Embedding First Order Logic into Kernel Machines

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Abstract. In this paper we propose a general framework to integrate supervised and unsupervised examples with background knowledge expressed by a collection of first-order logic clauses into kernel machines. In particular, we consider a multi-task learning scheme where multiple predicates defined on a set of objects are to be jointly learned from examples, enforcing a set of FOL constraints on the admissible configurations of their values. The predicates are defined on the feature spaces, in which the input objects are represented, and can be either known a priori or approximated by an appropriate kernel-based learner. A general approach is presented to convert the FOL clauses into a continuous implementation that can deal with the outputs computed by the kernel-based predicates. The learning problem is formulated as a semi-supervised task that requires the optimization in the primal of a loss function that combines a fitting loss measure on the supervised examples, a regularization term, and a penalty term that enforces the constraints on both the supervised and unsupervised examples. Unfortunately, the penalty term is not convex and it can hinder the optimization process. However, it is possible to avoid poor solutions by using a two stage learning schema, in which the supervised examples are learned first and then the constraints are enforced.

1 Introduction

This paper proposes a general framework to inject background knowledge expressed by first-order logic clauses into the regularized fitting of supervised examples carried out by kernel machines [7]. This approach has strong connections to studies of developmental psychology, where children have been shown to iteratively generalize their knowledge, initially derived from a set of punctual examples and then properly increased by the gradual acquisition of higher level concepts [4]. While the focus on biologically-plausible solutions has been playing a central role, scientists have mostly neglected those human behavioral principles, and have not been able to bridge learning processes based on examples and high level logic representations. Important exceptions concerning a unified treatment of learning with prior knowledge in logic form have been proposed in the field of probabilistic inductive logic programming (see e.g. [6] and [3]). In
this paper, we consider a multi-task learning scheme where multiple predicates defined on a set of objects are to be jointly learned from examples, enforcing a set of FOL constraints on the admissible configurations of their values. The predicates are implemented as generic functions getting as input a vector of features. A general approach is presented to convert any set of FOL clauses into a set of constraints on real-valued functions. We proposed a semi-supervised learning approach that requires the optimization of a function composed of a loss function, a regularization term, and a penalty term that enforces the constraints. When enforcing the constraint satisfaction term on the supervised and unsupervised examples only, we show that a representation theorem holds that dictates the optimal solution of the problem as a kernel expansion over the given examples. Unfortunately, unlike for classic kernel machines, the cost function is not guaranteed to be convex, unless for very simple FOL clauses. While direct optimization of the cost function is hopeless, we propose a solution inspired to stage-based learning in which we learn the supervised examples first and then we enforce the FOL constraints. The proposed approach is general and flexible. As an example, we show that it is related to manifold regularization [1], which also emerge in our logic setting. The experimental results show how the background knowledge increases the classification accuracy in the context of multi-task classification problems.

This is the outline of the paper. Section 2 introduces the proposed learning framework, while section 3 reports some experimental results. Finally, section 4 draws some conclusions.

2 Learning with first-order logic constraints

We consider a learning problem in which a set of predicates is to be inferred from examples. For the sake of simplicity, we assume that the arguments of each predicate can take values from the same domain, which is assumed to be a vectorial feature space $F \in \mathbb{R}^{m}$. However, it is easy to extend the framework to consider a different domain for each variable. The predicates are implemented as functions from a Cartesian product of the feature space to a scalar real value, such that $\pi_k : F^{n_k} \rightarrow \mathbb{R}, k = 1, \ldots, T$ being $n_k$ the grade of the predicate (i.e. the number of arguments). The value computed by the function $\pi_k$ can be interpreted as a continuous truth value, that is associated to the corresponding predicate for each configuration of the input variables.

