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Labelling Strategies for Hierarchical Multi-Label Classification Techniques

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Abstract

Many hierarchical multi-label classification systems predict a real valued score for every (instance, class) couple, with a higher score reflecting more confidence that the instance belongs to that class. These classifiers leave the conversion of these scores to an actual label set to the user, who applies a cut-off value to the scores. The predictive performance of these classifiers is usually evaluated using threshold independent measures like precision-recall curves. However, several applications require actual label sets, and thus an automatic labelling strategy.

In this article, we present and evaluate different alternatives to perform the actual labelling in hierarchical multi-label classification. We investigate the selection of both single and multiple thresholds. Despite the existence of multiple threshold selection strategies in non-hierarchical multi-label classification, they can not be applied directly to the hierarchical context. The proposed strategies are implemented within two main approaches: optimisation of a certain performance measure of interest (such as F-measure or hierarchical loss), and simulating training set properties (such as class distribution or label cardinality) in the predictions. We assess the performance of the proposed labelling schemes on 10 datasets from different application domains. Our results show that selecting multiple thresholds may result in

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an efficient and effective solution for hierarchical multi-label problems.

Keywords: Hierarchical multi-label classification, Threshold optimisation, Hierarchical loss, HMC-loss, F-measure

1. Introduction

Traditional classification problems deal with assigning a (single) class to an instance. However, many applications require assigning a *set* of classes (labels) to an instance. Examples are found in biology (e.g., gene function prediction [1, 2]), text or image classification [3, 4], etc. Multi-label classification algorithms have been proposed to tackle this task [5, 6, 7]. In many applications, the set of possible labels is structured as a hierarchy, representing a superclass/subclass relation. For instance, gene functions are organised as a tree structure in MIPS's FunCat hierarchy [8], or as a directed acyclic graph (DAG) in the Gene Ontology [9]. The corresponding classification task, that also takes into account this structure, is then called hierarchical multi-label classification (HMC) [10]. It thus involves predicting multiple and partial paths in a hierarchy of labels. Allowing partial paths means that the true and predicted paths need not necessarily to end in a leaf node. Several HMC algorithms have been proposed in the literature, e.g., [11, 12, 13]. They exploit the label set hierarchy when labelling instances. These systems also ensure (implicitly or using post-processing) that the hierarchy constraint is fulfilled in the predictions they make: whenever a class is predicted, its parent and ancestor classes are also predicted.

Rather than predicting an actual label set, most of the HMC algorithms actually predict a real valued prediction score p_i for every label l_i, that reflects the confidence that an instance should be annotated with label l_i. These values can be easily converted into a label set by applying a threshold on them: if p_i is above some threshold t_i, then the instance is predicted to belong to class l_i, otherwise not. To ensure that the predictions fulfil the hierarchy constraint, it suffices to choose $t_i \leq t_j$ whenever l_i is a super class of l_j.

Often, the decision as to which thresholds to choose is left to the end user, and the predictive performance of the classification algorithms is evaluated in a threshold independent way, for example by using precision-recall curves. However, in some situations, it is preferable or necessary to fix the thresholds. For instance, the gene function prediction task may be part of a larger pipeline of experiments, or the predicted image labels may be used as tags in image retrieval systems to locate images of interest. The objective of this article is to investigate and empirically compare different thresholding strategies.

HMC studies that fix the thresholds typically choose one threshold shared by all labels. In the non-hierarchical multi-label setting, however, studies exist that choose a separate threshold per label [14, 15]. It is currently an open question how these two options compare in HMC, and this is addressed in this article. Non-hierarchical optimisation techniques can not be straightforwardly applied in the HMC context, because of the aforementioned hierarchy constraint, and thus, we propose adapted techniques. Depending on the context, the user may want to set the thresholds such that the resulting classifier maximises predictive performance or such that training set properties (such as class distribution) are reflected in the predictions. We consider both approaches. In order to apply the former approach, we first critically review several performance measures used in HMC to compare a predicted label set to a true label set: hierarchical loss, HMC-loss and micro-averaged F-measure.

The contributions of this work are as follows. First, we describe measures that evaluate the predicted label sets, and we identify problems with the widely used (unweighted) hierarchical loss, which leads us to advise against its use (Section 2). Second, we devise a number of multiple-threshold-selection approaches for HMC (Section 3). Third, we empirically investigate the designed schemes and their single-threshold-selection counterparts on ten HMC datasets, showing that the multiple threshold approaches generally outperform their single threshold variants, both in predictive performance and computationally (Section 4). We draw some conclusions and further research directions (Section 5).

