Feature Construction for Relational Sequence Learning

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Abstract. We tackle the problem of multi-class relational sequence learning using relevant patterns discovered from a set of labelled sequences. To deal with this problem, firstly each relational sequence is mapped into a feature vector using the result of a feature construction method. Since, the efficacy of sequence learning algorithms strongly depends on the features used to represent the sequences, the second step is to find an optimal subset of the constructed features leading to high classification accuracy. This feature selection task has been solved adopting a wrapper approach that uses a stochastic local search algorithm embedding a naïve Bayes classifier. The performance of the proposed method applied to a real-world dataset shows an improvement when compared to other established methods, such as hidden Markov models, Fisher kernels and conditional random fields for relational sequences.

Key words: Relational Sequence Learning, Feature Construction/Selection, Stochastic Local Search, Statistical Relational Learning.

1 Introduction

Sequential reasoning is a fundamental task of intelligence. Indeed, sequential data may be found in a lot of contexts of the every day life. From a computer science point of view, sequential data may be found in many applications such as video understanding, planning, computational biology, user modelling, speech recognition, etc. The sequences are the simplest form of structured patterns and different methodologies have been proposed to face the problem of sequential pattern mining, firstly introduced in [1], with the aim of capturing the existent maximal frequent sequences in a given database. One of the many problems investigated concerns assigning labels to sequences of objects. However, some environments involve very complex components and features. Thus, the classical existing data mining approaches, that look for patterns in a single data table, have been extended to the multi-relational data mining approaches that look for patterns involving multiple tables (relations) from a relational database. This has led to the exploitation of a more powerful knowledge representation formalism as first-order logic.

Indeed, sequential learning techniques may be classified by the language they adopt to describe sequences. On the one hand we find algorithms adopting a

propositional language, such as hidden Markov models (HMMs) [2], allowing both a simple model representation and an efficient algorithm; on the other hand probabilistic relational systems are able to elegantly handle complex and structured descriptions where, on the contrary, an atomic representation could make the problem intractable to propositional sequence learning techniques. The aim of this paper is to propose a new probabilistic algorithm for relational sequence learning [3].

A way to tackle the task of learning discriminant functions in relational learning corresponds to reformulate the problem into an attribute-value form and then applying a propositional learner [4]. The reformulation process may be obtained adopting a *feature construction* method, such as mining frequent patterns that can then be successfully used as new Boolean features [5–7]. Since, the efficacy of learning algorithms strongly depends on the features used to represent the sequences, a *feature selection* task should be very useful. The aim of feature selection is to find an optimal subset of the input features leading to high classification performance, or, more generally, to carry out the classification task in a optimum way. However, the search for a variable subset is a NP-hard problem. Therefore, the optimal solution cannot be guaranteed to be acquired except when performing an exhaustive search in the solution space. The use of a *stochastic local search* procedure allows one to obtain good solutions without having to explore the whole solution space. Algorithms for feature selection can be divided into two categories: wrapper and filter methods [8]. When the feature selection algorithm embeds a classifier and selects subsets of features guided by their predictive power predicted by the classifier, it is using a wrapper approach. The filter approach selects the features adopting a preprocessing step using heuristics based on the intrinsic characteristic of the data and ignoring the learner.

In this paper we propose a new algorithm, named Lynx[1] for relational sequence learning that in the first step it adopts a classical feature construction approach. As we will see in the following, here the features are not considered as Boolean but we are able to associate a probability to each constructed feature. In the second step, the system adopts a wrapper feature selection approach, that uses a stochastic local search (non-exhaustive) procedure, embedding a naïve Bayes classifier to select an optimal subset of the constructed features. In particular, the optimal subset of patterns is searched using a Greedy Randomised Search Procedure (GRASP) and the search is guided by the predictive power of the selected subset computed using a naïve Bayes approach.

Hence the focus of the paper is on combining probabilistic feature construction and feature selection for relational sequence learning. The aim is to show that the proposed approach is comparable to other purposely designed probabilistic approaches for relational sequence learning.

The outline of the paper is as follows. After discussing related work in Section 2, we present the Lynx algorithm in Section 3. In particular we will briefly present the description language, followed by the description of the feature con-

[1] LYNX is public available at `http://www.di.uniba.it/~ndm/lynx/`.

struction and feature selection proposed methods. Before concluding the paper in Section 5, we experimentally evaluate Lynx on a real-world dataset.

