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A Comprehensive and Comparative Study on Hierarchical Multi Label Classification

Purvi Prajapati, Amit Thakkar, Amit Ganatra

Abstract: ***Multi label classification is variation of single label classification where each instance is associated with more than one class labels. Multi label classification is used in many applications like text classification, gene functionality, image processing etc. Hierarchical multi-label classification problems combine the characteristics of both hierarchical and multi-label classification problems. This paper introduced k binary classifier and one classifier approaches of hierarchical multi label classification. These approaches are explained with two algorithms to solve hierarchical multi label classification problems. One is the C4.5H algorithm (extension of multi label decision tree) and second is Predictive Clustering Tree (PCT) algorithm. From theoretical and experimental study on yeast data set shows that PCT algorithm is the best option for hierarchical multi label classification. PCT algorithm is implemented on Clus. This paper introduced three approaches of Clus: Single Classification (SC), Hierarchical Single Label Classification (HSC) and Hierarchical Multi label Classification (HMC). From theoretical and experimental study, HMC performs better compare to remaining two approaches.***

Index Terms: ***Classification, Decision Tree, Hierarchical Classification, Multi Label Classification, Predictive clustering tree.***

I. INTRODUCTION

In classification problems, each instance of a dataset is associated with just one class label. However, there are many classification tasks where each instance can be associated with one or more class labels. This group of problems represents an area known as Multi-Label Classification.

Basically there are two ways for representation of multiple labels: flat structure and hierarchical structure. In flat structure all class labels are arranged at same level. In hierarchical structure all class labels are organized in hierarchy according to label correlation ships.

In Hierarchical Classification, classes are organized in a hierarchy: an example that belongs to some class automatically belongs to all its super classes [1]. Hierarchical Multi-label Classification (HMC) problems combine the characteristics of both hierarchical and multi-label classification problems: (1) class labels are organized in a hierarchical structure (e.g. a tree or DAG structure); (2) Examples may be associated with more than one class labels [2, 12]. Here tree structure is used for hierarchical structure.

Applications of hierarchical multi label classification are found in many areas, including text classification [9, 10], functional genomics, image recognition, face recognition, emotion detection, etc.

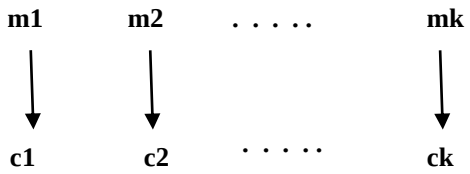
The rest of the paper is organized as follows. Section II explains approaches of hierarchical multi label classification. Decision tree for HMC and Multiple prediction tree for HMC discussed in Section III and IV respectively. Section V explains evaluation measures for HMC. Section VI shows experimental analysis on toyHMC and yeast dataset. At last current research challenges and conclusion presented in Section VII and VIII respectively.

II. APPROACHES FOR HMC

There are mainly two approaches for hierarchical multi label classification: k–Binary Classifier approach and Single Classifier approach.

A. *K-BINARY CLASSIFIER*

This approach transforms an HMC task into a separate



binary classfication task for each class in the hierarchy. This referred as k- Binary Classifier approach or Single classifier (SC) for each label.

After transformation apply basic classification algorithm for classification.

Figure I: Model for k-Binary Classifier

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Binary classification has several drawbacks. It is less efficient, because the learner has to run dataset |L| times, with L is set of class labels, which can be hundreds or thousands. It often results in strongly skewed class distributions: in HMC applications classes at lower levels of the hierarchy often have very small frequencies, while the frequency of classes at higher levels tends to be very high. Many learners have problems with strongly skewed class distributions. Hierarchical relationships between classes are not considered. Means an instance belonging to a class must belong to all its super classes is not automatically imposed. The learned models identify features relevant for one class, rather than identifying features with all classes. [1, 3, 4]

B. *ONE CLASSIFIER*

This approach developed one single multi-label model which predicts multiple class labels at once. Means it predicts all the classes of examples at once.