2. Evaluating HMC classifiers

In HMC we obtain for every instance and every label a prediction. As mentioned in the introduction, this prediction is often real-valued. Given a hierarchy of k labels, we represent the predicted multi-label of an instance x with a vector $p = (p_1, ..., p_k) \in \mathbb{R}^k$. The label hierarchy can be represented by a partial order $\leq_h$ that represents the superclass relationship. For all labels l_1 and l_2: $l_1 \leq_h l_2$ if and only if l_1 is a superclass of l_2. In the following discussion, we assume that p fulfils the hierarchy constraint: $p_{l_i} \geq p_{l_j}$ whenever $l_i \leq_h l_j$.

In order to evaluate the predicted multi-labels in a test set, there are two possible strategies. The first strategy keeps the real-valued predictions, and evaluates them independently of any fixed thresholds. This is often done by constructing an average precision-recall curve (PR curve) and reporting the area under the curve. Precision gives the proportion of positive predictions that are positive, while recall gives the proportion of positive instances that are correctly predicted positive. A precision-recall curve plots the precision of a model as a function of its recall. While a threshold corresponds to a single point in PR space, by varying the threshold a curve is obtained. Vens et al. [11] and Pillai et al. [15] describe how to compute PR curves in the context of multiple labels.

The second strategy is to convert the predicted multi-labels to binary vectors, by thresholding the predicted values, and to evaluate these binary multi-labels. In non-hierarchical multi-label classification several evaluation measures have been proposed for evaluating binary multi-labels. An overview is given by Tsoumakas et al. [6]. However, these measures are less suited for HMC tasks, exactly because they do not take into account the hierarchical structure in the labels. Kiritchenko et al. [16] formulate three requirements that should be fulfilled by a hierarchical evaluation measure (see the simple label hierarchy in Fig. 1, where {I,J} is indicated as the true multi-label to be predicted):

1. *The measure should give credit to a partially correct classification.* Thus, predicting node K should be better than predicting node C, as the prediction of K involves the path ABF that is part of the correct multi-label.
2. *The measure should punish distant errors more heavily.* This requirement is split further into two parts:
   (a) *The measure should give a higher evaluation for correctly classifying one level down, than to stay at the parent.* Thus, predicting F should be better than predicting B.
   (b) *The measure should give a lower evaluation for incorrectly classifying one level down than to stay at the parent.* Thus, predicting H should be worse than predicting C.
3. *The measure should punish errors at higher levels of the hierarchy more heavily.* This means that, e.g. predicting D when the true label is C should be worse than predicting K when the true label is I.

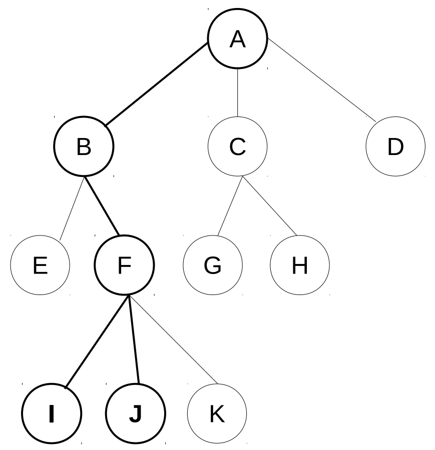


Figure 1: Toy class hierarchy.

Examples of evaluation measures for binary multi-labels that do take into account a hierarchical label structure are hierarchical loss functions and a hierarchical extension of the F-measure. In the following, we represent the thresholded (binary) predicted multi-label of an instance with a vector $\hat{p} = (\hat{p}_1, ..., \hat{p}_k) \in \{0,1\}^k$; similarly, we represent the true multi-label with a vector $l = (l_1, ..., l_k) \in \{0,1\}^k$. Without loss of generality, we also assume a single root node in the hierarchy. In case of a collection of separate hierarchies (such as the Gene Ontology, which consists of three independent sub-graphs), this means that we create an artificial root node, to which all instances belong. This node then has as children the individual root nodes of the sub-hierarchies.

