Unsupervised Constructive Learning

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Abstract

In constructive induction (CI), the learner's problem representation is modified as a normal part of the learning process. This is useful when the initial representation is inadequate or inappropriate. In this paper, I argue that the distinction between constructive and non-constructive methods is unclear. I propose a theoretical model which allows (a) a clean distinction to be made and (b) the process of CI to be properly motivated. I also show that although constructive induction has been used almost exclusively in the context of supervised learning, there is no reason why it cannot form a part of an unsupervised regime.

1 Introduction

Constructive induction (CI) is of use when the initial representation for a problem obstructs the application of ordinary inductive methods [1]. Wnek and Michalski [2] have divided constructive induction methods into several types including hypothesis-driven (HCI) methods, data-driven (DCI) methods and knowledge-driven (KCI) methods. Practical methods introduced in recent years include FRINGE [3], AQ17-HCI [2] and CN2-MCI [4].

Almost all CI methods seek to transform the initial representation space by introducing new *features*. However, in the literature, the term 'feature' has been used ambiguously. In most cases it has been used to denote any construct or mechanism which imposes a new partition(ing) on the representation space. However, this usage cannot be taken too literally since all supervised learning algorithms attempt to implement the *target* partitioning on the space and would thus all be potentially classified as constructive.

Explicitly discounting such degenerate cases still leaves us with methods such as C4.5 [5], Backpropagation [6] and CN2 [7, 8] which all make use of intermediate constructs (i.e., constructs not directly involved in production of output) that identify partitions on the representation space. These methods would seem to satisfy the criterion of being 'feature generators' in a non-degenerate sense and yet they are typically described as 'selective' and thus non-constructive (see [9,10,4,11,12] for a selection of views).

The decision criterion that is being applied in such cases is not completely clear. But it appears to be grounded in an evaluation of the *simplicity* of the partitioning introduced by the feature. Constructs that introduce simple, local partitions (e.g., the axis-parallel partitions created by internal, decision-tree nodes) tend *not* to be considered features. Algorithms such as C4.5 are thus effectively eliminated from the constructive class. But the notion of 'simple partitioning' is poorly defined and as a result, the whole enterprise of constructive induction is placed on an insecure footing.

In this paper, I will introduce an analysis of inductive justification and show how it permits this intuitive distinction to be recast in a secure theoretical context. I will also show how the process of CI can be properly motivated as a necessary response to hard, relational learning problems. Finally, I will show that the process is not necessarily confined to the domain of supervised methods but can easily be introduced in an unsupervised scenario.

2 Bayesian analysis of inductive justification

In recent years, researchers have made rapid progress in the theoretical analysis of learning. Early work by Gold [13] and Valiant [14,15] established a tradition which grew to encompass theoretical constructs such as VC-dimension [16] and led to the theoretical advances of Haussler and others, e.g., [17, 18, 19, 20, 21, 21, 22]. Much of this work is directed towards the goal of analyzing the complexity of learning but, at the time of writing, measuring the hardness of arbitrary learning problems (e.g., specific training sets) remains problematic [23]. However, it turns out that a useful, qualitative measure of problem hardness can be obtained via a Bayesian analysis of justification sources for generalisation.

Consider the following example. D is the body of data shown in Table 1. Each datum in D (i.e., each row in the table) is made up of the values of variables $x_1, x_2, x_3...x_n$. One of the values of x_4 is missing (see the '?' in

¹In the case of C4.5 the intermediate constructs are the internal decision-tree nodes while in the case of backpropagation the constructs are the hidden units in the network.

the fourth column). Can we use observations on the other data to predict this missing value? In other words, can we empirically *induce* the missing value?

\mathbf{x}_1	\mathbf{x}_2	Х3	X4	X_5	x_6
2	7	3	5	0	1
0	7	2	6	3	4
0	8	1	6	3	0
1	7	4	6	3	0
1	8	4	5	0	4
2	8	2	?	0	4
0	8	3	5	0	4
1	7	2	6	4	0
1	8	2	6	4	4
2	7	3	5	0	4
2	7	1	5	0	4

Table 1: Sample body of data.

If we find that every possible value of the relevant variable has an equal observed probability then we clearly cannot make any prediction at all. If all values do *not* have the same probability then we should predict the missing value to be the one which has the highest observed probability. However, there are several ways in which we can work out observed probabilities.

We can look at the unconditional probability of seeing a particular value v of x_i .

$$P(x_i = v)$$

Unfortunately, this does not help since both possible values of x_4 turn out to have the same observed probability. This is simply the chance value

$$P(x_i = v) = \frac{1}{|V|}$$

where V is the set of all possible values of x_i . (In this case the chance value is 0.5 since there are only two possible values.)

We can also look at the probability of seeing a particular value conditional on explicit instantiations of the other values, i.e.,

$$P(x_i = v_a | x_j = v_b \dots)$$

where v_a and v_b are possible values and '...' denotes the optional inclusion of other instantiations. This is more rewarding since it turns out that

$$P(x_4 = 5 | x_5 = 0) = 1$$

which is the observation that we always see $x_4 = 5$ whenever we see $x_5 = 0$. Finally, we can look at the probability of seeing a particular value conditional on there being an *implicit* property among the instantiations of other variables:

$$P(x_i = v | g(X) = v_q)$$

Here X is the entire datum and v_g is the value of a function g, which evaluates the implicit property. Looking at this sort of probability might have been rewarding if, for example, the missing value had been a value of x_2 , since it turns out that

$$P(x_2 = 7 | duplicatesin(X) = 0) = 1$$

where the duplicates in function tests whether there are duplicated values in the datum and the 0 value indicates a false result. (This probability is observed because 7 appears as the value of x_2 whenever there are no duplicates among the remaining values.)

