Maximum Entropy Modeling with Clausal Constraints*

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Abstract

We present the learning system *MACCENT* which addresses the novel task of stochastic MAXimum ENTropy modeling with Clausal Constraints. Maximum Entropy method is a Bayesian method based on the principle that the target stochastic model should be as uniform as possible, subject to known constraints. *MACCENT* incorporates clausal constraints that are based on the evaluation of Prolog clauses in examples represented as Prolog programs. We build on an existing maximum-likelihood approach to maximum entropy modeling, which we upgrade along two dimensions: (1) *MACCENT* can handle larger search spaces, due to a partial ordering defined on the space of clausal constraints, and (2) uses a richer first-order logic format. In comparison with other inductive logic programming systems, *MACCENT* seems to be the first that explicitly constructs a conditional probability distribution $p(C|I)$ based on an empirical distribution $\tilde{p}(C|I)$ (where $p(C|I)$ ($\tilde{p}(C|I)$) gives the induced (observed) probability of an instance I belonging to a class C). First experiments indicate *MACCENT* may be useful for prediction, and for classification in cases where the induced model should be combined with other stochastic information sources.

1 Introduction

Bayesian probability theory permits one to use prior knowledge, in the form of an empirical probability distribution, for making rational inferences about the behavior of a random process. *Maximum Entropy* [Jaynes, 1990] method is a Bayesian method based on the principle that the target stochastic model should be as uniform as possible, subject to constraints extracted from the training distribution. This principle is not new, it can in fact be traced back to Occam's razor, Laplace, and beyond, but relatively recent developments in computer science have boosted its popularity and have enabled its application to real-world problems, mainly in physics (cf. [Gull and Daniell, 1978]). As a starting point for our research we used the paper by Berger, Della Pietra, and Della Pietra [Berger *et al.*, 1996], which presents a maximum-likelihood approach to the construction of maximum entropy models of natural language.

We have combined the statistical approach of [Berger *et al.*, 1996] with techniques from the field of inductive logic programming to build the relational learner *MACCENT* that addresses the task of MAXimum ENTropy modeling with Clausal Constraints. The adjective "clausal" here refers to the fact that in *MACCENT* the constraints, which are the building blocks of maximum entropy modeling, are based on the evaluation of Prolog clauses in examples represented as Prolog programs. The integration of probabilistic methods with inductive logic programming has recently become a popular research topic (cf. [Karalič and Bratko, 1997; Muggleton, 1997; Pompe and Kononenko, 1995]), but, to the best of our knowledge, *MACCENT* is the first inductive logic programming algorithm that explicitly constructs a conditional probability distribution $p(C|I)$ based on an empirical distribution $\tilde{p}(C|I)$ (where $p(C|I)$ ($\tilde{p}(C|I)$) gives the induced (observed) probability of an instance I belonging to a class C).

We start our discussion with a brief introduction to the logical and mathematical foundations (Section 2). In the two next parts we then present the task addressed by

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animal	has_covering	has_legs	habitat	homeothermic	class
dog	hair	yes	land	yes	mammal
dolphin	none	no	water	yes	mammal
trout	scales	no	water	no	fish
shark	none	no	water	no	fish
herring	scales	no	water	no	fish
eagle	feathers	yes	air	yes	bird
penguin	feathers	yes	water	yes	bird
lizard	scales	yes	land	no	reptile
snake	scales	no	land	no	reptile
turtle	scales	yes	land	no	reptile

Table 1: The animals domain

MACCENT (Section 3), and the algorithm itself (Section 4). Finally, we report on classification and prediction experiments with a prototypical implementation of MACCENT (Section 5), and conclude (Section 6). Though throughout the paper we have restricted the logical notation to a minimum, we do assume some familiarity with the programming language Prolog [Bratko, 1986].