2.1. Hierarchical loss functions

The hierarchical loss (H-loss) function [17] was proposed specifically for HMC tasks. It assumes a tree structured label hierarchy. It is based on the Hamming or symmetric difference loss, which returns the symmetric difference between the predicted and true multi-label vector for an instance. However, the H-loss does not punish mistakes that have already been punished at a higher level in the hierarchy. In other words, whenever a classification mistake is made on a label in the hierarchy, the H-loss does not charge any loss for additional mistakes occurring in the subtree of that label:

$$\text{H-loss}(\hat{p}, l) = \sum_{i=1..k} c_i \{\hat{p}_i \neq l_i \quad and \quad \hat{p}_j = l_j, j \in anc(i)\}, \qquad (1)$$

where $anc(i)$ represents the set of ancestors of node i, and $c_1, ..., c_k > 0$ are fixed cost coefficients. Cesa-Bianchi et al. [18] propose two variants of the H-loss function: uniform H-loss with all coefficients set to one, and normalised H-loss, where each node's cost is equally split recursively among its children. The latter is achieved by setting the coefficients as follows: $c_{root} = 1$, and for the other nodes i in the hierarchy $c_i = c_j/|child(j)|$ with j the parent of i. For the label hierarchy in Fig. 1, this yields $c_A = 1$, $c_B = c_C = c_D = 1/3$, $c_E = c_F = c_G = c_H = 1/6$, and $c_I = c_J = c_K = 1/18$.

In practice, most HMC papers that use the H-loss use the uniform variant (e.g., [19, 20, 21, 22, 23, 13, 24]). Here, we identify two problems with this H-loss variant. First, surprisingly, none of the requirements by Kiritchenko et al. [16] is met by the uniform H-loss. This can be easily verified by calculating the H-loss for the examples given above. Second, it turns out that making zero predictions (i.e., predicting only the root, which is by default present in all instances) often results in a very good uniform H-loss score. Let us call a class that appears in the first level (i.e., directly under the root) of the class hierarchy a level1 class. If an instance has target labels that all belong to paths that pass through a single level1 class, then an empty prediction yields a H-loss of 1. This is the second best value that can be obtained. Only a completely perfectly predicted multi-label can yield a H-loss of 0. Since level1 classes are the most general classes in the taxonomy, it is to be expected that, even though an instance belongs to many paths, these paths will often pass through a single level1 class, and the multiple labels will only differentiate at lower, more specialised, levels of the hierarchy[1]. For instance, in gene function annotation, a gene involved in "aerobic respiration" (FunCat category 02.13.03) and in "photosynthesis" (02.30), which both belong to the level1 class "energy" (02) may be less likely to also have functions related to other level1 classes like "storage protein" (04) or "transcription" (11). Table 1 confirms the high rate of instances whose class(es) only pass(es) through a single level1 class. Clearly, the uniform H-loss function does not achieve what one would expect intuitively from a loss function designed for hierarchical classification. Cerri et al. [13] have observed that uniform H-loss can lead to results contradicting those of other evaluation measures, when comparing global versus local HMC prediction models.

[1]Remark that for hierarchical single-label classification tasks, there is always only a single level1 class involved.

Table 1: Number of instances belonging to a single root child.

Dataset	Total nb instances	Instances belonging to single root child
cellcycle_GO	3751	174
diatoms	3121	3121
enron	1649	319
expr_FUN	3779	1162
imclef07a	11006	11006
interpro_ara_FUN	3719	2895
reuters	6000	6000
seq_FUN	3919	1265
struc_ara_GO	11763	11763
wipo	1710	1710

The normalised H-loss mostly solves the issues discussed above, because (1) the coefficients decrease with increasing depth in the hierarchy, and (2) the total loss obtained for mistakes in a subtree can never exceed the cost associated with the root of the subtree. However, it still has a tendency to favour empty predictions, when used in a threshold selection scheme (see Section 4). Cesa-Bianchi et al. [18] list another disadvantage of this function: if the hierarchy has large branching factors in the upper levels, then the coefficients quickly become very small, which in turn yields very small H-loss values and makes it difficult to conduct comparisons among algorithms. Nevertheless, it should be stressed that the normalised H-loss should be preferred over the uniform H-loss.