The learning task is defined in a semi-supervised scheme by assigning a set of labeled examples for each predicate together with a set of unlabeled samples that are drawn from the feature vector distribution. In particular, the labeled examples for the $k$-th predicate are collected in the set $\mathcal{L}_k = \{([x_1^i, \ldots, x_{n_k}^i], y_k^i) \mid i = 1, \ldots, \ell_k\}$ where $x_j^i \in F, j = 1, \ldots, n_k$, is the $j$-th argument of the predicate, and $y_k^i \in \{0, 1\}$ is the target that encodes the truth value of the predicate for the given input configuration. The unlabeled set is $\mathcal{U} = \{x^i \mid x^i \in F, i = 1, \ldots, u\}$ and it is possible to collect all the available feature vectors in the set $\mathcal{S} = \{x \mid \exists k \exists i ([x_1, \ldots, x_i, \ldots, x_{n_k}], y_k) \in \mathcal{L}_k \land x = x_i\} \cup \mathcal{U}$. We assume that beside
the information provided by the given labeled and unlabeled examples, further
a priori knowledge on the given task is modeled by a set of First-Order Logic
(FOL) clauses defined over the unknown predicates \( \pi_k \) and a set of known pred-
icates \( \pi_{jK} \), \( j = 1, \ldots, T^K \). Basically the learning task requires to determine the
unknown predicates such that they provide an optimal fitting of the supervised
examples satisfying also the a priori FOL clauses on the feature space. We assume
that each unknown predicate \( \pi_k \) can be conveniently approximated in a given
Reproducing Kernel Hilbert Space (RKHS) \( \mathcal{H}_k \) by a function \( f_k : F_{nk} \to \mathbb{R} \),
such that the learning problem can be cast as an optimization task, where the
objective can be expressed as

\[
E(f) = R(f) + N(f) + V(f) \tag{1}
\]

where \( f = [f_1, \ldots, f_T]' \) is the array of the candidate predicates. The fitting of
the supervised examples is considered by the term

\[
R(f) = \sum_{k=1}^{T} \lambda_k^* \cdot \frac{1}{|\mathcal{L}_k|} \sum_{(x_1, \ldots, x_{nk}, y) \in \mathcal{L}_k} L_k^*(f_k(x_1, \ldots, x_{nk}), y),
\]

where \( L_k^*(z, y) \) is a loss function that measures the fitting quality of \( f_k(\cdot) \) with
respect to the target \( y \) and \( \lambda_k^* > 0 \) is the weight for the \( k \)-th predicate. Even
if extending this approach to employ multi-task kernels is trivial, in this paper
we consider scalar kernels that do not yield interactions amongst the different
predicates, that is \( N(f) = \sum_{k=1}^{T} \lambda_k^* \cdot ||f_k||_{H_k}^2 \), where \( \lambda_k^* > 0 \) can be used to impose
different weight to each predicate. The last term \( V(f) \) enforces the assigned
FOL constraints by penalizing their violation. The constraints are assumed to
hold for any valid configuration as defined by the quantified variables in the
FOL expression of each clause, however the penalty considers only the sampling
yielded by the points in \( S \). The constructive procedure to convert an FOL clause
into an appropriate penalty will be described in the following subsection.

It is easy to prove a straightforward extension of the Representer Theorem
for plain kernel machines \([7]\) that states that the solution of the optimization
problem involving the objective function of eq. (1) can be expressed by a kernel
expansion on the given examples available in the set \( S \). In fact, similarly to
the term corresponding to the empirical risk, the penalty term to enforce the
constraints only involves values of \( f_k \) sampled on a subset of \( S_{nk} \). Hence the
optimal approximation for the \( k \)-th predicate can be written as

\[
f_k(x_1, \ldots, x_{nk}) = \sum_{|x_1, \ldots, x_{nk}| \in S_k} w_{k,i} K_k([x_1^i, \ldots, x_{nk}^i], [x_1, \ldots, x_{nk}])
\]