2 Logical and statistical background

2.1 Logical paradigm: learning from interpretations

Consider the data in Table 1, which presents instances of four classes of animals. Traditional attribute-value learners represent each animal and candidate classification rule as a set of attribute-value pairs, such that simple subset test suffices in order to verify if a rule covers an instance. Alternatively, one can store the information available about a single animal in a Prolog knowledge base, encode candidate rules as Prolog queries, and apply the Prolog execution mechanism to verify whether or not a rule covers an instance. If the query succeeds, the rule covers the instance. If the query fails¹, the rule does not cover the instance. For example, the logical conjunction *has_legs* ∧ *habitat*(*land*) covers instance *dog* because the Prolog query $\leftarrow \text{has_legs}, \text{habitat}(\text{land})$ succeeds in the Prolog program dog:

```
animal(dog). has_covering(hair).
has_legs. habitat(land).
homeothermic. class(mammal).
```

Notice that the attribute-value and Prolog representations are equivalent in standard propositional domains. In Prolog notation however instances can be Prolog programs of deliberate size and complexity, rather than fixed-length vectors of attribute-value pairs. As a consequence, background knowledge can be added in a natural way as Prolog code shared by all instances. For example, with Prolog clause *kids_love_it* :- *homeothermic*, *habitat*(*water*) added as background knowledge to Table 1, rule *has_covering*(*none*) ∧ *kids_love_it* exclusively covers instance *dolphin*.

The above alternative and flexible Prolog based representation and verification method fits in the *learning*

¹Termination can be guaranteed by employing a depth-bound on the depth of the proof tree.

from *interpretations* paradigm, introduced by [De Raedt and Džeroski, 1994] and related to other inductive logic programming settings in [De Raedt, 1996].

2.2 Statistical paradigm: maximum entropy

Let us reconsider the data in Table 1, and interpret them as a sample of an expert biologist’s decisions concerning the class of animals. The observed behavior of the biologist can be summarized as an empirical conditional distribution $\tilde{p}(C|I)$ that, given the description of an instance in I in the first five columns, assigns probability 1 to the class specified in the last column, and 0 to all other classes. Sample $\tilde{p}$ can be used to support the construction of a stochastic model p to predict the behavior of the biologist. Given an instance I , this target model will assign to each class C_j an estimate $p(C_j|I)$ of the conditional probability that the biologist would classify I as C_j .

“Relevant” facts (statistics) extracted from the empirical distribution $\tilde{p}$ are the building blocks of the target distribution p . For example, with sample Table 1, $\tilde{p}$ assigns conditional probability 1 to exactly four classes C . If we are convinced this fact captures relevant information about the sample, we can construct our model p such that, for all instances I it meets the following constraint:

$$p(\text{mammal}|I) + p(\text{fish}|I) + p(\text{bird}|I) + p(\text{reptile}|I) = 1 \quad (1)$$

There is of course a whole family of models that meet constraint (1). However, some members of this family seem more justified than others, given the limited empirical evidence (1) we have gathered so far. More specifically, the model that assigns equal 0.25 probability to all classes seems intuitively more reasonable than one that grants probability 0.5 to *mammal* and *fish*, and 0 to the other classes. Though the latter model agrees with what we know, it contains information for which we have – as yet – no evidence. A stochastic model that avoids such bold assumptions, should be as “uniform” as possible, subject to the known constraints.

In the maximum entropy paradigm [Jaynes, 1990] conditional entropy

$$H(p) \equiv -\frac{1}{N} \sum_{C,I} p(C|I) \log p(C|I) \quad (2)$$

is used to measure uniformity², with N the number of instances in the sample. The *Maximum Entropy Principle* then states that, from the family of conditional probability distributions allowed by an empirically compiled set of constraints, we should elect the model with maximum conditional entropy $H(p)$.

²Throughout the paper log denotes natural logarithm.

