots, w_r\}, w_i \in \mathbb{R}^+ \). There exists a mapping function \( \zeta(w) : \mathbb{R}^r \to [0, 1]^r \) which transforms the weights to \( [0, 1]^r \) without modifying the solution of the inference problem \( y \) in PSL. The \( \zeta \) function is given by:

\[
\zeta(w) = \frac{w}{\max(w)}
\]

**Proof.** Similar to proof from Theorem 1. \( \square \)

Since we make an assumption that the user-defined metric depends only on the random variables, the metric value obtained is unaffected.

With regard to the second assumption, we constrain ourselves to only those metrics \( \omega(y, y^*) \) that are smooth with respect to the random variables (such as MSE). Note, our assumption is that the function \( \gamma \) is smooth and \( \gamma \) is parametrized with \( w \) and not the random variables \( y \). Hence, it is non-trivial to prove smoothness in \( \gamma \). With the above constraint on the possible metrics, we know that if a small change in \( w \) leads to a small change in \( y \), then the function \( \gamma \) is also smooth. We formally define smoothness of the function \( \gamma \) as follows:

**Definition 4.** Given two sets of weights \( w_1 \) and \( w_2 \) for a PSL program with \( r \) rules and random variables \( y \), the function \( \gamma \) is considered to be smooth if \( \Delta_{1,2} < \epsilon \) where \( \epsilon \to 0 \), then \( ||y_1 - y_2||_2 < \nu \) where \( \nu \to 0 \), \( y_1 \) and \( y_2 \) are the
random variables inferred using weights \( w_1 \) and \( w_2 \) respectively.

This directly leads to the conditioning of the problem. If a problem is well-conditioned then our assumption about the smoothness of \( \gamma \) is precise. If the problem is ill-conditioned then this assumption fails to hold and the function learned in BOWL could be a poor approximation of \( \gamma \).

Finally, in practice, it is inefficient to use GPR for high-dimensional problems (Wang et al. 2016); GPR works best when the number of dimensions is less than 50. This makes PSL weight learning an ideal use case for GPR, because typically PSL programs have just tens of rules and most often the number of rules does not exceed 50.

5 Empirical Evaluation

In this section, we evaluate BOWL on various realworld datasets. All our experiments were run on a machine with 16 cores and 64GB of memory. We investigate three research questions: [Q1] How does BOWL perform on realworld datasets compared to the existing methods? [Q2] Is BOWL-SS scalable? [Q3] Is BOWL-SS robust?

We selected five realworld datasets from different domains for which PSL models have promising results (Bach et al. 2017; Kouki et al. 2015). Details are as follows:

**Jester**: contains 2,000 users and 100 jokes (Goldberg et al. 2001). The task is to predict user’s preference to jokes.

**LastFM**: contains 1,892 users and 17,632 artists. The task is to recommend artists to users by predicting the ratings for user-artist pairs.

**Cora**: contains 2,708 scientific documents, seven categories, and 5,429 directed citations. The task is to assign a category to each document.

**Citeseer**: is similar to Citeseer dataset, but contains 3,312 documents, six categories and 4,591 directed citations.

**Epinions**: contains 2,000 users and 8,675 directed links which are positive and negative trust links between users. The task is to predict the trust relation.

5.1 Performance analysis

To address [Q1], we compare the performance of BOWL-SS, BOWL-OS, MLE, MPLE, and LME on several metrics. For each dataset, we use snowball sampling to create eight folds and perform cross validation. We perform a paired t-test \((p\text{-value} \leq 0.05)\) across methods. For BOWL-SS and BOWL-OS the maximum number of weight configurations to explore in order to approximate the user-defined metric function is set to \( t = 50 \). Although in our experiments, we observed that the best metric value is usually obtained at \( t < 25 \) (this is likely because the function we intend to learn has several flat regions). We also use a stopping criterion which terminates the exploration if the standard deviation at all sampled weight configurations is less than 0.5. MLE, MPLE, and LME were allowed to run for 100 iterations.