where \( K_k(\cdot, \cdot) \) is the reproducing kernel associated to the space \( \mathcal{H}_k \) and \( S_k \subseteq S_{nk} \)
is an appropriate subset of the \( n \)-tuples that can be formed from the available
sample points. The representer theorem shows that it is possible to optimize
eq (1) in the primal by gradient heuristics \([2]\). The weights of the kernel expansion
can be compactly organized in \( w_k = [w_{k,1}, \ldots, w_{k,|S_k|}]' \) and, therefore, the
optimization of eq. (1) turns out to involve the finite set of real-valued weights $w_k, k = 1, \ldots, T$. The overall error function might not be convex anymore due to the constraint penalty term. However, in case of positive kernel, the strict convexity is guaranteed when restricting the learning to the regularization and empirical risk terms. Please note that the labeled examples and the constraints are coherent, since they represent different reinforcing expressions of the concepts to be learned. If we start applying the constraint penalty term only after having learned the supervised examples then the penalty term should be null, when restricted to the supervised portion of examples and non-null only on the unsupervised portion. Hence, the proposed learning procedure consists of two consecutive stages: Labeled initialization, in which only a regularized fitting of the supervised examples is enforced, and abstraction stage during which we also start enforcing the constraints in the cost function. This technique has been proven to effectively tackle non-convex learning tasks.

2.1 Enforcing FOL clauses

To integrate FOL clauses into the proposed learning framework, we can exploit the classic association from Boolean variables to real-valued functions by using the t-norms (triangular norms) \[5\]. A t-norm is any function $T : [0, 1] \times [0, 1] \to \mathbb{R}$, that is commutative, associative, monotonic (i.e. $y \leq z \Rightarrow T(x, y) \leq T(x, z)$), and featuring a neutral element 1 (i.e. $T(x, 1) = x$). A t-norm fuzzy logic is defined by its t-norm $T(x, y)$ that models the logic AND, while the negation of a variable $\neg x$ is computed as $1 - x$. The $t$-conorm, modeling the logical OR, is defined as $1 - T((1 - x), (1 - y))$, as a generalization of the De Morgan’s law.

In the following we will consider the product t-norm $T(x, y) = x \cdot y$, but other choices are possible.

Hence, using a t-norm it is possible to define the logic operators that can be used to implement the continuous counterpart of a FOL expression. In particular, if $e_1$ and $e_2$ are the functions implementing two FOL expressions $E_1$ and $E_2$, eventually depending on a set of variables, when exploiting the product t-norm, we have that $E_1 \land E_2$ is implemented by $e_1 \cdot e_2$, $E_1 \lor E_2$ by $1 - (1 - e_1) \cdot (1 - e_2)$, and finally $\neg E_1$ as $1 - e_1$. The atoms in the expressions are represented by both the assigned predicates $\pi_{Kj}$ and the unknown predicates $\pi_k$, whose arguments are defined by a set of quantifiers. When considering the continuous implementation, the predicates $\pi_k$ are approximated by the corresponding kernel expansion $f_k$ that is not guaranteed to yield values in the interval $[0, 1]$ as required by the definition of t-norms. Hence, we apply a squashing function $\sigma : \mathbb{R} \to [0, 1]$ to constrain their values in $[0, 1]$, such that the atoms related to the predicates $\pi_k$ are implemented as $\sigma(f_k(x_1, \ldots, x_{n_k}))$. In the experimental setting, we exploited the targets $\{0, 1\}$ for the $\{false, true\}$ values in the supervised examples, and we decided to exploit the piecewise-linear squashing function $\sigma(y) = \min(1, \max(y, 0))$.

The expressions obtained by combining the predicates with logic operators contain variables corresponding to the arguments of each predicate. Each variable can range in the feature space $F$ and, when the same variable is shared among different arguments and/or predicates, it is assumed that same value
should be used in all its instances. The definition of the FOL clauses, that represent the given a priori constraints, requires each variable to be properly quantified in order to obtain an expression that should evaluate to the value true for all valid hypotheses for the unknown predicates π_k. In other words, the constraint can be thought as a functional, depending on the functions f_k, that should evaluate to 1 only for the solutions satisfying the constraint. Hence, if we denote by C_h the constraint represented by the h-th FOL clause, its dependence from the functions f_k can be made explicit by writing C_h(f_1, ..., f_T). The resulting expressions for all the clauses can be used to define the penalty term V(f) in eq. (1). We first consider how to implement the universal quantifier. If we assume that the expression E depends on the variable x ∈ F, a clause can be defined as ∀x E(x) meaning that the proposition E(x) should be true for all points in the feature space. Since it is infeasible to verify the constraint on all the feature space, we exploit the dataset S to evaluate the constraint. In particular, we force the t-norm expression of E(x) to be true in average by defining the penalty V_e(f) = \frac{1}{|S|} \sum_{x \in S} (1 - e(x)). In fact, the term 1-e(x) assumes values in [0, 1] and is null when the expression is verified in x. Hence, the penalty is null when the expression is verified over all the sample points. In general, when the expression depends on a set of variables that are universally quantified, i.e. the clause is in the form ∀x_1 ... ∀x_q E(x_1, ..., x_q), the penalty can be written as