2 Related Work

As already pointed out, the problem of sequential pattern mining is a central one in a lot of data mining applications and many efforts have been done in order to propose purposely designed methods to face it. Most of the works have been restricted to propositional patterns, that is, patterns not involving first order predicates. One of the early domains that highlights the need to describe with structural information the sequences was the bioinformatics. Thus, the need to represent many real world domains with structured data sequences became more unceasing, and consequently many efforts have been done to extend existing or propose new methods to manage sequential patterns in which first order predicates are involved. Related works may be divided into two categories. In the first category there are work belonging to the Inductive Logic Programming area [9], that reformulate the initial relational problem into an attribute-value form, by using frequent patterns as new Boolean features, and then applying propositional learners. To the second category belong all the systems purposely designed to tackle the problem of relational sequence analysis falling into the more specific Statistical Relational Learning area [10] where probabilistic models are combined with relational learning.

This work may be correlated to that in [7], where the authors presented one of the first Inductive Logic Programming feature construction method. They firstly construct a set of features adopting a declarative language to constraint the search space and to find discriminant features. Then, these features are used to learn a classification model with a propositional learner.

In [11] are presented a logic language, SeqLog, for mining sequences of logical atoms, and the inductive mining system MineSeqLog, that combines principles of the level-wise search algorithm with the version space in order to find all patterns that satisfy a constraint by using an optimal refinement operator for SeqLog. SeqLog is a logic representational framework that adopts two operators to represent the sequences: one to indicate that an atom is the direct successor of another and the other to say that an atom occurs somewhere after another. Furthermore, based on this language, the notion of subsumption, entailment and a fix point semantic are given.

These work even if may be correlated to our work, they tackle into account the feature construction problem only. Here, however we combine a feature construction process with a feature selection algorithm maximising the predictive accuracy of a probabilistic model. Systems very similar to our approach are those that combine a probabilistic models with a relational description such as logical hidden Markov models (LoHHMs) [12], Fisher kernels for logical sequences [13], and relational conditional random fields [14] that are purposely designed for relational sequences learning.

In [13] has been proposed an extension of classical Fisher kernels, working on sequences over flat alphabets, in order to make them able to model logical sequences, i.e., sequences over an alphabet of logical atoms. Fisher kernels were developed to combine generative models with kernel methods, and have shown promising results for the combinations of support vector machines with (logical) hidden Markov models and Bayesian networks. Successively, in [12] the same authors proposed an algorithm for selecting LoHMMs from data. HMM [2] are one of the most popular methods for analysing sequential data, but they can be exploited to handle sequence of flat/unstructured symbols. The proposed logical extension [15] overcomes such weakness by handling sequences of structured symbols by means of a probabilistic ILP framework.

Finally, in [14] an extension of conditional random fields (CRFs) to logical sequences has been proposed. In the case of sequence labelling task, CRFs are a better alternative to HMMs that makes it relatively easy to model arbitrary dependencies in the input space. CRFs are undirected graphical models that instead of learning a generative model, such as in HMMs, they learn a discriminative model designed to handle non-independent input features. In [14], the authors lifted CRFs to the relational case by representing the potential functions as a sum of relational regression trees learnt by a relational regression tree learner.

3 Lynx: a relational pattern-based classifier

This section firstly briefly reports the framework for mining (multi-dimensional) relational sequences introduced in [16] to manage patterns in which more than one dimension is taken into account. That framework has been used in Lynx due to its general logic formalism for representing and mining relational sequences. Over that framework Lynx implements a probabilistic pattern-based classifier. In particular, after introducing the representation language, the Lynx system along with its feature construction capability, the adopted pattern-based classification model, and the feature selection approach will be presented.

3.1 The language

As a representation language we used a first-order logic that we briefly review. The first-order *alphabet* consists of a set of *constants*, a set of *variables*, a set of *function symbols*, and a non-empty set of *predicate symbols*. Both function symbols and predicate symbols have a natural number (its *arity*) assigned to it. A *term* is a constant symbol, a variable symbols, or an n-ary function symbol f applied to n terms $t_1, t_2, \ldots, t_n$.

An atom $p(t_1, \ldots, t_n)$ (or atomic formula) is a predicate symbol p of arity n applied to n terms t_i. Both l and its negation $\overline{l}$ are said to be *literals* (resp. positive and negative literal) whenever l is an atomic formula.