Bi and Kwok [25] criticise H-loss, because it can never meet requirement 2b of Kiritchenko et al. [16]: when comparing two false positive predictions, where one prediction is more specific than the other, intuitively, the more specific prediction should receive a lower evaluation than the (more prudent) general one. However, this is in contrast to the idea behind H-loss, which gives them an equal evaluation. In response to this, Bi and Kwok designed the HMC-loss, which is also applicable to DAG label hierarchies:

$$\text{HMC-loss}(\hat{p}, l) = \alpha \sum_{i=1..k:\hat{p}_i=0,l_i=1} c_i + \beta \sum_{i=1..k:\hat{p}_i=1,l_i=0} c_i, \tag{2}$$

where $c_1, ..., c_k > 0$ are fixed cost coefficients, which are defined as in the normalised H-loss for tree hierarchies. For DAGs, the cost for non-root nodes is set as follows: $c_i = \sum_j c_j/|child(j)|$ with j the set of parents of i. The coefficients α and β allow a cost-sensitive learning setting, where false positives and false negatives are weighted differently. When $\alpha = \beta = 1$, the HMC-loss becomes equal to a weighted Hamming-loss, or to the uniform H-loss that does not disregard subtrees whenever a mistake is counted. The HMC-loss effectively solves the empty prediction issue of H-loss, because instead of only punishing the root node, every node belonging to the multi-label contributes to the loss. Moreover, all requirements for a hierarchical evaluation measure [16] are fulfilled.

2.2. Hierarchical F-measure

Precision and recall are traditionally defined for single-label classification problems. As these measures provide complementary information, they are often combined, resulting in the F-measure:

$$F_\beta = \frac{(\beta^2 + 1) \times precision \times recall}{\beta^2 \times precision + recall}, \beta \geq 0 \tag{3}$$

Parameter β weighs the importance of precision versus recall. In the rest of the paper, we use $\beta = 1$, resulting in the harmonic mean of precision and recall.

When dealing with multiple classes, precision, recall and F-measure are averaged. There are two strategies to calculate the average. Consider a prediction matrix, P, where each row represents an instance, each column a label, and the values the corresponding binary predictions. The macro-average computes the above measures for each column individually and then averages them over the columns. Thus, each class obtains an equal weight in the calculation. In contrast, the micro-average looks at all cells of the prediction matrix together. Micro-averaged precision (denoted by $precision^m$) is then the proportion of positively predicted cells that are positive and micro-averaged recall ($recall^m$) is the proportion of positive cells that are correctly predicted positive. The corresponding micro-averaged F_1 measure (F_1^m) is given by:

$$F_1^m = \frac{2 \times precision^m \times recall^m}{precision^m + recall^m} \tag{4}$$

While the macro-average gives an equal weight to each class, and thus tends to over-estimate the importance of rare classes, the micro-average implicitly gives more weight to more frequent classes. In the hierarchical setting, it thus makes more sense to consider the F_1^m measure. Moreover, Vens et al. [11] showed that PR curves generated from micro-averaged precision and recall can better capture overfitting issues. If the true label set fulfils the hierarchy constraint (which we assume in this article), i.e., whenever an instance belongs to some class it also belongs to the parent class, then Kiritchenko et al. [16] call the corresponding micro-averaged precision, recall and F_1 the *hierarchical* precision, recall and F_1 measures, respectively. In addition, they show that the hierarchical F_1 measure fulfils the requirements for hierarchical evaluation measures. Other papers that use the hierarchical F_1 measure include the work of Valentini [26] and Cesa-Bianchi et al. [27]. This measure can be applied to both tree and DAG structured hierarchies.

3. Threshold selection methods for HMC problems

In this section we present different alternatives to perform the final labelling of an HMC problem given a set of real-valued scores for the potential classes.

Let us assume we have trained a HMC classifier with a given training dataset TRS. Then, we classify a validation set VS, i.e. a set of N_v instances that did not play any role in the construction of the classifier, and for which the true multi-labels are known, i.e., we dispose of a binary matrix L_{val} that indicates for each validation instance the actual labels. Moreover, we classify a test set TS composed of N_t instances where the labels are unknown. As a result, we obtain two prediction matrices $P_{val} = \{\{p_1^1, .., p_k^1\}, ..., \{p_1^{N_v}, .., p_k^{N_v}\}\}$ and $P_{test} = \{\{p_1^1, .., p_k^1\}, ..., \{p_1^{N_t}, .., p_k^{N_t}\}\}$ that are composed of N_v and N_t prediction vectors p^i, respectively.

The final objective is to determine the best labelling of the TS instances. To do this, we utilise the P_{val} matrix as reference and we look for the best thresholds that convert it into a binary prediction matrix $\hat{P}_{val}$, which is evaluated against the actual labels L_{val}. Then, the learned thresholds are applied to the P_{test} matrix. There are two aspects in determining the best thresholding strategy.