3 Maximum entropy modeling with clausal constraints

As indicated in the previous section, the building blocks of a maximum entropy model are constraints such as Equation (1). MACCENT incorporates constraints based on *boolean clausal indicator functions* $f(I, C)$ with general form:

$$f_j(I, C) = \begin{cases} 1 & \text{if } C = C_j \text{ and query } \leftarrow Q_j \text{ succeeds in instance } I \\ 0 & \text{otherwise} \end{cases} \quad (3)$$

A clausal³ indicator function f_j , fully defined by the tuple $\langle C_j, \leftarrow Q_j \rangle$, gives rise to a *clausal constraint* of the form

$$CC_j : p(f_j) = \tilde{p}(f_j) \quad (4)$$

where $p(f_j)$ is the *expected value* of $f_j(I, C)$ in the target distribution, and $\tilde{p}(f_j)$ is the expected value of $f_j(I, C)$ in the empirical distribution. For any $f_j(I, C)$, the calculation of its expected value with respect to a conditional distribution proceeds as follows. First, we take the sum over all instances and classes $\sum_{I, C} f_j(I, C)$. For example, given the data in Table 1, if

$$f_1(I, C) = \begin{cases} 1 & \text{if } C = \text{fish and} \\ & \leftarrow \text{not}(\text{has_legs}), \text{habitat}(\text{water}) \text{ succeeds in } I \\ 0 & \text{otherwise} \end{cases}$$

then

$f_1(\text{dolphin}, \text{fish})$, $f_1(\text{trout}, \text{fish})$, $f_1(\text{shark}, \text{fish})$, and $f_1(\text{herring}, \text{fish})$ evaluate to one, and all other combinations of instances and classes evaluate to zero, hence $\sum_{I, C} f_1(I, C) = 4$. Next, we normalize the summation with constant N , the number of instances in the sample, for example $1/10 \sum_{I, C} f_1(I, C) = 0.4$. Finally, to obtain the expected value $p(f_j)$ of $f_j(I, C)$ in model p , we multiply $f_j(I, C)$ by $p(C|I)$. For the expected value of $f_j(I, C)$ in empirical distribution $\tilde{p}$, and in target distribution p this yields the equations

$$\tilde{p}(f_j) \equiv \frac{1}{N} \sum_{I, C} \tilde{p}(C|I) f_j(I, C) \quad (5)$$

$$p(f_j) \equiv \frac{1}{N} \sum_{I, C} p(C|I) f_j(I, C) \quad (6)$$

For example, with p a uniform conditional distribution, $p(\text{fish}|I) = 0.25$ for all instances in Table 1. As $f_1(I, \text{fish})$ equals one for only four for these, we have that $p(f_1) = 1/10 * (0.25 + 0.25 + 0.25 + 0.25) = 0.1$. On the other hand, in the sample we find that $\tilde{p}(\text{fish}|I) = 1$ for the three instances trout, shark, and herring, and $\tilde{p}(\text{fish}|I) = 0$ for all other instances, including dolphin. Hence, $\tilde{p}(f_1) = 1/10 * (1 + 1 + 1) = 0.3$. Function f_1 , through its expected value, thus reveals a discrepancy between the empirical and the target distribution. This

discrepancy disappears if we add the clausal constraint $p(f_1) = \tilde{p}(f_1) = 0.3$ to our initial constraint Equation (1), and construct a new model that maximizes conditional entropy subject to both constraints. As a second example, consider

$$f_2(I, C) = \begin{cases} 1 & \text{if } C = \text{reptile and} \\ & \leftarrow \text{not}(\text{has_covering}(\text{hair})), \text{not}(\text{has_legs}) \text{ succeeds in } I \\ 0 & \text{otherwise} \end{cases}$$

for which the expected values are $p(f_2) = 0.125$, and $\tilde{p}(f_2) = 0.1$. Notice that with respect to the sample the expected value $p(f_2)$ is 0.025 units too high, whereas $p(f_1)$ is 0.2 units too low.