A *clause* is a formula of the form $\forall X_1 \ldots \forall X_n (L_1 \vee \ldots \vee \overline{L}_i \vee \overline{L}_{i+1} \vee \ldots \vee \overline{L}_m)$ where each L_i is a literal and $X_j, j = 1, \ldots, n$, are all the variables occurring in the literals. The same clause may be written as $L_1, \ldots \leftarrow L_i, \ldots L_m$.

Clauses, literals and terms are said to be *ground* whenever they do not contain variables. A *Datalog clause* is a clause with no function symbols of non-zero arity; only variables and constants can be used as predicate arguments.

A *substitution* θ is defined as a set of bindings $\{X_1 \leftarrow a_1, \ldots, X_n \leftarrow a_n\}$ where $X_i, 1 \leq i \leq n$ is a variable and $a_i, 1 \leq i \leq n$ is a term. A substitution θ is applicable to an expression e, obtaining the expression $e\theta$, by replacing all variables X_i with their corresponding terms a_i.

Lynx includes the multi-dimensional relational framework, and the corresponding pattern mining algorithm, reported in [16] that here we briefly recall.

A *1-dimensional relational sequence* may be defined as an ordered list of Datalog atoms separated by the operator $<$: $l_1 < l_2 < \cdots < l_n$.

Considering a sequence as an ordered succession of events for each dimension, fluents have been used to indicate that an atom is true for a given event. For the general case of n-dimensional sequences, the operator $<_i$ has been introduced to express multi-dimensional relations. Specifically, $(e_1 <_i e_2)$ denotes that the event e_2 is the successor event of e_1 on the dimension i. Hence, A *multi-dimensional relational sequence* may be defined as a set of Datalog atoms, concerning n dimensions, where each event may be related to another event by means of the $<_i$ operators, $1 \leq i \leq n$.

In order to represent multi-dimensional relational patterns, the following dimensional operators have been introduced. Given a set $\mathcal{D}$ of dimensions, $\forall i \in \mathcal{D}$: $<_i$ (next step on dimension) indicates the direct successor on the dimension i; $\lhd_i$ (after some steps on dimension) encodes the transitive closure of $<_i$; and $\bigcirc_i^n$ (exactly after n steps on dimension i) calculates the n-th direct successor.

Hence, a *multi-dimensional relational pattern* may be defined as a set of Datalog atoms, regarding n dimensions, in which there are non-dimensional atoms and each event may be related to another event by means of the operators $<_i$, $\lhd_i$ and $\bigcirc_i^n$, $1 \leq i \leq n$.

The background knowledge $\mathcal{B}$ contains the definitions of the operators $\bigcirc_i^k$ and $\lhd_i$ used to prove the dimensional operators appearing in the patterns. Given S a multi-dimensional relational sequence, in the following we will indicate by Σ the set of Datalog clauses $\mathcal{B} \cup U$, where U is the set of ground atoms in S. In order to calculate the frequency of a pattern over a sequence it is important to define the concept of sequence subsumption.

Definition 1 (Subsumption). *Given $\Sigma = \mathcal{B} \cup U$, where U is the set of atoms in a sequence S, and $\mathcal{B}$ is a background knowledge. A pattern P* subsumes *the sequence S ($P \subseteq S$), iff there exists an SLD_{OI}-deduction of P from Σ.*

An SLD_{OI}-deduction is an SLD-deduction under Object Identity [17]. In the Object Identity framework, within a clause, terms that are denoted with different symbols must be distinct, i.e. they must represent different objects of the domain.

3.2 Feature Construction via pattern mining

The first step of the Lynx system corresponds to a feature construction process obtained by mining frequent patterns from sequences. The algorithm for fre-

quent multi-dimensional relational pattern mining is based on the same idea of the generic level-wise search method, known in data mining from the APRIORI algorithm [18]. The level-wise algorithm makes a breadth-first search in the lattice of patterns ordered by a specialization relation $\preceq$. The search starts from the most general patterns, and at each level of the lattice the algorithm generates candidates by using the lattice structure and then evaluates the frequencies of the candidates. In the generation phase, some patterns are taken out using the monotonicity of pattern frequency (if a pattern is not frequent then none of its specializations is frequent).