For each dataset, depending on the problem, we leverage the metric that has been used for the problem to measure its performance. Hence, we report \( MSE \) and \( AUROC \) for the Jester and LastFM datasets, categorical accuracy and \( F1 \) for the Cora and the Citeseer datasets, and \( AUROC \) and \( F1 \) for the Epinions dataset. We use UCB as our acquisition function with \( \psi = 5 \) to favor exploration. However, in Section 5.3 we show that similar performance can be obtained by using the other acquisition functions discussed in Section 3.8. The hyperparameters that we use for BOWL are: \( \sigma = 1.0, \rho = 1, \) and the mean function is a constant zero. We set the value of \( \rho \) to one after exploring different values in \([10^5, 10^{-5}]\), and we set \( \sigma \) to 1.0 as our metrics are in the range \([-1, 1]\).

Table 1 shows the comparison between BOWL and other methods across the different datasets. In each row of the table, the best performing method and those which are not significantly different from the best performing method are shown in bold. We observe that BOWL-SS is the best performing method across all the datasets and metrics. For the Epinions dataset, we observe that there is no statistically significant difference in \( F1 \) score between BOWL-SS, BOWL-OS, MLE, MPLE, and LME. However, it is interesting that for the same dataset when the evaluation metric is \( AUROC \), MPLE produces significantly lower values. For the LastFM, Jester, and Citeseer datasets, we observe that BOWL-SS significantly outperforms MLE, MPLE, and LME. For the Cora dataset, MPLE and MLE performs similar to BOWL-SS, while LME produces poorer results when \( F1 \) score is under consideration. Finally, BOWL-OS performs similar to or better than MLE, MPLE, and LME. However, the BOWL-SS approach yields the best performing results across all datasets.

5.2 Scalability

In this section, we compare the runtimes of BOWL-SS, MLE, MPLE, and LME to measure the scalability of BOWL-SS and address [Q2]. The number of parameters to learn in PSL is equal to the number of rules in the model and the data size translates to the number of groundings generated by the model. In Fig. 3a, we show the number of groundings generated by each of the datasets. We also show the number of rules in each model. The Jester dataset produces the largest number of groundings \((\sim 1M)\) using seven rules and the Epinions dataset produces the least number of groundings \((\sim 14K)\) using the largest model \((20\text{ rules})\).

In Fig. 3b, we observe that the learning times of MLE, MPLE, and LME are not correlated to the size of the model, i.e., the number of rules in the model, but correlated to the number of groundings. MLE increases by about a factor of \( \sim 40 \) from Epinions to the Jester dataset and MPLE by a factor of \( \sim 60 \). For LME, runtime increases based on the number of groundings and complexity of finding the margin. Therefore, LME takes longer to finish on the LastFM dataset compared to the Jester dataset. Next, we observe that the time taken to run BOWL-SS is almost the same for all five datasets with various sizes of rules and groundings. This is because the time taken to run BOWL depends mainly on the number of iterations it is allowed to run and the time it takes to solve MAP inference in PSL. Since the number of iterations is restricted to 50 for all models, this keeps the time almost the same for all datasets. Further, efficient infer-
Table 1: Performance of methods across datasets; the best scoring methods (with $p < 0.05$) are shown in bold.