Now that we have described the building blocks, we can formulate the task of *maximum entropy modeling with clausal constraints*:

- *Given:* A set $\mathcal{I}$ of N training instances, represented as Prolog programs;
- *Given:* An empirical conditional distribution $\tilde{p}(C|I)$, with $I \in \mathcal{I}$;
- *Given:* A language $\mathcal{L}$ of clausal constraints $p(f_j) = \tilde{p}(f_j)$;
- *Find:* An optimal set $\mathcal{CC} \subseteq \mathcal{L}$ of clausal constraints;
- *Find:* A stochastic model $p^{CC}(C|I)$ that maximizes conditional entropy $H(p)$ subject to the clausal constraints in $\mathcal{CC}$.

To restate, algorithms that address this task receive as input training instances, an empirical conditional distribution that relates training instances to classes, and a set of clausal constraints. In response, they must (1) select an “optimal” subset of clausal constraints, and (2) with these constraints build a model for use in classifying new instances.

We come back to the selection of $\mathcal{CC}$ later, and first concentrate on the modeling subtask. Given set $\mathcal{CC}$, the method of Lagrange multipliers from the theory of constrained optimization produces the model p that maximizes conditional entropy $H(p)$. As discussed thoroughly in [Della Pietra *et al.*, 1995; Berger *et al.*, 1996], the model in question has the parametric form

$$p_\Lambda(C|I) = \frac{1}{Z_\Lambda(I)} \exp \left(\sum_j \lambda_j f_j(I, C) \right) \quad (7)$$

where each parameter (Lagrange multipliers) λ_j from set Λ corresponds to a clausal constraint CC_j based on clausal indicator function f_j . The optimal parameter set Λ can be determined by maximizing the log-likelihood $L_{\tilde{p}}(p_\Lambda)$ of the empirical distribution $\tilde{p}$, which is defined by

$$L_{\tilde{p}}(p_\Lambda) = -\frac{1}{N} \sum_I \log Z_\Lambda(I) + \sum_j \lambda_j \tilde{p}(f_j) \quad (8)$$

³Recall that Prolog queries are a special type of Prolog *clauses* with **false** in the conclusion part.

Figure 1: The log-likelihood functions $F1 = L_{\tilde{p}}(p_{\{\lambda_1\}})$ and $F2 = L_{\tilde{p}}(p_{\{\lambda_2\}})$.

where $Z_{\Lambda}(I)$ is a normalization constant:

$$Z_{\Lambda}(I) = \sum_C \exp \left(\sum_j \lambda_j f_j(I, C) \right) \quad (9)$$

If we apply these equations to our running example, we obtain, after reduction,

$$L_{\tilde{p}}(p_{\{\lambda_1\}}) = -0.4 * \log(e^{\lambda_1} + 3) - 0.6 * \log(4) + 0.3 * \lambda_1$$

$$L_{\tilde{p}}(p_{\{\lambda_2\}}) = -0.5 * \log(e^{\lambda_2} + 3) - 0.5 * \log(4) + 0.1 * \lambda_2$$

where λ_1 and λ_2 correspond to f_1 and f_2 . The graph of these two equations is plotted in Figure 1. On the X axis of this graph, we find the λ values, on the Y axis the log-likelihood of the Table 1 training set. The graph shows that with $CC = \{CC_1\}$, the optimal parameter set $\{\lambda_1\}$ is obtained with a positive value for λ_1 . This agrees with the earlier finding that in the uniform distribution, $p(f_1) < \tilde{p}(f_2)$. The intuition here is that the appropriateness of CC_1 has been underestimated in p , and a positive weight λ_1 is required to correct this. The opposite holds for $CC = \{CC_2\}$, where the optimum for λ_2 is negative.