The generation of the frequent patterns is based on a top-down approach. The algorithm starts with the most general patterns. Then, at each step it tries to specialise all the potential frequent patterns, discarding the non-frequent patterns and storing the ones whose length is equal to the user specified input parameter *maxsize*. Furthermore, for each new refined pattern, semantically equivalent patterns are detected, by using the θ_{OI}-subsumption relation [17], and discarded. In the specialization phase, the specialization operator under θ_{OI}-subsumption is used. Basically, the operator adds atoms to the pattern.

The background knowledge The algorithm uses a background knowledge $\mathcal{B}$ (a set of Datalog clauses) containing the sequence and a set of constraints, similar to that defined in SeqLog [11], that must be satisfied by the generated patterns. In particular, some of the constraint included in $\mathcal{B}$ are (see [16] for more details):

- *maxsize(M)*: maximal pattern length;
- *minfreq(m)*: this constraint indicates that the frequency of the patterns must be larger than m;
- *type(p) and mode(p)*: denote the type and the input/output mode of the predicate's arguments p, respectively. They are used to specify a language bias indicating which predicates can be used in the patterns and to formulate constraints on the binding of variables;
- *negconstraint([$p_1, p_2, \ldots, p_n$])*: specifies a constraint that the patterns must not fulfill, i.e. if the clause $(p_1, p_2, \ldots, p_n)$ subsumes the pattern then it must be discarded;
- *posconstraint([$p_1, p_2, \ldots, p_n$])*: specifies a constraint that the patterns must fulfill. It discards all the patterns that are not subsumed by the clause $(p_1, p_2, \ldots, p_n)$;
- *atmostone([$p_1, p_2, \ldots, p_n$])*: this constraint discards all the patterns that make true more than one predicate among $p_1, p_2, \ldots, p_n$;
- *key([$p_1, p_2, \ldots, p_n$])*: it is optional and specifies that each pattern must have one of the predicates $p_1, p_2, \ldots p_n$ as a starting literal.

Frequency, Support and Confidence Given a set of relational sequences D defined over a set of classes C, then the *frequency* of a pattern p, freq(p, D), corresponds to the number of sequences $s \in D$ such that p subsumes s. The *support* of

a pattern p with respect to a class $c \in C$, $\text{supp}_c(p, D)$ corresponds to the number of sequences $s \in D$ whose class label is c. Finally, the *confidence* of a pattern p with respect to a class $c \in C$ is defined as $\text{conf}_c(p, D) = \text{supp}_c(p, D)/\text{freq}(p, D)$.

The refinement step The refinement of patterns is obtained by using a refinement operator ρ that maps each pattern to a set of specialisations of the pattern, i.e. $\rho(p) \subset \{p' | p \preceq p'\}$ where $p \preceq p'$ means that p is more general of p' or that p subsumes p'. In particular, given the set $\mathcal{D}$ of dimensions, the set $\mathcal{F}$ of fluent atoms, the set $\mathcal{P}$ of non-fluent atoms, for each $i \in \mathcal{D}$, the refinement operator for specialising the patterns is defined as follows:

adding a non-dimensional atom
- the pattern S is specialised by adding a non-dimensional atom;

adding a dimensional atom
- the pattern S is specialised by adding the dimensional atom $(x <_i y)$;
- the pattern S is specialised by adding the dimensional atom $(x \lhd_i y)$;
- the pattern S is specialised by adding the dimensional atom $(x \bigcirc_i^n y)$.

The dimensional atoms are added if and only if there exists a fluent atom referring to its starting event. The length of a pattern P is equal to the number of non-dimensional atoms in P.

For each specialisation level, before to start the next refinement step, Lynx records all the obtained patterns. Hence, it could happens to have in the final set a pattern p that subsumes a lot of other patterns in the same set. However, the subsumed patterns may have a different support, contributing in different way to the classification model.

3.3 Pattern-based Classification

After having identified the set of frequent patterns, now the task is how to use them as features in order to correctly classify unseen sequences. Let $\mathcal{X}$ be the input space of relational sequences, and let $\mathcal{Y} = \{1, 2, \ldots, Q\}$ denote the finite set of possible class labels. Given a training set $D = \{(X_i, Y_i) | 1 \leq i \leq m\}$, where $X_i \in \mathcal{X}$ is a single relational sequence and $Y_i \in \mathcal{Y}$ is the label associated to X_i, the goal is to learn a function $h : \mathcal{X} \to \mathcal{Y}$ from D that predicts the label for each unseen instance.