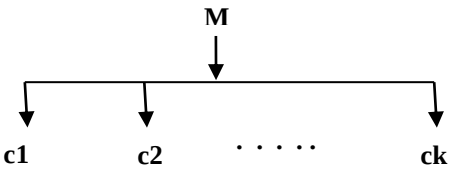

Figure II: Model for One Classifier

This approach takes hierarchical constraint into account. It is also able to identify features that are relevant to all classes. [1, 3, 4]

Table I: Comparision of Hierarchical Multi-label Classification Approach

k – Binary Classifier	**One classifier**
Time consuming prediction	Faster to learn
Model interpretation is difficult	Easy to interpret model
Difficult to generate hierarchical constraint	Hierarchical constraint automatically imposed

III. DECISION TREE FOR HMC

In Multi-Label Classification, we have multiple class labels. But decision tree predict only one class label, not a set of labels. Using decision tree, separate tree will be created for each label.

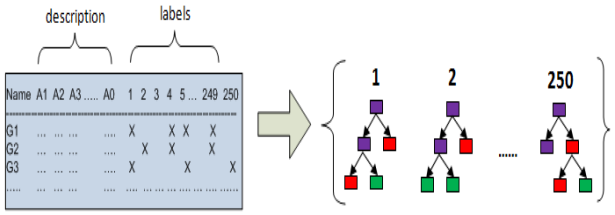

Figure III Decision Tree for each individual label

According to above figure, for 250 labels separate decision tree will be created.

C4.5H ALGORITHM

In this algorithm tree is constructed in top-down manner. Best attribute is chosen by considering information gain. Information gain is a difference between the entropy of whole set of remaining training examples and the weighted sum of the entropy of the subsets caused by partitioning on the values of that attribute.

$$Information\_gain(D, A) = entropy(D) - \sum_{v \in A} \frac{|Dv|}{|D|} * entropy(Dv) \quad (1)$$

Where A is the attribute being considered, D is the set of training examples being considered, and Dv is the subset of D with value v for attribute A.

Entropy (D) =

$$-\sum_{j=1}^{q} p(\lambda j)\log p(\lambda j) + q(\lambda j)\log q(\lambda j) \quad (2)$$

Where,

$p(\lambda j)$ = Relative frequency of class λj

$q(\lambda j) = 1 - q(\lambda j)$

For generating hierarchy of classes several modifications are required: reading and storing the class hierarchy, testing for membership of a class, finding the best class or classes to represent node and performing entropy calculations.

A. *READING AND STORING CLASS HIERARCHY:*

The class hierarchy is read from a file, along with the data values and attributes names. We require the user to unambiguously specify the hierarchical relationships by requesting the hierarchy already in tree format. The format uses indentation by spaces to show the parent and child relationships, with children indented more than their parents. Children can only have a single parent.

B. *TESTS FOR MEMBERSHIP OF A CLASS:*

Testing a data item for membership of a class is now trivial, due to our class representation: simply check if the appropriate array element is set to “true” or not. Membership of parent classes was calculated once at the start, and is now explicit. When doing calculations which involve looking at a specific level in the hierarchy, we can use a Boolean mask to hide classes belonging to other levels. Since the class array consists of Booleans, simply AND-ing a Boolean array mask with the class array will show the classes of interest.

C. *FINDING THE BEST CLASS OR CLASSES TO REPRESENT A NODE:*

Nodes in the decision tree are labeled with the classes which best represent the data in each node. These classes are the classification which is to be made by following a path from the root down to that node. Since we are still dealing with the multi-label problem, there may be several classes used to label a node in the tree. When dealing with the class hierarchy we could choose to label the node with all appropriate classes from most specific to most general, or just the most specific classes.

D. *ENTROPY CALCULATIONS:*

To deal with hierarchies the entropy calculations again need to be modified. The basic entropy calculations developed for multi-label learning still apply, but we also need to consider the differences between levels of the hierarchy.

Entropy (D) =

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$$-\sum_{j=1}^{q} p(\lambda j)\log p(\lambda j) + q(\lambda j)\log q(\lambda j) - \alpha(\lambda j)\log treesize(\lambda j) \quad (3)$$

Where,

$p(\lambda j)$ = Relative frequency of class λj

$q(\lambda j) = 1 - q(\lambda j)$

$\alpha(\lambda j) = 0, if \;\; p(\lambda j) = 0$

= a user defined constant otherwise (default=1)

$treesize(\lambda j) = 1$ + Number of descendant classes of class λj

MULTIPLE PREDICTION TREE VS. SEPARATE DECISION TREE

- Identify features with high relevance for multiple classes.
- Hierarchical constraint is maintained.
- More efficient than separate decision tree.
- Simpler models, if the classes are not independent.
- Learning from skewed distribution.

