Using Logical Decision Trees for Clustering

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Abstract. A novel first order clustering system, called C 0.5, is presented. It inherits its logical decision tree formalism from the TILDE system, but instead of using class information to guide the search, it employs the principles of instance based learning in order to perform clustering. Various experiments are discussed, which show the promise of the approach.

1 Introduction

A decision tree is usually seen as representing a theory for classification of examples. If the examples are positive and negative examples for one specific concept, then the tree defines these two concepts. One could also say, if there are k classes, that the tree defines k concepts.

Another viewpoint is taken in Langley's *Elements of Machine Learning* [11]. Langley sees decision tree induction as a special case of the induction of *concept hierarchies*. A concept is associated with each node of the tree, and as such the tree represents a kind of taxonomy, a hierarchy of many concepts. This is very similar to what many clustering algorithms do (e.g. COBWEB, [9]).

Concept hierarchies can be induced in a supervised or unsupervised manner. Decision trees are an example of the former, while typical clustering algorithms are unsupervised.

The ILP system TILDE [2] induces first order logical decision trees from classified examples. In this paper, we show how to adapt the TILDE system to perform clustering, resulting in the C 0.5 system. To realize this, principles from instance based learning are employed. More specifically, we assume that a distance measure is given that computes the distance between two examples. Furthermore, in order to compute the distance between two clusters (i.e. sets of examples), we employ a function that computes a prototype of a set examples. A prototype can be regarded as an example. The distance between two clusters is then defined as the distance between the prototypes of the two clusters. Now, the distance measure employed determines whether the learning process is supervised or unsupervised. If the distance measure employs class information, learning is supervised, if no class information is employed, learning is unsupervised.

All logical aspects of TILDE are inherited by C 0.5. This includes the logical representation of binary decision trees and the learning from interpretations setting (in which examples are logical interpretations).

2 The problem

We use the *learning from interpretations* setting. In this setting, each example is a Prolog program encoding the specific properties of the example. See [5,3] for more details on learning from interpretations.

For instance, examples for the well-known mutagenesis problem [14] can be described by interpretations. Here, an interpretation is simply an enumeration of all the facts we know about one single molecule: its class, *lumo* and *logp* values, the atoms and bonds occurring in it, certain high-level structures, ... We can represent it e.g. as follows: `{ logmutag(-0.7), lumo(-3.025), logp(2.29), atom(d189_1,c,22,-0.11), bond(d189_2,d189_3,7), ... }`.

A logical decision tree is a binary decision tree in which each node contains a conjunction of literals. This conjunction may share variables with nodes above it in the tree. The test that is to be performed at the node consists of its conjunction, together with the conjunctions on the path from the root of the tree to this node that share variables with this node or with other nodes sharing variables with it. This test has two possible outcomes (it may fail or succeed), upon which the splitting of a cluster of examples into two subclusters is based.

The format of logical decision trees makes them perfectly fit as a representation for a cluster hierarchy. Each node in the tree corresponds to a cluster of examples, and the hierarchical structure of the tree shows how clusters are split into subclusters. The test in a node can be seen as a discriminant description of the two clusters in which the current cluster of examples is divided. One cluster is described by saying that the test succeeds, the other by saying that it fails.

This view is in correspondence with Langley’s viewpoint that a test in a node is not just a decision criterion, but also a description of the subclusters formed in this node. In [2], we have shown how a logical decision tree can be transformed into an equivalent logic program. This procedure can be used to obtain descriptions of the clusters.

The purpose of conceptual clustering is to obtain clusters such that intra-cluster distance (i.e. the distance between examples belonging to the same cluster) is as small as possible and the inter-cluster distance (i.e. the distance between examples belonging to different clusters) is as large as possible.

In this paper, we assume that a distance measure d that computes the distance $d(e_1, e_2)$ between examples e_1 and e_2 is given. Furthermore, there is also a need for measuring the distance between different clusters (i.e. between sets of examples). Therefore we will assume as well the existence of a prototype function p that computes the prototype $p(E)$ of a set of examples E . The distance between two clusters C_1 and C_2 is then defined as the distance $d(p(C_1), p(C_2))$ between the prototypes of the clusters. This shows that the prototype should be considered as (possibly) partial example descriptions.

For instance, on the mutagenesis problem, the distance could be the Euclidean distance d_1 between the activities of the two compounds, or the Euclidean distance d_2 between the points in the three-dimensional space corresponding to the *lumo*, *logp* and *activity* values of the two compounds, or it could be the distance d_3 as measured by a first order distance measure.