Let us now return to the selection of an optimal set $CC \subset \mathcal{L}$. For the time being we assume an exhaustive search through $2^{\mathcal{L}}$ and focus on an evaluation function for $S \subset \mathcal{L}$. Notice that maximum entropy and maximum likelihood are dual problems and that, of all models of parametric form (7), the maximum entropy model is the one that maximizes the the likelihood of the sample. As might be clear from the above discussion of Figure 1, this maximum is function of the set S of clausal constraints. We are interested in the set S that produces the highest likelihood of the training sample $\tilde{p}$. Formally, if we let p^S denote the maximum entropy model obtained with a set S of clausal constraints then

$$CC \equiv \operatorname{argmax}_{S \subset \mathcal{L}} L_{\tilde{p}}(p^S) \quad (10)$$

Algorithm 1 : MACCENT

- Inputs: Language $\mathcal{L}$; empirical distribution $\tilde{p}(C|I)$
Outputs: Set CC of clausal constraints; model p^{CC}
1. Start with $CC = \emptyset$; thus p^{CC} is uniform
 2. Select next clausal constraint $\hat{c}c$ from $\mathcal{L}$ using Algorithm 2
 3. Check the termination condition
 4. Adjoin $\hat{c}c$ to CC
 5. Compute p^{CC} using Equation (7)
 6. Go to step 2
-

For an illustration of this evaluation function consider again Figure 1. The graph shows that with $\{CC_1\}$ we can obtain log-likelihood around -1.17, whereas with $\{CC_2\}$ we only reach -1.38. Hence, of these two sets, $\{CC_1\}$ is to be preferred.

4 The MACCENT Algorithm

In this section we present the learning system MACCENT which addresses the task of MAXimum ENTropy modeling with Clausal Constraints. The task as described in the previous section does not directly translate to a tractable algorithm. Usually, with millions of clausal constraints in $\mathcal{L}$, it is prohibitive to inspect all subsets of $\mathcal{L}$ in search for the optimal one. In our description of MACCENT we will gradually abandon the request for optimality of CC . We first discuss a greedy search method and an approximate gain evaluation function, both due to [Berger *et al.*, 1996]. In addition, we then propose a structure on $\mathcal{L}$ that one can use to organize the search process.

As shown in Algorithm 1, MACCENT carries out a greedy search, adjoining clausal constraints one at a time, using an evaluation function to select the next constraint at each step. Given a set S of constraints collected so far, a natural evaluation function for a candidate clausal constraint $\hat{c}c$ returns the gain $\Delta L_{\tilde{p}}(S, \hat{c}c)$ in the log-likelihood of the training data obtained by that adding $\hat{c}c$ to S

$$\Delta L_{\tilde{p}}(S, \hat{c}c) \equiv L_{\tilde{p}}(p^{S \cup \hat{c}c}) - L_{\tilde{p}}(p^S) \quad (11)$$

As $L_{\tilde{p}}(p^S)$ remains constant, this comes down to adding at each step the constraint CC that maximizes $L_{\tilde{p}}(p^{S \cup CC})$. We have thus reduced the selection task to the discovery of the best $CC \in \mathcal{L}$. For instance, consider again our running example and the graph in Figure 1. Knowing that $L_{\tilde{p}}(p^{\emptyset}) = -\log(4) \simeq -1.39$, we can compute that the gain obtained by adding CC_1 and CC_2 is something round 0.22 and 0.01 respectively. Hence, CC_1 is a better initial choice.

Still, given the “old” set $\mathcal{S} = \{CC_1, \dots, CC_n\}$, log-likelihood gain requires for each candidate $\hat{cc} \in \mathcal{L}$ the computation of the set of parameters $\Lambda = \{\lambda_1, \dots, \lambda_n, \alpha\}$ that maximizes $L_{\tilde{p}}(p_\Lambda)$, where α is the parameter that corresponds to $\hat{cc}$. Various numerical methods have been applied to this problem, including problem specific algorithms such as BROWN [Brown, 1959] or ITERATIVE SCALING [Darroch and Ratcliff, 1972]. However, none of these methods allow for a sufficiently efficient computation of gain $\Delta L_{\tilde{p}}(\mathcal{S}, \hat{cc})$. As a remedy, [Berger *et al.*, 1996] introduce the notion of *approximate gain* which no longer requires the computation of $n + 1$ parameters. The “old” parameter set $\{\lambda_1, \dots, \lambda_n\}$ is retained, and the approximation is made that the addition of constraint $\hat{cc}$ affects only parameter α . Given candidate constraint $\hat{cc}$ derived from indicator function $\hat{f}$, Equation (8) then reduces to

$$G_{\mathcal{S}, \hat{f}}(\alpha) = -\frac{1}{N} \sum_{I, C} \log \left(p^{\mathcal{S}}(C|I) e^{\alpha \hat{f}(I, C)} \right) + \alpha \tilde{p}(\hat{f}) \quad (12)$$