\[
V_e(f) = \frac{1}{|S|^q} \sum_{x_1 \in S} \cdots \sum_{x_q \in S} (1 - e(x_1, ..., x_q)).
\]

Clearly, the complexity of the penalty is combinatorial in the cardinality of the sample set, but we can usually exploit the fact that some correlations among the different variables are present in the real problem. For instance, we can model the fact that some configurations of the quantified variables are not admissible by introducing the predicate d(x_1, ..., x_q) that is true only for the valid (or more probable) configurations of the variables and by enforcing the proposition d(x_1, ..., x_q) ⇒ e(x_1, ..., x_q). In fact, the proposition is equivalent to ¬(d(x_1, ..., x_q) ∧ ¬e(x_1, ..., x_q)) whose t-norm implementation is 1 - d(x_1, ..., x_q) · (1 - e(x_1, ..., x_q)). Thus the term involved in the penalty is d(x_1, ..., x_q) · (1 - e(x_1, ..., x_q)) that is null whenever the variable configuration is not valid. This result is implemented by computing the sum only on the n-tuples observed in the dataset.

The implementation of the existential quantifier is more tricky, since it requires to verify the existence in the feature space of a point that satisfies a given proposition. Given the expression ∃x E(x), we have no a priori general rule to find the feature vectors x ∈ F that make E(x) true for the current hypothesis of f_k. Assuming that at least one of such points is available in the sample set S, the existence operator can be rewritten as ∨_{x_i \in S} E(x_i). This expression can be transcribed in a continuous t-norm form as: 1 - \prod_{x_i \in S} (1 - e(x_i)). Please note that an efficient implementation of this operator needs further studies.
3 Experimental results

This section presents an experimental analysis on some artificial benchmarks properly created to show how the FOL logic clauses can be used in the context of semi-supervised learning with plain kernel machines. The two-stage learning algorithm described in section 2 is exploited in all the experiments.

A first synthetic task consists of a multi-class classification problem over four different classes: \(A, B, C, D\). The patterns for each class are assumed to be uniformly distributed over the following rectangles:

- \(A = \{(x, y) : 0 \leq x \leq 3, 0 \leq y \leq 3\}\)
- \(B = \{(x, y) : 1 \leq x \leq 4, 1 \leq y \leq 4\}\)
- \(C = \{(x, y) : 2 \leq x \leq 5, 2 \leq y \leq 5\}\)
- \(D = \{(x, y) : (1 \leq x \leq 3, 1 \leq y \leq 3) \lor (2 \leq x \leq 4, 2 \leq y \leq 4)\}\)

The reported results are based on a test set of 100 patterns per class, which are selected via the same sampling schema used to generate the training set. We used a Gaussian kernel with fixed \(\sigma\) set to 0.4 and averaged the accuracy results over 10 different runs performed on different instances of the training and test sets.

Let \(a(x), b(x), c(x), d(x)\) be a set of predicates representing whether a pattern \(x\) belongs to the classes \(A, B, C, D\), respectively. The following two FOL clauses are supposed to be known a-priori about the geometry of the classification task:

\[
\forall x \ (a(x) \land b(x)) \lor (b(x) \land c(x)) \Rightarrow d \quad \text{and} \quad \forall x \ a(x) \lor b(x) \lor c(x) \lor d(x).
\]

Figure 1 reports the classification accuracy obtained when using the constraints and the unsupervised data versus when no constraints are employed in learning the classification task. The classifier trained using the constraints outperforms the one learned without using the constraints by a statistically significant margin, which ranges between 2\% and 5\% depending on the training configuration.