Let $\mathcal{P}$, with $|\mathcal{P}| = d$, be the set of constructed features obtained in the first step of the Lynx system (the patterns mined from D). For each sequence $X_k \in \mathcal{X}$ we can build a d-component vector-valued $\mathbf{x} = (x_1, x_2, \ldots, x_d)$ random variable where each $x_i \in \mathbf{x}$ is 1 if the pattern $p_i \in \mathcal{P}$ subsumes the sequence x_k, and 0 otherwise.

Using the Bayes' theorem, if $p(Y_j)$ describes the prior probability of the class Y_j, then the posterior probability $p(Y_j|\mathbf{x})$ can be computed from $p(\mathbf{x}|Y_j)$ by

$$p(Y_j|\mathbf{x}) = \frac{p(\mathbf{x}|Y_j)p(Y_j)}{\sum_{i=1}^{Q} p(\mathbf{x}|Y_i)p(Y_i)}. \quad (1)$$

Given a set of discriminant functions $g_i(\mathbf{x})$, $i = 1, \ldots, Q$, a classifier is said to assign the vector $\mathbf{x}$ to the class Y_j if $g_j(\mathbf{x}) > g_i(\mathbf{x})$ for all $j \neq i$. Taking $g_i(\mathbf{x}) = P(Y_i|\mathbf{x})$, the maximum discriminant function corresponds to the *maximum a posteriori* (MAP) probability. For minimum error rate classification, the following discriminant function will be used

$$g_i(\mathbf{x}) = \ln p(\mathbf{x}|Y_i) + \ln P(Y_i). \tag{2}$$

Here, we are considering a multi-class classification problem involving discrete features, multi-class problem in which the components of the vector $\mathbf{x}$ are binary-valued and conditionally independent. In particular, let the component of the vector $\mathbf{x} = (x_1, \ldots, x_d)$ be binary valued (0 or 1). We define

$$p_{ij} = \text{Prob}(x_i = 1|Y_j)_{\substack{i=1,\ldots,d \\ j=1,\ldots,Q}}$$

with the components of $\mathbf{x}$ being statistically independent for all $x_i \in \mathbf{x}$. In this model each feature x_i gives us a yes/no answer about the pattern p_i. However, if $p_{ik} > p_{it}$ we expect the i-th pattern to subsume a sequence more frequently when its class is Y_k than when it is Y_t. The factors p_{ij} can be estimated from the training examples as frequency counts, as follows

$$\begin{aligned} p_{ij} &= \text{Prob}(x_i = 1|Y_j) \\ &= \text{support}_{Y_j}(p_i)_{\substack{i=1,\ldots,d \\ j=1,\ldots,Q}}. \end{aligned}$$

In this way, the constructed features p_i may be viewed as *probabilistic features* expressing the relevance for the pattern p_i in determining the classification Y_j.

By assuming conditional independence we can write $P(\mathbf{x}|Y_i)$ as a product of the probabilities of the components of $\mathbf{x}$. Given this assumption, a particularly convenient way of writing the class-conditional probabilities is as follows:

$$P(\mathbf{x}|Y_j) = \prod_{i=1}^{d} (p_{ij})^{x_i} (1 - p_{ij})^{1-x_i} \tag{3}$$

Hence, the Equation 2 yields the discriminant function

$$\begin{aligned} g_j(\mathbf{x}) = \; & \ln p(\mathbf{x}|Y_j) + \ln p(Y_j) = \\ & \ln \prod_{i=1}^{d} (p_{ij})^{x_i} (1 - p_{ij})^{1-x_i} + \ln p(Y_j) = \\ & \sum_{i=1}^{d} \ln \left((p_{ij})^{x_i} (1 - p_{ij})^{1-x_i} \right) + \ln p(Y_j) = \\ & \sum_{i=1}^{d} x_i \ln \frac{p_{ij}}{1 - p_{ij}} + \sum_{i=1}^{d} \ln(1 - p_{ij}) + \ln p(Y_j) \end{aligned} \tag{4}$$

The factor corresponding to the prior probability for the class Y_j can be estimated from the training set as

$$p(Y_i) = \frac{|\{(X,Y) \in D \text{ s.t. } Y = Y_i\}|}{|D|}, 1 \leq i \leq Q.$$