Equation (12) in turn simplifies the computation of the *approximate gain*

$$\sim \Delta L_{\tilde{p}}(\mathcal{S}, \hat{cc}) \equiv \max_{\alpha} G_{\mathcal{S}, \hat{f}}(\alpha) \quad (13)$$

to a one-dimensional optimization problem which can be solved, for instance, with Newton’s method.

Though [Berger *et al.*, 1996] has shown one can implement a high-performance algorithm on the basis of the above approximations, we still assume an exhaustive search through a flat, unstructured space $\mathcal{L}$ of clausal constraints. To further speed up the search, and enable the exploration of bigger search spaces, MACCENT extends these approximations with classical machine learning techniques. The key observation here is that generality imposes a partial ordering on $\mathcal{L}$. To be precise, this generalisation relation is defined between tuples of class names and Prolog queries⁴: $\langle C_g, \leftarrow Q_g \rangle$ is more general than $\langle C_s, \leftarrow Q_s \rangle$ if and only if $C_g \leftarrow Q_g$ is logically more general (under θ subsumption, cf. [Plotkin, 1970]) than $C_s \leftarrow Q_s$. One can specify a lattice for clausal constraints with a set of most general descriptions $\langle C_j, \leftarrow true \rangle$ at the top, and a specialisation operator for top-down exploration of this lattice. In MACCENT we handle both tasks with the declarative language bias formalism DLAB [Dehaspe and De Raedt, 1996].

As shown in Algorithm 2, MACCENT exploits the lattice structure of $\mathcal{L}$ to carry out a general-to-specific heuristic beam search for clausal constraints with satisfactory, rather than optimal, approximate gain. At each

Algorithm 2 : Select next clausal constraint

Inputs: Language $\mathcal{L}$; empirical distribution $\tilde{p}(C|I)$; current set CC

Outputs: Clausal constraint $\hat{cc}$

1. Initialize current best approximate gain $Best := -1$
 2. Initialize $Beam := \{\langle C_j, \leftarrow true \rangle \mid \text{class } C_j \in \mathcal{L}\}$
 3. Select cc from Beam
 4. For each cc in Beam, and for each specialisation $cc' \in \mathcal{L}$ of cc :
 - (a) Compute $Gain = \Delta L_{\tilde{p}}(CC, cc')$ using Equation (13),
 - (b) If $Gain > Best$ then update $Best := Gain$ and $\hat{cc} := cc'$,
 - (c) Add cc' to Beam
 5. Prune Beam
 6. If Beam is not empty, go to step 3
-

level of its search, MACCENT considers all specialisations of clausal constraints in the beam, and if necessary updates the current best solution.

We still have to specify a stopping criterion (Algorithm 1, step 3) and a procedure for pruning Beam (Algorithm 2, step 5). For our stopping criterion we use Equation (8) to calculate the log-likelihood $L_{\tilde{p}}(p^{CC \cup \hat{cc}})$ of a separate empirical distribution $\tilde{p}$. If the log-likelihood of this withheld portion of the training set decreases⁵ with the addition of $\hat{cc}$, this is taken as an indication of over-training, and MACCENT terminates.