Given the distance at the level of the examples, the principles of instance based learning can be used as to compute the prototypes. E.g. on the mutagenesis problem, d_1 would result in a prototype function p_1 that would simply compute the average activity of the compounds in the cluster, d_2 would result in a prototype function p_2 that would compute the average instance along the *lumo*, *logp* and *activity* values of the compounds in the cluster, whereas d_3 could result in function p_3 that would compute the (possibly reduced) least general generalisation¹ of the compounds in the cluster.

Notice that although we employ - in this paper - only propositional distance measures, we obtain first order descriptions of the clusters through the representation of logical decision trees. Hence, one could say that we realize 0.5th order Clustering, which explains the name of our system C 0.5.

By now we are able to formally specify the clustering problem:

Given

- a set of examples E (each example is a definite clause theory),
- a background theory B in the form of a definite clause theory,
- a distance measure d that computes the distance between two examples or prototypes,
- a prototype function p that computes the prototype of a set of examples,

Find: clusters in the form of a logical decision tree.

Notice that in this problem-setting, the interpretation i corresponding to an example e is the least Herbrand model of $B \wedge e$. So, conceptually, the clustering process learns from interpretations. This is similar to the Claudien [4], ICL [6] and TILDE [2] systems.

3 C 0.5 : Clustering of order 0.5

C 0.5 employs the basic TDIDT framework as it is also incorporated in TILDE. The only point where our algorithms C 0.5 and TILDE differ from the propositional TDIDT algorithm is in the computation of the tests to be placed in a node. To this aim, we employ a classical refinement operator under θ -subsumption [12], see [2] for details.

Another point where C 0.5 deviates from the classical TDIDT algorithm is in its heuristics. TDIDT algorithms typically use two heuristics: a splitting criterion to select the best test in a node, and a stopping criterion to decide whether a given node or cluster should be turned into a leaf or should be split further.

The splitting criterion used in C 0.5 works as follows. For a given a cluster C , and a test T that will result in two disjoint subclusters C_1 and C_2 of C , C 0.5 computes the distance $d(p(C_1), p(C_2))$. The best test T is then the one

¹ Using Plotkin's [12] notion of θ -subsumption or the variants corresponding to structural matching [1, 13].

that maximizes this distance. This reflects the principle that the inter-cluster distance should be as large as possible.

Stopping criteria for conceptual clustering are usually less clear. Typically, the stopping criterion depends on the number and size of clusters one wants to obtain. In C 0.5, we consider right now only that each leaf of the tree should contain a minimal number of examples.

4 Applications of Clustering in ILP

We see a number of interesting applications of clustering in ILP. We will divide these into characterisation, classification and regression tasks. But first, we make an observation that will be important to all these tasks.

Once a decision tree has been induced, there can be two separate arguments for saying that an example belongs to a cluster. One is based on the tests in the tree. If an example is sorted into a specific node based on those tests, one has reason to say that the example really belongs to the cluster corresponding to that node. A second argument is based on the distance metric. Without performing any tests in the tree, one can still say that an example belongs to a cluster because it is close to the examples in that cluster. Both arguments are quite independent from one another (cf. also [10]).

This means that information can flow in two opposite directions. One can assign an example to a cluster based on the tree, and predict that its distance to the examples in that cluster will be small; or one can assign it to a cluster based on its distance to the examples in the cluster, and predict that it will satisfy the description of that cluster that the tree gives. While the first information flow has a flavour of classification, the second comes closer to characterisation (although the difference between the two is not always very clear-cut).

4.1 Characterisation of clusters

The fact that logical decision trees offer a first order description of clusters makes it possible to perform a kind of abduction. Based on the fact that an example belongs to a specific cluster (according to the distance metric that is used), one can predict that it fulfills the intensional description of that cluster.

4.2 Classification

It is quite clear that first order clustering can be used for classification; in fact, the original TILDE system is such a classification system. Following Langley's viewpoint, it is basically a clustering system where the "distance" metric is the class entropy within the clusters : lower class entropy within a cluster means that the examples in that cluster are more similar with respect to their classes.

Since TILDE needs information about the classes of its training examples, it is a supervised learning system. However, clustering can also be done in an unsupervised manner. The distance metric used to form clusters may or may not

use information about the classes of the examples. Even if it does not use class information, clusters may be coherent with respect to the class of the examples in them. This will be illustrated in our experiments.