IV. MULTIPLE PRIDICTION TREE

Predictive Clustering Tree (PCT) can be constructed with a standard "Top-Down Induction of Decision Tree" algorithm, similar to CART and C4.5. PCT generates multiple prediction trees, which makes multiple predictions at once. PCT framework views decision tree as a hierarchy of clusters. Top node corresponds to one cluster containing all data, which is recursively partitioned into smaller clusters. Each split reduces intra-cluster variance. [4, 5]

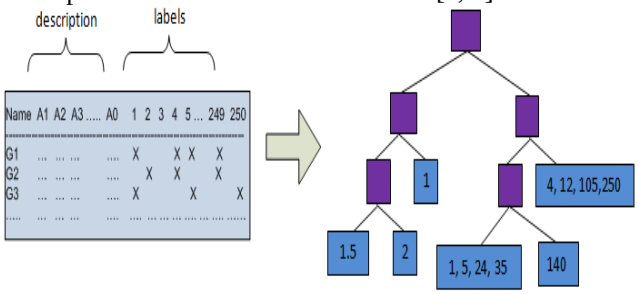

Figure IV multiple prediction tree for multiple labels

PCT: ALGORITHM

I is the current training instances, t is an attribute value test, p is the partition induced by t on I, h is the heuristic value of t. The superscript * indicates the current best test and its corresponding partition and heuristic.

Input: Current training instances I

Output: Tree

Procedure: PCT (I)

1. (t*, p*) = BestTest(I)
2. if t* ≠ none
3. for each $I_k \in P*$
4. $tree_k$ = PCT(I_k)
5. return node (t* , $U_k\{tree_k\}$)
6. else
7. return leaf(Prototype(I))

Procedure: BestTest(I)

1. (t* , h* , p*) = (none , 0, ϕ)
2. for each possible test t
3. p = partition induced by t on I
4. h = Var(I) - $\sum_{I_k \in p} \frac{|I_k|}{|I|} Var(I_k)$
5. if (h > h*) ^ Acceptable(t , p)
6. (t*, h*, p*) = (t , h , p)
7. return (t*, p*)

The algorithm takes as input a set of training instances I. The main method searches for the best acceptable attribute-value test that can be put in a node. If such a test t* can be found then the algorithm creates a new internal node labeled t* and calls itself recursively to construct a sub tree for each subset in the partition p* induced by t* on the training instances. To select the best test, the algorithm scores the tests by the reduction in variance. Maximizing variance reduction maximizes cluster homogeneity and improves predictive performance. If no acceptable test can be found, that is, if no test significantly reduces variance, then the algorithm creates a leaf and labels it with a representative case of the given instances.[4, 5]

Here toyHMC dataset is used to trace the PCT algorithm which generates hierarchical tree. This dataset has three attributes. From that one attribute is used to represent class hierarchy.

```
@relation simple

@attribute A     {a,b}
@attribute B     {1,2}
@attribute class hierarchical
rec/sport/swim, rec/sport/run, rec/auto

@data
a, 1, rec/sport/swim
a, 2, rec/sport/run
a, 2, rec/sport/run@rec/sport/swim
b, 1, rec/sport
b, 2, rec/auto
```

Figure V toyHMC.arff data set

The resulting tree using PCT algorithm:

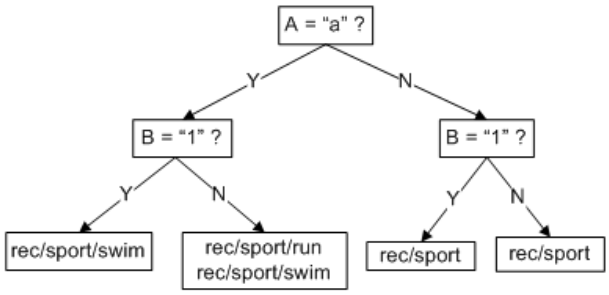

Figure VI Tree using PCT

Clus is a decision tree and rule induction system that implements the predictive clustering framework. This framework unifies clustering and predictive modeling and allows for a natural extension to more complex prediction settings such as multi-task learning and multi-label classification. It uses ideas

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of: C4.5 and CART. Most decision tree learners induce classification or regression trees, Clus generalizes this approach by learning trees that are interpreted as cluster hierarchies We call such trees predictive clustering trees or PCTs. Depending on the learning task at hand, different goal criteria are to be optimized while creating the clusters, and different heuristics will be suitable to achieve this. [6]