Given a beam size BS , the default strategy for pruning Beam is to rank the clausal constraints cc' in Beam according to their *Gain* and keep at most BS of the best scoring constraints. However, in cases where the input empirical distribution assigns only probabilities 1 and 0, as for instance in Table 1, we can apply a more sophisticated heuristic. Thereto, we define the notion of *potential approximate gain* as an upper bound to the maximum *Gain* that can be obtained via further specialisation of cc' . We cannot go into details here, but under the circumstances mentioned, potential approximate gain can easily be computed. One has to select the instances for which $\tilde{p}(C'|I) = 1$, compute the approximate gain counting only this subset, do the same for the complementary subset, and take the maximum of both computations. The potential approximate gain upper bound allows a branch-and-bound search in which clausal constraints are pruned that after specialisation can never produce an approximate gain above the current best. Apart from that, potential approximate gain can also be used in combination with actual approximate

⁴Recall (cf. Equations (3) and (4)) that the tuple $\langle C_j, \leftarrow Q_j \rangle$ fully identifies clausal constraint CC_j .

⁵A delay is built in to allow recovery from a temporary decrease.

gain to better rank the constraints in *Beam*⁶.

5 Experiments

In this section we report on some first classification and prediction experiments with a prototypical Prolog implementation of MACCENT. Both classification and numeric prediction could in fact be considered as special cases of the task of learning from a conditional probability distribution $\tilde{p}(C|I)$: with classification $\tilde{p}(C|I)$ only takes values 0 and 1; with numeric prediction there are only two classes C . We would like to stress that the full power of MACCENT should best be demonstrated on the general case of multi-class datasets where $\tilde{p}$ can take any real value between 0 and 1 (e.g. distribution of votes for more than two candidates in different districts). At present however, such data do not seem to be readily available.

First, we round off the running example with the application of MACCENT to the multi-class animals domain. With the hold-out stopping criterion suppressed, MACCENT found 13 constraints before the log-likelihood of Table 1 was reduced to 0. The first four of these clausal constraints are, in order of discovery,

$\langle C, \leftarrow Q \rangle$	gain	λ	llh
$\langle \text{reptile}, \leftarrow \text{has_cov}(\text{scales}), \text{habitat}(\text{land}) \rangle$	0.27	1.59	-1.11
$\langle \text{fish}, \leftarrow \text{not}(\text{has_legs}), \text{not}(\text{hom}) \rangle$	0.23	1.56	-0.88
$\langle \text{bird}, \leftarrow \text{has_cov}(\text{feath}) \rangle$	0.18	1.59	-0.70
$\langle \text{mammal}, \leftarrow \text{not}(\text{has_cov}(\text{feath})), \text{hom} \rangle$	0.18	1.59	-0.52

with the approximate gain, best λ , and log-likelihood of the sample in columns 2, 3, and 4 respectively.

5.1 Classification

When compared to other inductive logic programming classifiers, MACCENT has the advantage that it induces a conditional probability distribution that can directly be combined with other stochastic information sources. To illustrate this point we conducted a relatively small experiment with natural language data extracted from the Wall Street journal corpus [Marcus *et al.*, 1993].

In this corpus the words are tagged with so-called Parts-of-Speech (POS). We grouped the tags into 16 classes, the most important of which are noun, adjective, verb, punctuation, determiner, pronoun, adverb. Next, based on frequency counts in the corpus, we set up a dictionary that, given a word w assigns to each class pos a lexical probability $p_{dict}(pos|w)$. For instance, $p_{dict}(\text{adjective}|\text{cross}) = 0.03$, $p_{dict}(\text{noun}|\text{cross}) = 0.69$, $p_{dict}(\text{verb}|\text{cross}) = 0.28$. Then we selected from the corpus the first 1000 occurrences of words, such as *cross*, that are ambiguous between exactly the three classes noun, adjective, and verb. We stored each word, with

⁶MACCENT mainly employs the average of the actual and the potential approximate gain.

its class label, and the tagged left and right context in a separate instance. As background knowledge we specified Prolog predicates $left(Index, Limit, Pos)$, and $right(Index, Limit, Pos)$ that check whether a certain tag Pos appears in the context of a word within distance $Limit$, where $Index$ is the position the word in the sentence. In the language $\mathcal{L}$, with a size of order 10^{15} , we allowed combinations of these two predicates, with $Limit$ taking values 1, 2, 3, 4, 5, and *unlimited*, and with Pos instantiated to one of the 16 morphological categories. Finally, we ran MACCENT on this 3-class problem to construct a probability distribution $p_{context}(pos|w)$ based on the context of the word.