The minimum probability of error is achieved by the following decision rule: decide Y_k if $g_k(\mathbf{x}) \geq g_j(\mathbf{x})$ for all j and k, where $g_i(\cdot)$ is defined as in Equation 4. Let we note that this discriminant function is linear in the x_i and thus we can write

$$g_j(\mathbf{x}) = \sum_{i=1}^{d} \alpha_i x_i + \beta_0, \tag{5}$$

where $\alpha_i = \ln(p_{ij}/(1-p_{ij}))$, and $\beta_0 = \sum_{i=1}^{d} \ln(1-p_{ij}) + \ln p(Y_j)$. Recall that we decide Y_i if $g_i(\mathbf{x}) \geq g_k(\mathbf{x})$ for all i. The magnitude of the weight α_i in $g_j(\mathbf{x})$ indicates the relevance of a subsumption for the pattern p_i in determining the classification Y_j. This is the probabilistic characteristic of the features obtained in the feature construction phase, opposed to the Boolean feature.

3.4 Feature Selection with stochastic local search

After having constructed a set of features, and presented a method to use those features to classify unseen sequences, now the problem is how to find an optimal subset of these features that optimise the prediction accuracy. The optimisation problem of selecting a subset of features (patterns) with a superior classification performance may be formulated as follows. Let $\mathcal{P}$ be the constructed original set of patterns, and let $f : 2^{|\mathcal{P}|} \rightarrow \mathbb{R}$ a function scoring a selected subset $X \subseteq \mathcal{P}$. The problem of feature selection is to find a subset $\widehat{X} \subseteq \mathcal{P}$ such that

$$f(\widehat{X}) = \max_{Z \subseteq \mathcal{P}} f(Z).$$

An exhaustive approach to this problem would require examining all $2^{|\mathcal{P}|}$ possible subsets of the feature set $\mathcal{P}$, making it impractical for even low values of $|\mathcal{P}|$. The use of a stochastic local search procedure allows us to obtain *good* solutions without having to explore the whole solution space.

Given a subset $P \subseteq \mathcal{P}$, for each sequence $X_j \in \mathcal{X}$ we let the classifier finds the MAP hypothesis adopting the discriminant function reported in Eq. 2:

$$\widehat{h}_P(X_j) = \arg\max_i g_i(\mathbf{x}_j), \tag{6}$$

where $\mathbf{x}_j$ is the feature based representation of the sequence X_j obtained using the patterns P. Hence the initial optimisation problem corresponds to minimise the expectation

$$\mathrm{E}[\mathbf{1}_{\widehat{h}_P(X_i) \neq Y_i}]$$

where $\mathbf{1}_{\widehat{h}_P(X_i)\neq Y_i}$ is the characteristic function of the training example X_i, defined as

$$\mathbf{1}_{\widehat{h}_P(X_i)\neq Y_i} = \begin{cases} 1 & \text{if } \widehat{h}_P(X_i) \neq Y_i \\ 0 & \text{otherwise} \end{cases}$$

Finally, given D the training set with $|D| = m$ and P a set of features (patterns), the number of classification errors made by the Bayesian model is

$$err_D(P) = m\mathrm{E}[\mathbf{1}_{\widehat{h}_P(X_i)\neq Y_i}]. \tag{7}$$

GRASP$^{\mathbf{FS}}$ Consider a *combinatorial optimisation* problem, where one is given a discrete set X of solutions and an objective function $f : X \to \mathbb{R}$ to be minimised and seeks a solution $x^* \in X$ such that $\forall x \in X : f(x^*) \leq f(x)$. A method to find high-quality solutions for a combinatorial problem is a two steps approach consisting of a greedy construction phase followed by a perturbative local search [19]. The greedy construction method starts the process from an empty candidate solution and at each construction step adds the best ranked component according to a heuristic selection function. Then, a perturbative local search algorithm, searching a local *neighborhood*, is used to improve the candidate solution thus obtained. Advantages of this search method are the much better solution quality and fewer perturbative improvement steps to reach the local optimum.

Greedy Randomised Adaptive Search Procedures (GRASP) [20] solve the problem of the limited number of different candidate solutions generated by a greedy construction search method by randomising the construction method. GRASP is an iterative process combining at each iteration a construction and a local search phase. In the construction phase a feasible solution is built, and then its neighbourhood is explored by the local search.