Clus is written in Java programming language. So to run Clus, it suffices to install the Java Runtime Environment (JRE). Clus uses two input files and these are named filename.s and filename.arff. The file filename.s contains the parameter settings for Clus. The file filename.arff contains the training data to be read. The results of Clus run are put in an output file filename.out.[6]

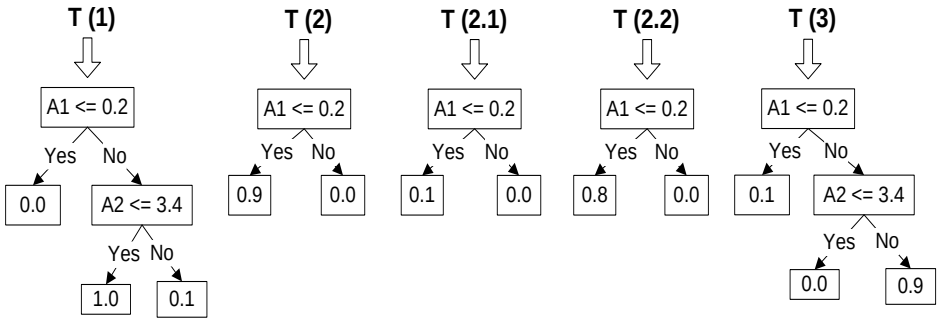

Figure VII (a) Clus-SC

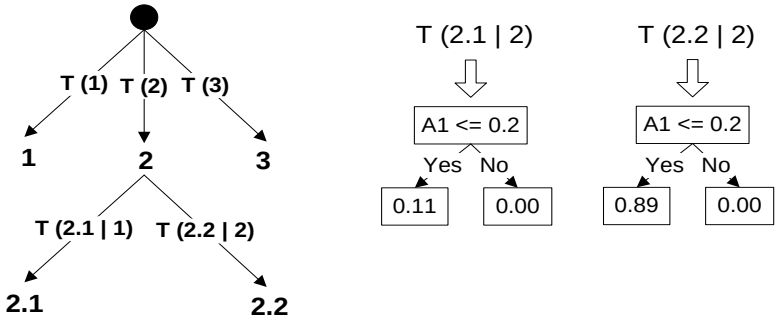

Figure VII(b) Clus-HSC

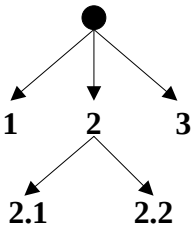

Figure VII(c) Class hierarchy

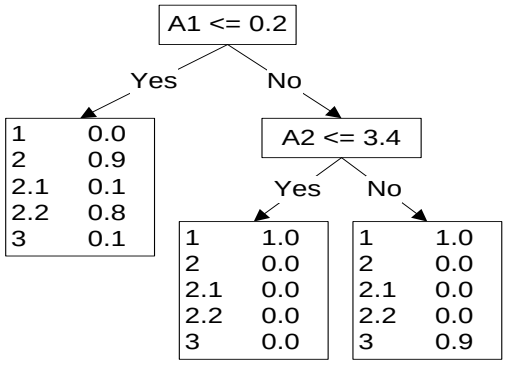

Figure VII(d) Clus-HMC approach

There are three approaches of Clus: Clus-SC, Clus-HSC and Clus-HMC [1, 5]. Class Hierarchy: Figure VII(c) shows small class hierarchy. Class label names reflect the position in the hierarchy, e.g., '2.1' is a subclass of '2' [1].

Clus-SC:

In this approach, separate tree is created for each class label. Each of these trees is a single label binary classification tree. So this approach is an independent single label classification problem. The hierarchy introduces dependencies between class labels. But hierarchy is ignored by this approach. This approach has several disadvantages:

1. It is inefficient, because the learner has to be run |C| times, with |C| the total number of classes.
2. It often results in learning from strongly skewed class distribution: classes at lower levels of the hierarchy often have very small frequencies, while the frequency of classes at higher levels tends to be very high.

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3. The knowledge discovery point of view, the learned models identify features relevant for one class, rather than identifying features with high overall relevance.
4. The hierarchical constraint is not taken into account, i.e. it is not automatically imposed that an instance belonging to a class should belong to all its super classes.