First, we distinguish the number of thresholds that is considered. Numbers reported in the HMC literature range from a single global threshold used for all datasets [13] to a single threshold per dataset [28, 29, 30, 31]. Although it has been done in non-hierarchical multi-label classification, to our knowledge the selection of a separate threshold per class has not been performed in the HMC context. In this work, we consider the problem of single and multiple thresholds selection. Both approaches are optimisation schemes that are generically illustrated in Algorithms 1 and 2.

Algorithm 1 Generic STS pseudo-code

```
Require: A validation prediction matrix $P_{val}$.
Ensure: A global threshold $t$.
 1: CutPoints= all different values from $P_{val}$ sorted in ascending order.
 2: bestThreshold = -1
 3: bestPerformance = worst value // e.g., $\infty$ if performance is to be minimised
 4: for each cutpoint in CutPoints do
 5:    performance = ComputePerformance($P_{val}$, cutpoint,$L_{val}$)
 6:    if betterThan(performance,bestPerformance) then
 7:       bestPerformance = performance
 8:       bestThreshold = cutpoint;
 9:    end if
10: end for
11: return bestThreshold
```

- Single-threshold selection (STS) consists of computing a single cut-off per dataset that optimises some value. A threshold t that is shared between all the classes is obtained and used to transform P_{val} into $\hat{P}_{val}$. Most HMC classifiers provide a P_{val} that preserves the hierarchy constraint, so that the probability of belonging to label l_j cannot be higher than the probability associated to l_i whenever $l_i \leq_h l_j$ (l_i is an ancestor of l_j). Therefore, the application of a single threshold over all classes keeps the hierarchy constraint.

- Multiple-thresholds selection (MTS) optimises a threshold t_i for every label of a dataset, resulting in a vector $t = (t_1, ..., t_k)$. As such, the STS approach can be considered a particular case of the MTS in which all the thresholds are forced to be equal. However, in this case, the hierarchy constraint must be ensured during the selection process by keeping any threshold $t_i \leq t_j$ whenever $l_i \leq_h l_j$.

Finding the optimal threshold value for the validation set in STS requires the evaluation of all possible candidate threshold values, which in worst case corresponds to the number of instances times the number of possible classes,

Algorithm 2 Generic MTS pseudo-code

```
Require: A validation prediction matrix $P_{val}$.
Ensure: A threshold vector $t = (t_1, ..., t_k)$.
 1: for each class i do
 2:     CutPoints[i] = all different values from column $i$ of $P_{val}$ sorted in ascending order.
 3: end for
 4: bestThresholdVector = [-1,-1,...,-1]
 5: bestPerformance = worst value // e.g., $\infty$ if performance is to be minimised
 6: for each possible threshold vector $t$ from CutPoints do
 7:     performance = ComputePerformance($P_{val}$,$t$,$L_{val}$)
 8:     if betterThan(performance,bestPerformance) then
 9:         bestPerformance = performance
10:         bestThresholdVector = t;
11:     end if
12: end for
13: return bestThresholdVector
```

so, $O(N_v \times k)$. In general, however, the number of possible threshold values is lower than $N_v \times k$ because of repeated values. The complexity of STS can easily be reduced though, at the cost of a decrease in accuracy, by using a sub-optimal approach. This approximation may consist of the evaluation of limited number of possible candidate threshold values, which are equally distributed in the range of the score values. For instance, if the score values belong to the range $[0, 1]$, we may investigate 100 thresholds as {0.01, 0.02, ..., 1}.

In MTS, for every class l_i we have to find a threshold $t_i \in [min(P_{val}(i)), max(P_{val}(i))]$, where $P_{val}(i)$ represents the column vector i of P_{val}. Thus, the number of possible thresholds per class is upper bounded by the number of instances in VS. For non-decomposable measures, seeking for the optimal solution in this validation set requires to explore all the possible combinations at first sight, resulting in an exponential complexity $O((N_v)^k)$. However, the hierarchy constraint drastically reduces the number of possible valid combinations. If the performance measure is decomposable over classes, it takes the same complexity as STS. Nonetheless, the hierarchy complicates the search process as the classes need to be processed in a hierarchical order. The set of possible thresholds for each class is then constrained by the classes already processed. Thus, both for decomposable and non-decomposable measures, the hierarchy has a positive influence on computational complexity.

Obtaining single or multiple thresholds according to the validation set does not guarantee that the threshold/s is/are the most suitable for the test set, due to overfitting phenomena. For this reason, in the proposed MTS approaches, we do not pursue optimal approaches that may not be feasible in time, but rather efficient search processes that guarantee that only coherent threshold vectors (w.r.t. the hierarchy constraint) are evaluated.

