Probability Measures for Prediction in Multi-table Information Systems

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Abstract. Rough Set Theory is a mathematical tool to deal with vagueness and uncertainty. Rough Set Theory uses a single information table. Relational Learning is the learning from multiple relations or tables. This paper presents a new approach to the extension of Rough Set Theory to multiple relations or tables. The utility of this approach is shown in classification experiments in predictive toxicology.

1 Introduction

Rough set theory [Paw82, Paw91, KPPS99], introduced by Zdzislaw Pawlak in the early 1980s, is a mathematical tool to deal with vagueness and uncertainty. Rough set theory defines an indiscernibility relation that partitions the universe of examples into elementary sets. The indiscernibility relation is defined based on a single table. Relational Learning is based on multiple tables. A survey of research in Rough Sets and Relational Learning is presented in [MUS04]. *Statistical relational learning* (SRL) is a recent area of research, concerned with developing techniques to learn statistical models from relational data, and information is available at <http://robotics.stanford.edu/srl/>.

In this paper, a Multi-Table Information System (MTIS) is defined that extends the single information table of rough set theory to multiple information tables. The formalism used in this paper is based on tables and rows, rather than on universes and elements. Notions from the Variable Precision Rough Set model are introduced along with the notion of significant elementary sets (elementary sets in the β -positive or β -negative regions that also have a sufficiently large number of examples). This is used for prediction. An illustrative experiment in toxicology is then presented.

Another formalism for MTIS based on universes and elements is presented in [MUS05]. The universes correspond to the tables and the elements of the universes correspond to the rows of the tables. That formalism is applied in that paper to two special cases of MTIS. Whereas the formalism used in this paper is applicable to a general MTIS. The decision class of an unknown example

is computed using the probability measures of the significant elementary sets in the individual tables. However, this formalism needs further study into the relationship between the probability measures of the overall system and those of the individual tables. A formal study based on probabilistic measures and distributed tables is found in [Š05].

2 Multi-table Information System

2.1 Definitions

A table T is a set of rows $\{x_1, \dots, x_m\}$ and is denoted as $T = (I, A, V, \rho)$, where I is a finite set of row indices (or row identifiers), with each row index $p, 1 \leq p \leq m$, corresponding to a particular row x_p of the table; A is a finite set of attributes; $V = \bigcup_{a \in A} V_a$ is the set of attribute values of all attributes, where V_a is the domain of attribute a ; and $\rho : I \times A \rightarrow V$ is an information function such that for every row index $p \in I, \rho(p, a) \in V_a$ is the value of attribute a in the row x_p corresponding to the row index p . In other words, a row $x_p \in T = (I, A, V, \rho), p \in I$, has the value $\rho(p, a) \in V_a$ for every $a \in A$. This definition is based on the definition of Rough Set Information System in [Paw82].

We define a Multi-Table Information System (MTIS) as a finite set of tables denoted as $T = \{T_0, T_1, \dots, T_n\}$, where $T_0 = \{I_0, A_0, V_0, \rho_0\}$ is a decision table with two attributes in A_0 , one of which is the example identifier which has a unique value for every row, and the other is a binary valued decision attribute. A similar definition is also found in [Wro00]. Here, each row of table T_0 corresponds to an example from the universe of examples as in the Rough Set Information System [Paw82].

An example MTIS follows. Let $T = \{T_0, T_1, T_2, T_3\}$. The values of $I_i, A_i, V_i, \rho_i, i = 0, 1, 2, 3$ can be easily seen from the figures of the tables given below.

Table T_0

drug	decision
d1	true
d10	true
d102	true
d110	false
d114	false

Table T_1

drug	atom	element	type	charge
d1	a1_1	h	1	p
d102	a102_1	h	2	p
d1	a1_2	o	1	n
d12	a12_1	o	2	n
d10	a10_1	c	1	p
d10	a10_2	c	2	p

Table T_3

drug	property	val
d12	salmonella	p
d205	chromaberr	n
d108	cytogen_sce	n
d1	cytogen_ca	p
d101	cytogen_ca	n

Table T_2

drug	atom1	atom2	bond-type
d12	d12_1	d12_2	7
d12	d12_1	d12_7	1
d1	d1_14	d1_22	2
d1	d1_17	d1_24	1
d101	d101_8	d101_9	2

2.2 Link Relation

Let $T_i, T_j \in T$ ($i \neq j$) be two tables in a MTIS T . T_i is said to be linked to T_j if there exists a set of common attributes $K_{ij} \subseteq (A_i \cap A_j) \neq \emptyset$, known as *link attributes*, between them. Let $x_{i,p}$ be the row in table T_i with row index $p \in I_i$, and $x_{j,q}$ be the row in table T_j with row index $q \in I_j$. We say that $x_{i,p}$ is *linked* to $x_{j,q}$ through the link attributes K_{ij} if $\rho_i(p, b) = \rho_j(q, b)$ for every $b \in K_{ij}$.