Figure VII(a) shows Clus-SC approach for the given class hierarchy (Figure VII(c)).

Clus-HSC:

This approach learns a separate tree for each hierarchical edge. For a non top-level class c, it holds that an instance can only belong to c if it belongs to c's parent par(c). An alternative approach to learning a tree that directly predicts c, is therefore to learn a tree that predicts c given that the instance belongs to par(c). Learning such a tree requires fewer training instances: only the instances belonging to par(c) are relevant. The subset of these instances that also belong to c become the positive instances and the other instances the negative instances. The resulting tree predicts the conditional probability P(c/par(c)). To make predictions for a new instance, we use the product rule P(c) = P(c/par(c)) P(par(c)). This rule applies the trees recursively, starting from the tree for a top-level class. Figure VII(b) shows Clus –HSC approach.

Clus-HMC:

This approach is to develop learners that learn a single multi-label model that predicts all the classes of an example at once. It considers hierarchy constraint into account. This approach is also able to identify features that are relevant to all classes. This approach follows PCT algorithm for hierarchical multi-label classification. Clus-HMC approach is shown in Figure VII(d) for given class hierarchy in Figure VII(c).

Table II Comparing the three Clus approach

	SC	HSC	HMC
Efficiency	-	√	√
Hierarchical constraint	-	√	√
Identifying global features	-	-	√

V. EVALUATION MEASURES

Let D be a multi-label evaluation data set, consisting of |D| multi-label instances (x_i, y_i), i=1 …..|D|, y_i Y. Y= {1,2,….k} is a set of labels. Let z_i be the set of labels predicted by classifier for example x_i. Three metrics are defined below. [1, 7]

Label Cardinality of D is the average number of labels of the instances in D.

$$LC(D) = \frac{1}{|D|}\sum_{i=1}^{|D|}|Yi| \quad (4)$$

Label Density of D is the average number of labels of the instances in D divided by |L|.

$$LD(D) = \frac{1}{|D|}\sum_{i=1}^{|D|}\frac{|Yi|}{|L|} \quad (5)$$

Precision is the percentage of predicted labels that were correct.

$$\text{Precision}(H,D) = \frac{1}{|D|}\sum_{i=1}^{|D|}\frac{|Y_i \cap Z_i|}{|Z_i|} \quad (6)$$

Recall is the percentage of correct labels that were predicted.

$$\text{Recall}(H,D) = \frac{1}{|D|}\sum_{i=1}^{|D|}\frac{|Y_i \cap Z_i|}{|Y_i|} \quad (7)$$

F-score is a combination of precision and recall. It is the harmonic average of the two metrics and it is used as an aggregated performance score.

$$F-score = \frac{2*\text{precision} * \text{recall}}{\text{precion} + \text{recall}} \quad (8)$$

There is common characteristic for above measures, the larger measure value, and the better classification performance. The performance is perfect value when its value equals one.

Coverage is defined as the distance to cover all possible labels assigned to a sample x. It is loosely related to precision at the level of perfect recall. The smaller value of coverage is, the better the performance is.

$$Coverage = \frac{1}{N}\sum_{i=1}^{N}\max r_i(\lambda) - 1 \quad (9)$$

Hierarchical Loss considers mistakes made at higher levels in the class hierarchy more important than mistakes made at lower levels.

$$l_H = \sum_i [v_{k,i} \neq y_{k,i} \text{ and } \forall c_j \leq_h c_i : v_{k,j} = y_{k,j}] \quad (10)$$

VI. EXPERIMENT

To simulate toyHMC.arff (Figure V) file on Clus, this generates hierarchy of class labels in one text document. Class hierarchy is given as below:

```
Hier #nodes: 5
Hier classes by level: [1, 1, 2, 2]
rec: 10
    auto: 2
    sport: 8
        run: 4
        swim: 4
```


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Figure VII hierarchy,txt file

Below figure shows output file generated on Clus :

```
A = a
+--yes: B = 1
|      +--yes: [1,0.1,0.9,0.2,0.7]: 1
|      +--no:  [1,0.066667,0.933333,0.8,0.466667]: 2
+--no:  B = 1
       +--yes: [1,0.1,0.9,0.2,0.2]: 1
       +--no:  [1,0.6,0.4,0.2,0.2]: 1
```

Figure VIII toyHMC.out - Output file in Clus

In table III, the data sets describe different aspects of the genes. (yeast dataset for biology) Each gene included in the datasets is annotated with one or more classes selected from the MIPS FunCat hierarchical classification scheme. In below table, |D| is the number of instances, and |A| number of attributes.