Classifying words into the class with highest probability as predicted by the model we ran a 10-fold crossvalidation based on a random partition over 1000 instances, and each time measured the performance in terms of classification accuracy. The model $p_{context}(pos|w)$ induced by MACCENT achieved an average accuracy of 70.4%(± 4.8). The model $p_{dict}(pos|w)$ based on the dictionary had a much better score of 81.2(± 3.0). The best score however was obtained from the combination of the two models $p_{context}(pos|w) * p_{dict}(pos|w)$ which achieved an accuracy of 85.4(± 3.0).

Though MACCENT by itself is likely to perform better in the presence of more sophisticated background knowledge, this initial experiment with POS-tagging demonstrates the (poor) output of MACCENT can successfully be combined with other stochastic information sources. For a more mature application of maximum entropy method to the general POS-tagging problem, we refer to [Ratnaparkhi, 1996].

5.2 Numeric prediction

Recall that one of the inputs to MACCENT is an empirical distribution $\tilde{p}(C|I)$. In the previous examples, $\tilde{p}$ took only the values 0 and 1. Multi-class datasets where $\tilde{p}$ can take any real value between 0 and 1, do not seem to be readily available. There are however enough tasks available that involve regression, the prediction of a numeric value. These values can always be projected onto a scale from 0 to 1. With some abuse of the intuitions behind a conditional probability model, MACCENT can now interpret the rescaled values as estimates of the probability that the example belongs the single “positive” class. The inverse “unscaling” projection allows one to calculate predictions from the induced model. Like the FORS system [Karalič and Bratko, 1997], which incorporates linear regression techniques, MACCENT can then perform first order regression from positive data only.

We applied this technique to two benchmark domains well known in the inductive logic programming community: mutagenicity [Srinivasan *et al.*, 1996], and mesh design [Dolšak and Muggleton, 1992].

In the first domain the task is to predict the log mutagenicity of molecules on the basis of structural information on the compounds. We used the full set of available background predicates and defined a language $\mathcal{L}$ with size order 10^{24} . With a 10-fold crossvalidation we obtained an average standard error of $1.38(\pm 0.18)$, with log-mutagenicity ranging from -3 to 5.39.

The second domain requires a prediction about the coarseness of a mesh model used to approximate physical structures. For every edge of the structure one has to decide on the number, ranging from 1 to 17, of subedges on the basis of properties of the edge and of related edges. We focused our experiments on the 5 structure (A,B,C,D,E) dataset. With a language $\mathcal{L}$, with size of order 10^7 , we tried both a 5-fold leave-one-structure-out (mesh-xv5) and a random 10-fold crossvalidation (mesh-xv10). We calculated standard error of the estimate, and accuracy. For accuracy we rounded MACCENT's predictions to the nearest class. The table below summarizes results for MACCENT and ICL [De Raedt and Van Laer, 1995].

Algorithm	Accuracy		Standard error	
	mesh-xv5	mesh-xv10	mesh-xv5	mesh-xv10
ICL	0.80	0.70(± 0.05)	2.82(± 1.19)	1.84(± 1.03)
MACCENT	0.25	0.44(± 0.11)	2.83(± 0.42)	1.54(± 0.33)

The above table shows roughly the same picture for mesh-xv5 and mesh-xv10: MACCENT scores a lot worse on accuracy, but comparable or even slightly better on standard error. We take this as an indication that the scaling technique indeed makes sense, and that MACCENT can be considered for solving regression tasks.

6 Conclusion

We have presented a framework for combining maximum entropy modeling with inductive logic programming techniques, and a number of approximations that led to the definition and implementation of the MACCENT algorithm. First experiments indicate the first order statistical modeling algorithm MACCENT may be useful for prediction, and for classification in cases where the induced model should be combined with other stochastic information sources.

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