Formally, a binary relation $L(K_{ij})$ ($K_{ij} \neq \emptyset$), called *link relation*, is defined between two tables T_i and T_j as

$$L(K_{ij}) = \{(x_{i,p}, x_{j,q}) \in T_i \times T_j \mid \forall b \in K_{ij}. \rho_i(p, b) = \rho_j(q, b), \text{ where } p \in I_i, q \in I_j\}$$

A row $x_{i,p}$ in table T_i is linked to row $x_{j,q}$ in table T_j if $(x_{i,p}, x_{j,q}) \in L(K_{ij})$.

In general, a row x_{i,p_i} in table T_i is linked to another row x_{j,p_j} in table T_j iff there exist tables $T_f, T_g, \dots, T_h \in T$, with rows such that $(x_{i,p_i}, x_{f,p_f}) \in L(K_{if})$, $(x_{f,p_f}, x_{g,p_g}) \in L(K_{fg})$, $\dots$, $(x_{h,p_h}, x_{j,p_j}) \in L(K_{hj})$. We say that row x_{i,p_i} is *linked through* the rows $x_{f,p_f}, x_{g,p_g}, \dots, x_{h,p_h}$ to row x_{j,p_j} , and the set of rows

$$C(p_i) = \{x_{f,p_f}, x_{g,p_g}, \dots, x_{h,p_h}, x_{j,p_j}\}$$

is said to form of a *combination* of rows associated with x_{i,p_i} . We note that a row x_{i,p_i} in table T_i could have a number of such combinations of rows.

In this paper, we restrict K_{ij} to a singleton set, and consider only a single link attribute between any pair of tables. In the illustration, table T_0 is linked to tables T_1, T_2 and T_3 through the link attribute **drug**.

2.3 Elementary Sets

Let B_i be a subset of attributes in a table $T_i = (I_i, A_i, V_i, \rho_i)$, $B_i \subseteq A_i$, such that no attribute in B_i is either a link attribute or a primary key. A binary relation $R(B_i)$, called *indiscernibility relation*, is defined on a table T_i as

$$R(B_i) = \{(x_{i,p}, x_{i,q}) \in T_i \times T_i \mid \forall b \in B_i. \rho_i(p, b) = \rho_i(q, b), \text{ where } p, q \in I_i\}$$

We say that two rows $x_{i,p}$ and $x_{i,q}$ of table T_i are indiscernible and belong to the same elementary set iff $\rho_i(p, b) = \rho_i(q, b)$ for $p, q \in I_i$ and every $b \in B_i$.

The elementary set of table T_i , with respect to the indiscernibility relation $R(B_i)$, containing the row $x_{i,p}$ is

$$[x_{i,p}]_{R(B_i)} = \{x_{i,q} \in T_i \mid \forall b \in B_i, \rho(p, b) = \rho(q, b), \text{ where } p, q \in I_i\}$$

$[x_{i,p}]_{R(B_i)}$ is denoted as $[x_{i,p}]$ when B_i is known from the context. Even though each table is partitioned into elementary sets based on the attributes in B_i , yet it continues to have all the original entries.

2.4 Conditional Probabilities of Elementary Set

Each row in table $T_i \in T$, $i \neq 0$, is linked to one row in the decision table T_0 . Hence, each row $x_{i,p}$ in an elementary set $[x_{i,p}]$ can be considered to be associated with a decision class. For a boolean decision class, let $[x_{i,p}]^+([x_{i,p}]^-)$ be the subset of the elementary set $[x_{i,p}]$ containing rows associated with the positive (negative) decision class.

The conditional probability that a row in the elementary set $[x_{i,p}]$ is positive is

$$P(+|[x_{i,p}]) = \frac{|[x_{i,p}]^+|}{|[x_{i,p}]|}$$

and $P(-|[x_{i,p}])$ is similarly defined.

2.5 Prediction

We now consider the prediction of the decision class of a test case. We assume that the test case has a row in the decision table T_0 , but does not yet have a value for the decision attribute. The associated data for this test case is introduced as rows in the other tables.

A *combination* of rows $C(p) = \{x_{1,q}, \dots, x_{n,t}\}$ linked to a test case $x_{0,p}$, has one row from each of the tables with rows linked to $x_{0,p}$. Every row in the combination is linked to the test case either directly or through other rows in the combination.