In a second benchmark, we assume to have patterns laying in a \(IR^2\) feature space and belonging to two classes \(A, B\), according to the well-known two moon-like shaped distributions. We assume to be assigned an a-priori similarity relation \(r(x, y)\) between a set of pairs of patterns \((x, y)\). The semantic meaning of the relation \(r\) can differ in different applications. For example, it could be used to represent the hyperlink connections between documents in Web retrieval tasks, or the co-citations among authors, etc. In this experiment, we assume that \(r\) models
Table 1. Moon benchmark: classification accuracy on the test set obtained with and without using the manifold regularization expressed in FOL form.

<table>
<thead>
<tr>
<th>num labeled patterns</th>
<th>4</th>
<th>8</th>
<th>12</th>
</tr>
</thead>
<tbody>
<tr>
<td>with FOL knowledge</td>
<td>59.6%</td>
<td>68.5%</td>
<td>72.3%</td>
</tr>
<tr>
<td>without FOL knowledge</td>
<td>40.4%</td>
<td>53.5%</td>
<td>71.2%</td>
</tr>
</tbody>
</table>

the geometric closeness of the patterns in the feature space. This assumption is very general and can be applied in any application where the input patterns lay in a metric space. In particular, the following FOL clause is used to express the knowledge that the input patterns featuring a similarity relation should yield the same predicate output:

$$\forall x \forall y r(x, y) \Rightarrow (f(x) \land f(y)) \lor (\neg f(x) \land \neg f(y)). \quad (2)$$

This is a reformulation of the well known assumption made in manifold regularization [1] in a continuous logic setting. This assumption expresses the fact that the input patterns are distributed along a manifold, over which the functions to be learned should be smooth, e.g. connected inputs on the manifold should tend to correspond to similar function outputs. The FOL clause in equation 2 can be rewritten as: $\forall \forall \forall y (r(x, y) \land f(x) \land f(y)) \land (\neg f(x) \land f(y))$. Using the product t-norm and the mapping to a continuous cost function as explained in section 2, we obtain the following constraint term for the cost function:

$$V(f) = \sum_{x \in S} \sum_{y \in S} r(x, y)(1 - f(x)f(y))(1 - (1 - f(x))(1 - f(y))) =$$

$$\sum_{(x, y) : x, y \in S, r(x, y) \neq 0} r(x, y)(1 - f(x)f(y))(1 - (1 - f(x))(1 - f(y))).$$

In our experimental setting, the strength of the relation is computed as $r(x, y) = e^{-\|x - y\|/\sigma_d}$, where $\sigma_d = 2/3$. The constraint part is then plugged into equation 1 and optimized by gradient descent. Figure 2 plots the output map of the learned predicate $f$. The effect of the knowledge expressed by the FOL clause over the unsupervised data smoothes the predicate output value over the regions where scarce labeled data is available. The activation map perfectly reconstructs the boundaries of the regions where the input patterns are distributed for the two classes. Table 1 reports the accuracy values for different numbers of the labeled and unlabeled patterns. When learning using the FOL prior knowledge, the
training data was augmented with 100 unlabeled patterns. The accuracy values have been obtained as an average over 10 different random generations of the training and test data. The accuracy gain is very significant when little labeled data is available.

4 Conclusions

This paper presents a framework to learn a set of predicates, each implemented as a kernel machine, starting from a collection of supervised training data and prior knowledge in form of FOL clauses. The FOL clauses can be compiled into a set of real-valued function constraints that are subsequently converted to a penalty function added to the classic loss and regularization term of kernel machines. The experimental results show how it is possible to impose smoothness over a manifold of points using the FOL formalism. The regularized fitting of the supervised data along with the penalty term that expresses the logic clauses is optimized by a two-stage process, inspired to development psychology, that is shown to be very effective especially when small sets of supervised data are available. The proposed framework opens the doors to a new class of semantic-based regularization machines, in which it is possible to integrate prior knowledge using high level abstract representations.

References