Methods which attempt to discover and exploit such probabilities for inductive purposes, without using any other source of information, are **empirical** learning algorithms. There are a large number of these, see [24, 25, 26].

3 Statistical v. relational learning

The analysis of justification sources allows us to divide methods of inductive learning into two basic types. A method that attempts to exploit either of the first two forms of probability confronts a tractable task. Only cases that are *explicitly* observed in the data need to be taken into account. There are a finite number of these. The task thus involves deriving frequency statistics (probabilities) over a *finite* dataset.

A method that attempts to exploit probabilities of the third form confronts a less tractable task since it has to first identify the appropriate evaluation function for the implicit property (i.e., it has to guess what the property is). Since there are an infinite number of possible functions that might be considered, the task is infinitely hard in general.²

The general implication is that exploiting probabilities of the first and second form is easier than exploiting probabilities of the third form. It is no surprise that practical learning methods tend to be predisposed towards the easier task,

² Although the domain of these functions is finite, the range is necessarily infinite. Assuming a finite range is tantamount to assuming an arbitrary boundary on the space of possible relationships.

i.e., they tend to exploit probabilities of the first and second form, rather than of the third form. [27]

Interestingly, we can deduce that the evaluation function used in the third form must measure a relational property of its inputs. To understand why, we need to think about the way in which the function differentiates different types of input. Let us say that the function produces a particular value whenever the input variables have certain absolute values. In this case, the evaluation is effectively a label for an explicit case. If all the values of the function are derived this way, the conditional probability can be reduced to a set of probabilities of the second form. If the probability is a valid example of the third form, the evaluation function must therefore measure a non-absolute — i.e., relational — property of its inputs.

Learning problems whose solutions involve exploiting probabilities of the third form are thus **relational**. Problems which involve exploitation of probabilities for explicit cases are **statistical**, since they simply involve the derivation of frequency statistics over a finite dataset. Learning *methods* can be classified the same way. Learning procedures which exploit probabilities of the first and second form are statistical while ones which exploit probabilities of the third form are relational.

4 Recursive relational exploitation is constructive learning

It is important to note that relational learners are potentially recursive. The identification of any set of relational effects involves the application of evaluations (functions) to the original data. This creates new values and thus new data. These new data can themselves be processed for statistical and relational effects in a recursive manner. Thus the process of recursively exploiting relational effects is manifestly a constructive process. Since the process of exploiting statistical effects is manifestly non-constructive — and since there are no alternative methods of exploitation — it can be deduced that the process of constructive induction is, precisely, the process of recursive exploitation of relational effects. This provides an operational definition of the the distinction between constructive and non-constructive methods. It also gives the former type of process a clear motivation: constructive methods are necessitated just in case the relevant problem is of the hard, relational type.

Equating 'constructive induction' with recursive, relational learning is generally compatible with conventional interpretations of the meaning of the term. In particular, it is compatible with the intuition that constructive induction involves the creation of 'non-local' partitions. Any feature/function which computes a statistical property of its arguments will tend to define a partitioning involving contiguous regions of the original input space, whereas a feature which

computes a relational property will not do so.

The values of a function which computes a statistical property of its inputs are, by definition, correlated with the absolute values of the inputs to that function. Thus values of the function are correlated with absolute 'coordinates' of the representation space and the function must, therefore, define sets of objects which tend to share the same coordinates, i.e., be located within the same region of that space. In contrast, the values of a function that computes a relational property of its inputs are not correlated with the absolute values of the function's inputs and thus not correlated with absolute 'coordinates' of the representation space. The feature implemented by the function will therefore tend to instantiate a complex, non-local partition of the space.

The proposed model also allows us to understand why practical CI methods typically involve some sort of search for relational functions. Oliveira and Sangiovanni-Vincentelli [12], for example, describe a system that effectively searches for a minimal set of features each of which tests for a conjunctive property of the input variables. Kramer [4] describes a system that tries to detect and exploit relations over variables which tend to appear together in useful rules. Matheus [28] describes the CITRE system which, to a first approximation, tries to capitalize on the presence of disjunctive regions in decision tree descriptions. Other systems involve a search (i.e., operator-based) process working with some sort of relational description language, e.g., [29, 11,10]. In several recent cases, this type of approach has focussed on what are known as 'counting' or M-of-N features, i.e., features which effectively count the number of occurrences of a particular variable value, cf. [30,31,2,9,32,33].

It is worth noting, finally, that although all these approaches place the constructive process within the domain of supervised methods, there is no reason why constructive induction cannot form a part of an unsupervised process. The justification analysis shows that it can form a part of any inductive process provided that the underlying problem is relational.

5 Concluding comments

It is widely agreed that existing learning methods are extremely effective provided the 'right' representation of the problem or environment is used. Thus constructive induction — the problem of finding the right representation — is a key challenge. Overcoming it might enable us to construct learning mechanisms which begin to approximate the power and generality of natural (e.g., animate) learners. In this paper I have shown that constructive learning is effectively the recursive form of the relational exploitation procedure and that as such it is a necessary requirement for the solving of hard, relational learning problems. I have also shown that there is no reason whatsoever why this process has to be confined to the supervised scenario. It can be used quite legitimately in unsupervised scenarios. Further research on this topic may clarify whether the

process of unsupervised constructive learning may have any useful application.

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