Algorithm 1 reports the GRASP$^{\mathrm{FS}}$ procedure included in the Lynx system to perform the feature selection task. In each iteration, it computes a solution $S \in \mathcal{S}$ by using a randomised constructive search procedure and then applies a local search procedure to S yielding an improved solution. The main procedure is made up of two components: a constructive phase and a local search phase.

The constructive search algorithm used in GRASP$^{\mathrm{FS}}$ iteratively adds a solution component by randomly selecting it, according to a uniform distribution, from a set, named *restricted candidate list* (RCL), of highly ranked solution components with respect to a greedy function $g : \mathcal{S} \to \mathbb{R}$. The probabilistic component of GRASP$^{\mathrm{FS}}$ is characterised by randomly choosing one of the best candidates in the RCL. In our case the greedy function g corresponds to the error function $err_D(P)$ previously reported in Eq. 7. In particular, given $err_D(P)$, the heuristic function, and $\mathcal{S}$, the set of feasible solutions,

$$\underline{s} = \min\{err_D(S)|S \in \mathcal{S}\}$$

and

$$\overline{s} = \max\{err_D(S)|S \in \mathcal{S}\}$$

Algorithm 1 GRASP$^{\text{FS}}$

Input: D: the training set; $\mathcal{P}$: a set of patterns (features); *maxiter*: maximum number of iterations; $err_D(P)$: the evaluation function (see Eq. 7)
Output: solution $\widehat{S} \subseteq \mathcal{P}$

```
Ŝ = ∅, err_D(Ŝ) = +∞
iter = 0
while iter < maxiter do
    α = rand(0,1)
    /* construction */
    S = ∅; i = 0
    while i < n do
        S = {S' | S' = add(S, A)}
        s̄ = max{err_D(T) | T ∈ S}
        s̲ = min{err_D(T) | T ∈ S}
        RCL = {S' ∈ S | err_D(S') ≤ s̲ + α(s̄ − s̲)}
        select the new S, at random, from RCL
        i ← i + 1
    /* local search */
    N = {S' ∈ neigh(S) | err_D(S') < err_D(S)}
    while N ≠ ∅ do
        select S ∈ N
        N ← {S' ∈ neigh(S) | err_D(S') < err_D(S)}
    if err_D(S) < err_D(Ŝ) then
        Ŝ = S
    iter = iter + 1
return Ŝ
```

are computed. Then the RCL is defined by including in it all the components S such that

$$err_D(S) \geq \underline{s} + \alpha(\overline{s} - \underline{s}).$$

The parameter α controls the amounts of greediness and randomness. A value $\alpha = 1$ corresponds to a greedy construction procedure, while $\alpha = 0$ produces a random construction. As reported in [21], GRASP with a fixed nonzero RCL parameter α is not asymptotically convergent to a global optimum. The solution to make the algorithm asymptotically globally convergent, could be to randomly select the parameter value from the continuous interval $[0, 1]$ at the beginning of each iteration and using this value during the entire iteration, as we implemented in GRASP$^{\text{FS}}$. Hence, starting from the empty set, in the first iteration all the subsets containing exactly one pattern are considered and the best is selected for further specialisation. At the iteration i, the working set of patterns S is refined by trying to add a pattern belonging to $\mathcal{P} \setminus S$.

To improve the solution generated by the construction phase, a local search is used. It works by iteratively replacing the current solution with a better solution taken from the neighbourhood of the current solution while there is a better solution in the neighbourhood. In order to build the neighbourhood of a solution S, *neigh(S)*, the following operators have been used. Given $\mathcal{P}$ the set of patterns, and $S = \{p_1, p_2, \ldots, p_t\} \subseteq \mathcal{P}$ a solution:

add: $S \rightarrow S \cup \{p_i\}$ where $p_i \in \mathcal{P} \setminus S$;
remove: $S \rightarrow S \setminus \{p_i\} \cup \{p_k\}$ where $p_i \in S$ and $p_k \in \mathcal{P} \setminus S$.

In particular, given a solution $S \in \mathcal{S}$, the elements of the neighborhood $neigh(S)$ of S are those solutions that can be obtained by applying an elementary modification (add or remove) to S. Local search starts from an initial solution $S^0 \in \mathcal{S}$ and iteratively generates a series of improving solutions $S^1, S^2, \ldots$. At the k-th iteration, $neigh(S^k)$ is searched for an improving solution S^{k+1} such that $err_D(S^{k+1}) < err_D(S^k)$. If such a solution is found, it is made the current solution. Otherwise, the search ends with S^k as a local optimum.