The second aspect in the thresholding strategy is how to compute the performance, which corresponds to the procedure *ComputePerformance* in Algorithms 1 and 2:

- Compute the predictive performance in the validation set, using the evaluation measure that will be used to evaluate the test set predictions (Section 3.1).
- Reflect training or validation set properties in the test set predictions.

We now discuss each of these in detail.

3.1. Optimising the evaluation measure

One obvious strategy is to optimise the performance measure that will be used in the end to evaluate the test set predictions. In the experiments (Section 4), three evaluation measures will be used that were discussed in Section 2: the normalised H-loss, the HMC-loss and the F_1^m. Optimising them under the STS scheme is straightforward following Algorithm 1. For every possible threshold value, calculate the corresponding measure, and take the threshold that yielded the best value. However, under the MTS scheme, the optimisation process becomes more complicated. In what follows, we propose three optimisation processes associated to the hierarchical loss (Section 3.1.1), the HMC-loss (Section 3.1.2) and the micro-averaged F-measure (Section 3.1.3), respectively.

3.1.1. Multiple Threshold Selection for the Normalised Hierarchical Loss.

The computation of the normalised H-loss can be partially decomposed over classes. Observing Equation 1, we can see that the loss calculation for one label directly depends on the predictions made for its ancestors. Therefore, we need to establish the thresholds for the ancestor labels before the threshold of a child label, giving rise to a top-down procedure as follows.

We start by fixing the root's threshold to zero: every instance belongs to the root, so any threshold between 0 and 1 would be valid. However, as the thresholds need to increase while going down the hierarchy, it is better to set the root threshold as low as possible. Then we recursively move to the child nodes, and for each of these nodes select the threshold that minimises the normalised H-loss, only considering the nodes on the path from this node to the root, and only considering candidate thresholds equal to or higher than the parent's threshold, to enforce the hierarchy constraint. This efficient procedure results in an optimal threshold vector, because the total loss incurred in the subtree of a node can never exceed the loss associated with the node itself.

The procedure is outlined in Algorithm 3. The $NormHLoss$ function calculates the normalised H-loss given a label matrix, a prediction matrix on which it applies the previously calculated and current thresholds, and the hierarchy path from the current node to the root.

For DAGs datasets we set the coefficients as in the HMC-loss (See Section 2.1). However, the optimality is not guaranteed in this case, because the coefficients may increase while moving down in the hierarchy.

3.1.2. Multiple Threshold Selection for the HMC-loss

The HMC-loss simply adds the losses (false positives and false negatives) for each label of the hierarchy. As stated by Equation 2, it takes into account the hierarchy by using coefficients that decrease with the depth. As such, this measure could be decomposed over the different classes. However, an independent optimisation per class, as proposed for the normalised H-loss, is not applicable, even though a top-down approach is considered. The reason is that now the total loss incurred in the subtree of a node *can* exceed the loss associated with the node itself. For example, in Fig. 1, node B has coefficient 1/3, but the subtree below it has total coefficient of 1/2. Thus, the subtree needs to be considered when selecting a threshold for node B.

Algorithm 4 defines the MTS procedure for the HMC-loss. As in the previous case, the root's threshold is set to zero, while the other thresholds are optimised in a top-down fashion. Following this top-down approach, for each label i, we look for the best threshold that optimises the HMC-loss in node i and its subtree at the same time. Following the previous example, when analysing node B, we minimize the sum of the losses for nodes B, E, F, I, J and K with their corresponding weights. Moreover, we limit the search to appropriate values of the thresholds to take into consideration the hierarchy

Algorithm 3 MTS for the Normalised H-loss

Require: A validation prediction matrix P_{val} and label matrix L_{val}.
Ensure: A threshold vector $t = (t_1, ..., t_k)$.

```
 1: bestThresholds[1,...,$k$] = [0,-1,...,-1]
 2: for each non-root node $i$ (top-down approach) do
 3:    bestLoss = $\infty$
 4:    $H_i$ = hierarchy path starting in the root node and ending in $i$
 5:    CutPoints = all different values from the column of $P_{val}$ that corre-
       spond to $i$, that are equal to or larger than the threshold selected for
       $i$'s parent
 6:    for each cutpoint in CutPoints do
 7:       loss = $NormHLoss(P_{val}, L_{val}, cutpoint, bestThresholds, H_i)$
 8:       if loss < bestLoss then
 9:          bestLoss = loss
10:          bestThresholds[i] = cutpoint
11:       end if
12:    end for
13: end for
14: return  bestThresholds
```

constraint: the threshold for i should be equal to or larger than the threshold for i's parent.