This principle leads to a classification technique that is very robust with respect to missing class information. Indeed, even if only a small percentage of the examples is labelled with a class, one could perform unsupervised clustering, and assign to each leaf in the concept hierarchy the majority class in that leaf. If the leaves are coherent with respect to classes, this method would yield high classification accuracy with a minimum of class information available. This is similar to Emde’s method for learning from few classified examples, implemented in the COLA system [7].

4.3 Regression

The above shows that first order clustering can be used for characterisation of clusters in the data, as well as for classification. An application that has a flavour of both, is predicting numerical values. If clusters are coherent with respect to some numerical attribute of the examples, one can compute the average value for a cluster of examples and use this to predict the value of unseen examples. This is basically what Kramer’s SRT system [10] does. SRT builds so-called structural regression trees: trees in which each leaf predicts a numerical value instead of a symbolic class and the tests in the nodes are conjunctions of literals.

5 Experiments

We have evaluated some of the ideas proposed in this paper using a preliminary implementation of C 0.5. Concerning the evaluation of a clustering system, there is the fundamental problem of how to evaluate the quality of a set of clusters as there is no clear and objective criterion to measure this. The situation is different in concept-learning, where the quality of the output of a system is measured in terms of accuracy. Therefore, as frequently done in conceptual clustering (cf. [9]), we will measure the quality of the obtained clusters using the accuracy with which these clusters can be used for prediction.

5.1 Experimental setup

Originally, mutagenicity was represented by a number on a logarithmic scale. For prediction purposes, a molecule is considered to be of class *positive* if this number is positive, and is of class *negative* otherwise. In all experiments we use euclidean distance metrics based on the numerical information about molecules, i.e. their *logp*, *lumo* and *logm* (which stands for *log-mutagenicity*, the number describing the activity of the molecule) values. Several distance metrics have been tried out. First of all, supervised learning (using *logm* for distance computation) was compared to unsupervised learning (using *logp* and *lumo*). This was done for three different hypothesis languages corresponding to the background

knowledges BG1-BG3 as defined in [14]. BG1 contains only structural information (atoms and bonds), BG2 adds to this the charges of each individual atom, BG3 adds to BG2 the *lumo* and *logp* values of each molecule.

In order to evaluate the results of the clustering algorithm, we have computed accuracies as follows. For a whole cluster the *logm* value of the prototypical element is computed. If this is a positive number, then the whole cluster is predicted to be positive, otherwise negative. The observed class of an example is then compared with the class of its cluster. Classification accuracy on the regression-friendly set is based on tenfold crossvalidation, for the regression-unfriendly set a leave-one-out procedure was adopted.

5.2 Classification Accuracy

In a first experiment we compare supervised and unsupervised clustering, on both the regression-friendly and regression-unfriendly datasets. Table 1 shows the results of our experiments. The results for supervised learning can be compared with results obtained with other systems (Progol, TILDE), but for unsupervised learning this comparison is harder in the case of BG1 and BG2, since C 0.5 does use *logp* and *lumo* information during the induction process, even if the theories that are derived do not use them. For the regression-friendly data we have included results obtained with the TILDE system. The refinement operator and other parameters were exactly the same in C 0.5 as in TILDE, only the minimal coverage of clusters was higher (10 examples for the regression-friendly data, 4 for the regression-unfriendly data) because C 0.5 does not have a good stopping criterion yet. We have not tried to find an optimal value for the minimal coverage, but consistently used 10 (or 4).

Table 1 shows that the results of both supervised and unsupervised learning are comparable with results for TILDE (with the exception of BG3 where a significantly lower score is obtained). Especially for unsupervised learning this is a surprise. It shows that *lumo* and *logp* are very closely related to the class; examples with similar *lumo* and *logp* values often have the same class. This explains in part why FOIL, on the Mutagenesis dataset with BG3, finds a theory simply consisting of a large number of intervals for *logp* and *lumo* (see [14]).

In order to check this out in more detail, we have additionally experimented (on BG2) with distances based on *logp* only, on *lumo* only, and on the three numerical values together. Results are shown in Table 2 (first row). There are no significant differences for the different distance functions.

The results on the regression-unfriendly set (Table 1) are much harder to explain. The expected behaviour (less accuracy for unsupervised than for supervised learning) occurs clearly in BG3, but not in BG1 and BG2. We do not have an explanation for this.

5.3 Learning From Incomplete Examples

Next to comparing different distance functions, Table 2 also shows what happens if numerical information is missing. The dataset was changed so that the *lumo*

information was removed in approximately 50% of the models, chosen at random (every model has probability 0.5 of having this value removed), and the same was done independently for *logp* and *logm* values. This was repeated with removal of 75% or 90% of the information.