<table>
<thead>
<tr>
<th>Method (Metric)</th>
<th>Jester (MSE)</th>
<th>Jester (AUROC)</th>
<th>LastFM (MSE)</th>
<th>LastFM (AUROC)</th>
<th>Citeeseer (Acc)</th>
<th>Citeeseer (F1)</th>
<th>Cora (Acc)</th>
<th>Cora (F1)</th>
<th>Epinions (AUROC)</th>
<th>Epinions (F1)</th>
</tr>
</thead>
<tbody>
<tr>
<td>MLE</td>
<td>0.058</td>
<td>0.733</td>
<td>0.081</td>
<td>0.581</td>
<td>0.710</td>
<td>0.671</td>
<td>0.832</td>
<td>0.869</td>
<td>0.815</td>
<td>0.960</td>
</tr>
<tr>
<td>MPLE</td>
<td>0.060</td>
<td>0.737</td>
<td>0.083</td>
<td>0.568</td>
<td>0.729</td>
<td>0.754</td>
<td>0.832</td>
<td>0.869</td>
<td>0.744</td>
<td>0.958</td>
</tr>
<tr>
<td>LME</td>
<td>0.055</td>
<td>0.740</td>
<td>0.126</td>
<td>0.554</td>
<td>0.728</td>
<td>0.689</td>
<td>0.831</td>
<td>0.849</td>
<td>0.826</td>
<td>0.960</td>
</tr>
<tr>
<td>BOWL-GS</td>
<td>0.055</td>
<td>0.767</td>
<td>0.082</td>
<td>0.599</td>
<td>0.740</td>
<td>0.796</td>
<td>0.832</td>
<td>0.869</td>
<td>0.812</td>
<td>0.962</td>
</tr>
<tr>
<td>BOWL-SS</td>
<td>0.053</td>
<td>0.767</td>
<td>0.078</td>
<td>0.599</td>
<td>0.743</td>
<td>0.798</td>
<td>0.833</td>
<td>0.868</td>
<td>0.825</td>
<td>0.960</td>
</tr>
</tbody>
</table>

Figure 3: Analyzing scalability of BOWL-SS on number of rules and groundings. BOWL-SS is minimally affected by both the number of rules and groundings.

5.3 Robustness
To address [Q3], we run two sets of experiments: the first experiment is to test the effects of choosing an acquisition function on the performance of BOWL-SS and the second experiment is to check how robust BOWL-SS is w.r.t. different initialization. In Table 2 we compare the performance of BOWL-SS using four different acquisition functions (UCB, TS, PI, and EI) for all five datasets. We observe that using BOWL-SS with different acquisition functions yields similar results. This indicates that the performance of BOWL-SS is robust to these exploration strategies. For our second experiment, we perform weight learning with BOWL-SS using 100 random initializations and report the mean and standard deviation (std) of a metric per dataset in Table 2. Note that for this experiment we use UCB as our acquisition function. Further, we use only one (of the eight) folds per dataset as we intend to measure the variance introduced by different initializations. In Table 2, we also observe that the standard deviation is small for all datasets which indicates that BOWL-SS is robust to initialization.

Table 2: We observe that the performance of BOWL-SS is unaffected by both acquisition function and initialization.

<table>
<thead>
<tr>
<th>Datasets</th>
<th>Different acquisition functions</th>
<th>Varied initializations</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>UCB</td>
<td>TS</td>
</tr>
<tr>
<td>Jester (MSE)</td>
<td>0.053</td>
<td>0.052</td>
</tr>
<tr>
<td>LastFM (MSE)</td>
<td>0.078</td>
<td>0.078</td>
</tr>
<tr>
<td>Citeeseer (F1)</td>
<td>0.797</td>
<td>0.797</td>
</tr>
<tr>
<td>Cora (F1)</td>
<td>0.868</td>
<td>0.869</td>
</tr>
<tr>
<td>Epinions (F1)</td>
<td>0.962</td>
<td>0.960</td>
</tr>
</tbody>
</table>

6 Conclusion and Future work
In this paper, we introduce BOWL, a BO approach to learn weights in PSL. BOWL yields improved performance across several metrics on a variety of different real-world datasets. There are many avenues for expanding our work. To perform weight learning using BOWL, the SRL model needs to be fully grounded. There are a variety of approaches for avoiding full grounding (Sarkhel, Singla, and Gogate 2015; Sarkhel et al. 2016) that would be interesting to integrate into our approach. Further, performance of GPs are highly dependent on the kernel function used. Therefore, an exploration of different kernels for BOWL could further improve the performance of our method.

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