4 Experiments

Experiments have been conducted on protein fold classification, an important problem in biology since the functions of proteins depend on how they fold up. The dataset, already used in [13, 12, 14] is made up of logical sequences of the secondary structure of protein domains. The task is to predict one of the five most populated SCOP folds of alpha and beta proteins (a/b): TIM beta/alpha-barrel (c1), NAD(P)-binding Rossmann-fold domains (c2), Ribosomal protein L4 (c23), Cysteine hydrolase (c37), and Phosphotyrosine protein phosphatases I-like (c55). The class of a/b proteins consists of proteins with mainly parallel beta sheets (beta-alpha-beta units). Overall, the class distribution is 721 sequences for the class c1, 360 for c2, 274 for c23, 441 for c37 and 290 for c55.

Conf.	Lynx	Folds										Mean
		1	2	3	4	5	6	7	8	9	10	
0.95	w/o GRASP^{FS}	0.84	0.88	0.83	0.83	0.85	0.76	0.85	0.81	0.82	0.80	0.826
	w GRASP^{FS}	0.88	0.92	0.88	0.88	0.89	0.84	0.93	0,87	0.90	0.93	**0.878**
1.0	w/o GRASP^{FS}	0.89	0.94	0.84	0.92	0.94	0.88	0.91	0.89	0.88	0.87	0.896
	w GRASP^{FS}	0.94	0.97	0.93	0.95	0.95	0.93	0.93	0.97	0.90	0.94	**0.942**

Table 1. Cross-validated accuracy of Lynx with and without feature selection on two values for the confidence.

As in [14], we used a round robin approach [22], treating each pair of classes as a separate classification problem, and the overall classification of an example instance is the majority vote among all pairwise classification problems.

Table 1 reports the experimental results of a 10-fold cross-validated accuracy of Lynx. Two experiments have been conducted, one with a confidence level equal to 0.95 and the other with a confidence level of 1.0. In particular, given the training data D, we imposed that $\text{conf}_c(p, D) = 0.95$ (resp. $\text{conf}_c(p, D) = 1$). For each experiment, Lynx has been applied on the same data with and without feature selection. In particular, we applied the classification on the test instances without applying GRASP^{FS} in order to have a baseline accuracy value. Indeed, as we can see, the accuracy grows when GRASP^{FS} optimises the feature set, proving the validity of the method adopted for the feature selection task. Furthermore, the accuracy level grows up when we mine patterns with a confidence level equal to 1.0 corresponding to save *jumping emerging patterns*[2] only. This proves that jumping patterns have a discriminative power greater than *emerging patterns*[3] (when the confidence level is equal to 0.95).

As as second experiment we compared Lynx on the same data to other statistical relational learning systems, whose cross-validated accuracies are summarised in Table 2. In particular, LoHHMs [12] were able to achieve a predictive accuracy of 75%, Fisher kernels [13] achieved an accuracy of about 84%, TildeCRF [14] reaches an accuracy value of 92.96%, while Lynx obtains an accuracy of 94.15%. Hence, we can conclude that Lynx performs better than established methods on real-world data.

System	Accuracy
LoHMMs [12]	75%
Fisher kernels [13]	84%
TildeCRF [14]	92.96%
Lynx	94.15%

Table 2. Cross-validated accuracy of LoHHMs, Fisher kernels, TildeCRF and Lynx

[2] A jumping emerging pattern is a pattern with non-zero support on a class an a zero support on all the other classes, i.e. with a confidence equal to 1.

[3] An emerging pattern is a pattern with a grow rate greater that 1.

5 Conclusions

In this paper we considered the problem of multi-class relational sequence learning using relevant patterns discovered from a set of labelled sequences. We firstly applied a feature construction method in order to map each relational sequence into a feature vector. Then, a feature selection algorithm to find an optimal subset of the constructed features leading to high classification accuracy has been applied. The feature selection task has been solved adopting a wrapper approach that uses a stochastic local search algorithm embedding a naïve Bayes classifier. The performance of the proposed method applied to a real-world dataset shows an improvement when compared to other established methods.

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