Table III Dataset Properties

	Data set	|D|	|A|
D1	Sequence (seq)	3932	478
D_2	Phenotype (phenol)	1592	69
D_3	Secondary structure (struc)	3851	19628
D_4	Homology search (hom)	3867	47034
D_5	Spellman et al. (cellcycle)	3766	77
D_6	Roth et al. (church)	3764	27
D_7	DeRisi et al. (derisi)	3733	63
D_8	Eisen et al. (eisen)	2425	79
D_9	Gash et al. (gasch1)	3773	173
D_{10}	Gash et al. (gasch2)	3788	52
D_{11}	Chu et al. (spo)	3711	80
D_{12}	All microarray (expr)	3788	551

Below table shows comparison of Clus and C4.5H algorithm on yeast dataset mentioned in table III.

Table IV

Average precision and coverage for all data sets[5]

	Precision		Coverage	
Name	**Clus**	**C4.5H**	**Clus**	**C4.5H**
Seq	61	71	80.18	14.16
Phenol	67	68	3.09	3.26
Struc	68	58	29.71	2.05
Hom	64	55	81.41	12.06
Cellcycle	82	54	0.86	71.34
Church	75	53	8.18	58.64
Derisi	77	61	2.90	8.39
Eisen	88	48	5.73	37.63
gasch1	67	38	15.77	47.24
gasch2	96	60	3.09	64.06
Spo	79	46	3.70	12.82
Expr	77	75	27.28	5.56

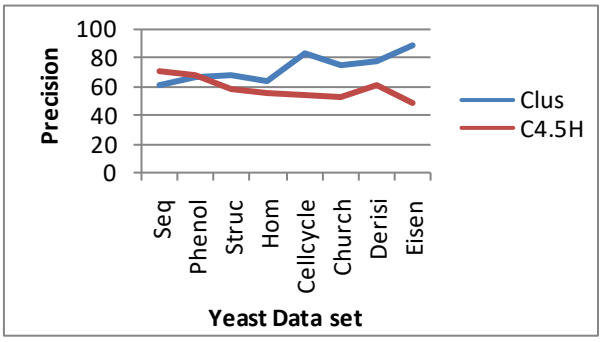

Figure IX Precision for Clus and C4.5H

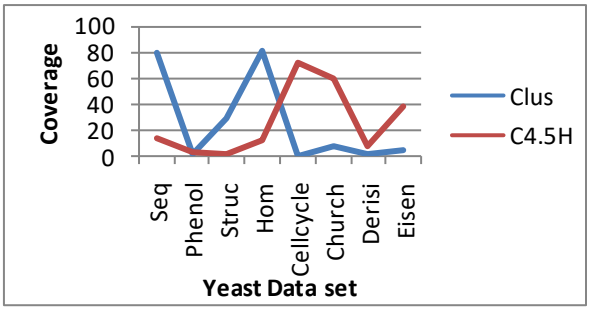

Figure X Coverage for Clus and C4.5H

Table IV presents the obtained average precision and coverage for each data set. The average precision obtained by Clus is higher than C4.5H, this increased precision comes in most cases at the expense of lower coverage. The coverage of Clus is lower than C4.5H.

VII. CURRENT RESEARCH CHALLENGES

Following are the research challenges of the existing hierarchical multi label classification problem:

- Some of the instances are less informative because of irrelevant labels are existing in dataset. So try to extract only relevant label set from multi label set.
- To apply data preprocessing techniques such as pruning, feature selection etc. to improve the performance of multi label classification problem.
- One critical issue is to build hierarchical structure for large dataset with large number of attributes.
- In most of the cases instances are ignored who has missing values. So training instances are reduced.

VIII. CONCLUSION

This paper presented study of two approaches for hierarchical multi label classification. From comparative study concluded that learning a single HMC tree is much faster than learning many regular trees. Clus-HMC has a better predictive performance than Clus-SC and Clus-HSC and for all evaluation measures. This paper also presented comparative analysis of PCT and C4.5H algorithm for precision and coverage measure. PCT performs better compare to C4.5H for generating hierarchical tree.

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