Algorithm 4 MTS for the HMC-loss

```
Require: A validation prediction matrix $P_{val}$ and label matrix $L_{val}$.
Ensure: A threshold vector $t = (t_1, ..., t_k)$.
 1: bestThresholds[1,...,$k$] = [0,-1,...,-1]
 2: for each non-root node $i$ (top-down approach) do
 3:     bestLoss = $\infty$
 4:     $Sub_i$ = subtree of node $i$ (including $i$ itself)
 5:     CutPoints = all different values from the columns of $P_{val}$ that correspond to $Sub_i$, that are equal to or larger than the threshold selected for $i$'s parent
 6:     for each cutpoint in CutPoints do
 7:         loss = $HMCLoss(P_{val}, L_{val}, cutpoint, Sub_i)$
 8:         if loss < bestLoss then
 9:             bestLoss = loss
10:             bestThresholds[i] = cutpoint
11:         end if
12:     end for
13: end for
14: return bestThresholds
```

Note that this approach is sub-optimal: if the optimal threshold would be 0.6 for node B, and 0.7 for nodes E, F, I, J and K, then this can only be found if, during the selection of B's threshold, using 0.6 for all nodes (too many false positives) is better than 0.7 for all nodes (too many false negatives).

3.1.3. Multiple Threshold Selection for the micro-averaged F-measure

The micro-averaged F-measure cannot be decomposed over classes, what makes the optimisation of this measure non trivial. Pillai et al. [15] proposed a technique to compute the global maximum micro-average F-measure with a low computational cost (upper bounded by $O(N_v^2 k^2)$), in non-hierarchical multi-label classification. This method initialises the threshold vector to the smallest possible cut-off values. Then, iteratively, each threshold is considered for an update, and this is continued until no threshold can be updated. The updates consist in increasing the value of a threshold, so that it maximises the micro-averaged F-measure, while keeping the other thresholds fixed. The main problem in extending this approach towards HMC, is that increasing the value of a single threshold will violate the hierarchy constraint. Indeed, if a threshold for node i is increased, all thresholds corresponding to i's descendants need to be increased as well, as they should be larger than or equal to i's threshold. Here, we propose to set the thresholds of the descendants equal to the threshold being updated, thus keeping the computational cost advantage, at the cost of providing a sub-optimal solution, in the same sense as when optimising the HMC-loss.

Following Pillai's notation for sake of clarity, let $t = (t_1, ..., t_k)$ denote a specific value of the thresholds, and $T = (T_1, ..., T_k)$ the thresholds considered as variable. Let us assume that all the score prediction vectors per class $P_{val}(i) = \{P_{val}(i, 0), P_{val}(i, 1), ..., P_{val}(i, N_v)\}$ have been sorted in ascending order, so that, $P_{val}(i, j) \leq P_{val}(i, j + 1), \forall j = 1, ..., N_v - 1$. Algorithm 5 presents the pseudo-code of the modified algorithm. In what follows we describe the main changes performed to the method, referring to the lines in the pseudo-code.

First of all, all the thresholds t_i are originally initialised to any random value between $(0, P_{val}(i, 0))$. In contrast, we set all thresholds to zero, in order to ensure the hierarchy constraint is fulfilled at the start.

Then, based on two main properties, Pillai et al. demonstrated that an iterative updating process is globally optimal. In this process, each threshold T_i is increased to any value that locally increases the F^m_β, while keeping all the other $T_j, j \neq i$ fixed, until no improvement is achieved by changing any of the thresholds (lines 6-29). This means that even though the F^m_β cannot be decomposed over classes, the optimisation can be implemented in an iterative way, and thereby reducing complexity.

In the original proposal, every T_i is checked with all the values contained in the prediction vector $P_{val}(i)$. Lines 2-4 extract all potential cut points for every class from P_{val}.

When investigating the value of a given T_i, we have to check that the fixed threshold values of the descendants of label l_i satisfy the hierarchy. In this way, the descendant thresholds may become variable T_d, where l_d is any children of class l_i (See lines 12-16).