Each row $x_{i,p}$ in a combination falls in an elementary set of table T_i with the associated conditional probabilities $P(+|[x_{i,p}])$ and $P(-|[x_{i,p}])$. Hence, a row can be considered to have the conditional probabilities $P(+|[x_{i,p}])$ and $P(-|[x_{i,p}])$. We have also noted that a test case could have a number of combinations of rows.

Simple Approach: A simple approach that can be used for prediction follows. For every combination of rows corresponding to the test case with index p_0 of the decision table T_0 , the product of positive conditional probabilities of rows is defined as

$$posprod = \prod_{x \in C_k(p_0)} P(+|[x])$$

Similarly, the product of negative conditional probabilities *negprod* is defined. If the sum of the *posprods* of all the combinations is greater than the sum of

negprods of all the combinations, then the test case is predicted as positive; otherwise, it is predicted as negative. The *posprod* is the measure of the positive trend shown by the values of the attributes in each table. The summation of the *posprod* addresses the situation where a particular test case may be related to multiple rows in a table.

Significant Elementary Sets Approach: Many of the elementary sets are too small to be considered as representative of either positive or negative trend. We consider an elementary set to be a *significant elementary set*, if it has sufficiently large number of examples, and its $P(+|[x_{i,p}]) \geq \beta_u$ or $P(-|[x_{i,p}]) \leq \beta_l$, where $\beta_u \geq 0.5$ and $\beta_l \leq 0.5$. When $\beta_u = 1 - \beta_l$, we denote it as β , and note that $\beta_l = 1 - \beta$. An elementary set $[x_{i,p}]$ is said to be significant if and only if

$$|[x_{i,p}]| \geq \alpha \wedge ((P(+|[x_{i,p}]) \geq \beta_u \vee P(-|[x_{i,p}]) \leq \beta_l))$$

where α is a user-defined parameter.

If only k rows in the combination of rows fall in significant elementary sets, then we define the *Positive Conditional Probability* of the combination of rows as

$$\mathcal{P}_+ = \sqrt[k]{\prod P(+|[x_{i,p}])}$$

where $P(+|[x_{i,p}])$ s are of significant elementary sets. Similarly, *Negative Conditional Probability* $\mathcal{P}_-$ is defined.

A combination of rows predicts the test case as positive if $\mathcal{P}_+ \geq \mathcal{P}_-$ and as negative otherwise. If the number of combinations predicting the test case as positive is greater than the number of combinations predicting it as negative, the final prediction of the test case is positive; otherwise, it is negative.

3 Application to Predictive Toxicology

The dataset used is the Predictive Toxicology Evaluation Challenge dataset found at <http://web.comlab.ox.ac.uk/oucl/research/areas/machlearn/cancer.html>. The database of compounds have been classified as carcinogens or otherwise. The challenge is to predict the carcinogenicity of previously untested chemicals. The dataset is in the form of the Multi-Table Information System described in Section 2.1.

An illustrative experiment is performed using this dataset, and the results of the ten-fold cross-validation and the summary of the results are presented in the the following tables. The results of one of the folds are not available due to an error in the experiment.

The average prediction accuracy using the simple approach is 60%, and that using the significant elementary sets approach is 59.6%. It is to be noted that there is no improvement in the prediction accuracy. However, the space requirement for the significant elementary sets approach is much less when compared to the simple approach. This is a difficult dataset and *progol* achieves only 64% even with the use of more background knowledge.

Simple approach					Significant elementary set approach				
Positive		Negative		Accuracy	Positive		Negative		Accuracy
+	−	+	−		+	−	+	−	
13	5	9	6	0.58	14	4	11	4	0.55
16	2	8	7	0.70	17	1	9	6	0.70
14	4	10	5	0.58	15	3	11	4	0.58
14	4	13	2	0.48	15	3	10	5	0.61
14	4	12	3	0.52	13	5	11	4	0.52
15	3	6	9	0.73	14	4	6	9	0.70
11	7	8	7	0.55	11	7	9	6	0.52
18	0	13	2	0.61	17	1	15	0	0.52
15	5	5	8	0.70	15	5	5	8	0.70

Simple approach				Significant elementary set approach			
	Actual +	Actual −			Actual +	Actual −	
Predicted +	130	84	214	Predicted +	131	87	218
Predicted −	34	49	83	Predicted −	33	46	79
	164	133	297		164	133	297

4 Conclusions

This paper presents an approach to learning from a Multi-Table Information System. The results of an illustrative example in toxicology are presented.

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