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Regression learning based on incomplete relationships between attributes

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A B S T R A C T

In recent years, machine learning researchers have focused on methods to construct flexible and interpretable regression models. However, the method of obtaining complete knowledge from incomplete and fuzzy prior knowledge and the trade-off between the generalization performance and the interpretability of the model are very important factors to consider. In this paper, we propose a new regression learning method. Complete relationships are obtained from the incomplete fuzzy relationships between attributes by using Markov logic networks [29]. The complete relationships are then applied to constrain the shape of the regression model in the optimization procedure to solve the trade-off problem. Finally, the benefits of our approach are illustrated on benchmark data sets and in real-world experiments.

1. Introduction

Several machine learning algorithms have been developed during recent years. However, domain experts do not readily adopt machine learning algorithms and prediction models because the mathematical form of the model and the theoretical basis of machine learning do not take the specialized knowledge of domain experts into account. To resolve this problem, machine learning researchers have focused on methods that can be used to construct flexible and interpretable regression models. What are the elements required to ensure the interpretability of the model, and how is the regression model constructed using these elements? James et al. [12] noted that the following elements may be useful for the construction: an open-ended language that can describe the model, a search procedure for the model, a principled method for evaluating the model, and a procedure for automatically generating reports. Based on this, an automated statistical modeling method was proposed that used a greedy search algorithm for constructing the portfolio of all kinds of kernel functions. In this method, detailed reports were automatically generated that describe patterns in the data captured by the model. Brodersen et al. [3] proposed a novel generative-embedding approach that incorporates neurobiologically interpretable generative models into discriminative classifiers based on dynamic causal models for achieving more accurate predictions and mechanistic interpretability of clinical classifications. Chen et al. [4] investigated fault diagnosis in the model space and fitted a series of

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models using a series of signal segments selected for discriminating faulty models from healthy models and improve the interpretability of the fault diagnosis model.

However, according to Zhang [42], interpretability is closely related to the domain knowledge of experts in practical engineering areas for two reasons. First, the model should provide the causal explanation of the predication results considering the knowledge of domain experts. Second, in the case of insufficient training data, domain knowledge helps improve the machine learning performance.

It is generally known that various types of prior knowledge or domain knowledge are usually associated with practical engineering areas. However, this knowledge is usually heterogeneous, fuzzy, incomplete, and informal and cannot be strictly defined by mathematical formulas. Thus, we posit that deriving a comprehensive inference from the incomplete and fuzzy prior knowledge regarding the model, and formulating a method to improve the interpretability of the model based on the results of the inference are also very important for a flexible and interpretable regression model.

In this study, incomplete and fuzzy relationships between the input attributes and the output attribute are taken as the prior knowledge. A set of weighted predicates is first constructed by domain experts to represent the incomplete and fuzzy relationship between the input attributes and the output attribute. Then, the complete relationships between the attributes are obtained by inference based on Markov logic networks (MLNs) [7,29,30].

Good statistical modeling requires not only interpretability but also generalization performance [12]. Because the generalization performance and the interpretability are entirely different in nature, the method to solve the trade-off problem between them using the complete knowledge is also very important. In this paper, the complete knowledge is represented as a prior vector function, and shape constraints obtained from the prior vector function are applied to the function space of the regression learning algorithm to evaluate the interpretability in the optimization procedure. A new regularization learning framework is proposed for resolving the trade-off problem based on these shape constraints. Meanwhile, in the learning process, the complete knowledge can be revised according to the training samples. After learning, the revised knowledge can also offer explanations for the predicted results of the optimal regression model.

The remainder of this paper is organized as follows. The regression learning problem based on the incomplete relationships between attributes is stated in Section 2. Section 3 introduces various related works. Section 4 proposes the predicates that represent fuzzy relationships between attributes and the prior vector function. The new regression learning algorithm is introduced in Section 5. Section 6 describes how the proposed method is tested on benchmark data sets and application examples, and discusses the experimental results. Section 7 reports the conclusions. Detailed proofs related to the method and some proposed theorems are provided in the appendix.

2. Problem statement

In a regression problem, we consider a triplet $(\mathcal{A}, X, C)$, where $\mathcal{A} = \{a_1, \cdots, a_i, \cdots a_M, o\}$ is an attribute set, a_i is the ith input attribute, and o is the output attribute. The training data set in the sample space is $X = \{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \cdots, (\mathbf{x}_N, y_N)\}$, where $\mathbf{x}_i = \{x_{i1}, x_{i2}, \cdots, x_{iM}\} \in \mathbf{R}^M$, $y_i \in \mathbf{R}$, $i = 1, 2, \cdots, N$, N is the number of training data, and every data $\mathbf{x}_i$ has M attributes. C is an attribution relationship set between an element a_i and the output attribute o. Every element in X is a two-tuple $(\mathbf{x}_i, y_i)$. Each y_i,$1 \le i \le N$, is a single value that has a vector $\mathbf{x}_i$ associated with it. In the regression problem, a regression model will be found based on the training data set X and the attribution relationship set C, which includes some incomplete and fuzzy relationships between the input attributes and the output attribute. It is necessary to formulate a method to simultaneously improve the interpretability and generalization performance of the regression model. The optimization problem can be expressed as

$$\underset{\mathbf{w}\in R^m, \lambda \in R}{argmin}\ Q(\mathbf{w}, \mathbf{x}_i) + \lambda \tilde{Q}(\boldsymbol{\mu}, \gamma, \mathbf{x}_i), i = 1, ..., N, \tag{1}$$

where $Q(\mathbf{w}, \mathbf{x}_i)$ is a loss function that can assess the generalization performance of the regression model and $\tilde{Q}(\boldsymbol{\mu}, \gamma, \mathbf{x}_i)$ is a pseudo-regression loss function that can assess the interpretability of the model.

3. Related works

Building a bridge between logic and learning is a key to constructing a flexible and interpretable regression model [6]. Many regression and classification learning techniques based on statistical relational learning theory (SRL) have recently been proposed to act as a bridge between logic and learning. The kFoil algorithm [14] implemented a dynamic propositionalization approach with kernel methods. Its key idea is to dynamically induce a small set of clauses using a Foil-like covering algorithm and to use these clauses as features in support vector machines (SVMs) to directly tackle classification or regression problems. Bicer et al. [1] proposed the construction of an R-convolution kernel for each clause and the calculation of the similarities between two data points by measuring the number of other points that can be reasoned from them. Melacci et al. [21] proposed a box kernel that incorporates supervised points and supervised sets. Veillard [34] proposed a method for the incorporation of prior knowledge via an adaptation of the standard radical basis function(RBF) kernel. However, because all the above methods solve regression and classification problems by applying relation rules to a kernel function, the interpretability is very hard to improve.

Some scientists directly incorporated relation rules into the learning mechanism [16]. Fung et al. [8] proposed incorporating prior knowledge into a linear SVM classifier in the form of convex constraints in the input space. Based on the method,