Table 2 shows that in the absence of a lot of information, classification accuracy slowly decreases. However, when using a distance measure that combines several numerical attributes, prototypes can be computed more accurately than if only one numerical attribute is used. Absence of information about one attribute can be compensated for by knowledge of another value. This causes the distance function using all three attributes (*lumo*, *logp*, *logm*) to be very robust w.r.t. missing information; predictive accuracy decreases more slowly.

These results suggest that even if more complicated distance functions do not yield higher accuracy when all information is present, they make learning from incomplete examples more feasible.

	Regression friendly			Regression unfriendly		
	unsupervised	supervised	TILDE	unsupervised	supervised	TILDE
BG1	0.73	0.74	0.75	0.76	0.76	0.83
BG2	0.81	0.80	0.79	0.74	0.76	0.83
BG3	0.79	0.78	0.85	0.71	0.86	0.79

Table 1. Comparison of supervised and unsupervised clustering on both regression-friendly and unfriendly data; results with TILDE included for reference.

available numerical data	lumo	logp	lumo+logp	logm	lumo+logp+logm
100%	0.79	0.79	0.81	0.80	0.81
50%	0.77	0.79	0.81	0.78	0.79
25%	0.73	0.72	0.73	0.72	0.77
10%	0.65	0.65	0.67	0.67	0.74

Table 2. Classification accuracies obtained on BG2 with several distance functions, and on several levels of missing information.

6 Related Work

Our work is related to KBG [1], which performs first order agglomerative clustering but employs a first order distance measure, to RIBL [8], a first order instance based learner, and to Kramer’s SRT [10], which builds first order regression trees. Our work also exploits many of the ideas contained in Langley’s book, as he makes the link between TDIDT and clustering.

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References

1. G. Bisson. Conceptual clustering in a first order logic representation. In *Proceedings of the 10th European Conference on Artificial Intelligence*, pages 458–462. John Wiley & Sons, 1992.
2. H. Blockeel and L. De Raedt. Experiments with top-down induction of logical decision trees. Technical Report CW 247, Dept. of Computer Science, K.U.Leuven, January 1997. Also in Periodic Progress Report ESPRIT Project ILP2, January 1997.
3. L. De Raedt. Induction in logic. In R.S. Michalski and Wnek J., editors, *Proceedings of the 3rd International Workshop on Multistrategy Learning*, pages 29–38, 1996.
4. L. De Raedt and L. Dehaspe. Clausal discovery. *Machine Learning*, 26:99–146, 1997.
5. L. De Raedt and S. Džeroski. First order jk -clausal theories are PAC-learnable. *Artificial Intelligence*, 70:375–392, 1994.
6. L. De Raedt and W. Van Laer. Inductive constraint logic. In *Proceedings of the 5th Workshop on Algorithmic Learning Theory*, volume 997 of *Lecture Notes in Artificial Intelligence*. Springer-Verlag, 1995.
7. W. Emde. Inductive learning of characteristic concept descriptions. In S. Wrobel, editor, *Proceedings of the 4th International Workshop on Inductive Logic Programming*, volume 237 of *GMD-Studien*, pages 51–70, Sankt Augustin, Germany, 1994. Gesellschaft für Mathematik und Datenverarbeitung MBH.
8. W. Emde and D. Wettschereck. Relational instance-based learning. In L. Saitta, editor, *Proceedings of the 13th International Conference on Machine Learning*, pages 122–130. Morgan Kaufmann, 1996.
9. D. H. Fisher. Knowledge acquisition via incremental conceptual clustering. *Machine Learning*, 2:139–172, 1987.
10. S. Kramer. Structural regression trees. In *Proceedings of the 13th National Conference on Artificial Intelligence (AAAI-96)*, 1996.
11. P. Langley. *Elements of Machine Learning*. Morgan Kaufmann, 1996.
12. G. Plotkin. A note on inductive generalization. In *Machine Intelligence*, volume 5, pages 153–163. Edinburgh University Press, 1970.
13. L. De Raedt, P. Idestam-Almqvist, and G. Sablon. Theta-subsumption for structural matching. In *Proceedings of the 9th European Conference on Machine Learning*, 1997.
14. A. Srinivasan, S.H. Muggleton, and R.D. King. Comparing the use of background knowledge by inductive logic programming systems. In L. De Raedt, editor, *Proceedings of the 5th International Workshop on Inductive Logic Programming*, 1995.