When the best threshold has been determined for the current T_i and its associated T_d's, the algorithm checks if this optimisation has yielded a better performance. If yes, the thresholds values of t_i and its descendants are established accordingly (lines 23-26). Once again, this iterative process needs to follow a top-down approach to ensure that the threshold of the

Algorithm 5 MTS for the micro-averaged F-measure

```
Require: A validation prediction matrix $P_{val}$ and label matrix $L_{val}$.
Ensure: A threshold vector $t = (t_1, ..., t_k)$.
1: bestThresholds[1,...,$k$] = [0,0,...,0]
2: for all classes do
3:     CutPoints[i] = All different values from column $i$ of $P_{val}$ sorted in ascending order.
4: end for
5: bestPerformance = $-\infty$
6: repeat
7:     $updated < -false$
8:     for each node $i$ (top-down approach) do
9:         $Descendants$=listOfDescendants($i$)
10:        for all values $T_i$ in $CutPoints[i] \geq t_i$ do
11:            %Enforce hierarchy
12:            for each node $d$ in $Descendants$ do
13:                if $T_i > t_d$ then
14:                    $T_d = T_i$
15:                end if
16:            end for
17:            performance=$F^m_\beta(P_{val}, L_{val}, \{t_1, .., T_i, T_d, ..., t_k\})$ with $T_d = T_i$ for all descendants
18:            if $better\_than(performance, bestPerformance)$ then
19:                bestPerformance = performance
20:                bestThresholds= $T_i$, $T_d$ (if $T_d$ has been modified);
21:            end if
22:        end for
23:        if $better\_than(performance, bestPerformance)$ then
24:            $\{t_i, t_d\} = bestThresholds$
25:            updated=true
26:        end if
27:    end for
28: until updated==False
29: return bestThresholds
```

parent of the current analysed label is already fixed.

3.2. Reflecting training set properties

Apart from optimising a certain error measure of interest, a second potential strategy is to choose thresholds in such a way that some properties of the training or validation sets remain in the predictions of the test set. Specifically, we analyse two different strategies:

- To reflect the positive/negative distributions for each label in the resulting predictions (Subsection 3.2.1).
- To make the label cardinalities as similar as possible (Subsection 3.2.2).

The aim of these proposals is to check whether a simple and fast approach may yield successful thresholds, even though performance measures are not considered.

3.2.1. Reflecting class distribution

The idea behind this strategy is to perform a STS or MTS process in which the function to be optimised is the distance to the true class distribution. The thresholds are chosen based on the validation set, in such a way that they result in a positive/negative split for each class that is as close as possible to the true positive/negative split. Therefore, the true class distribution is also estimated from the validation set (and not from the training set, since this might introduce noise if the training set class distributions differ slightly from those of the validation set). To do so, we use the label matrix L_{val} and for each class i compute the percentage of positive instances CD_i.

Under STS, we follow Algorithm 1 in which the *computePerformance* function computes, for a given cut point and the prediction matrix P_{val}, the predicted percentage of positive instances CD'_i for each label. The threshold that minimises the Euclidean distance between the CD and CD' vectors is chosen.

Under MTS, we simply put the threshold for every label at the value that gives an equal positive/negative ratio as in the true class distribution. To make sure that the hierarchy constraint is guaranteed, a top-down approach is again required. Thus, if the class distribution of a certain class implies a lower threshold than the threshold established for (one of) its parent class(es), it must be set to the same value as that parent.

A very similar labelling strategy has been used in text categorisation, it is referred to as PCut by Yang [32], and as proportional assignment by Lewis and Ringuette [33] and Wiener et al. [34]. The difference is that these authors did not use a separate validation set to determine the thresholds, they immediately pick the positive/negative split in the test set that corresponds to the class distribution of the training set. The disadvantage of their approach is that, if the test set is changed (e.g., it grows because new instances become available), then the prediction of individual test instances may change.

3.2.2. Reflecting label cardinalities

This alternative aims at reflecting the label cardinality of the validation samples. Label cardinality is defined as the average number of labels associated with an instance [6]. This is related to the strategy used in [35] where the authors compared the label cardinality of the predictions in the test set to the label cardinality over the training set. Instead of using an averaged label cardinality, we compare instance per instance the true number of labels and the predicted number of labels over a validation set.

In STS, we count for each validation instance how many labels are present, obtaining a vector of true label counts per example LC_i, where $1 < i < n$. When analysing the different thresholds, we compute the resulting predicted label counts $LC_i^{'}$. Afterwards, the Euclidean distance between both vectors is minimised.

An MTS label cardinality approach is not applicable, since label cardinalities are computed per instance, and not per class.

4. Experimental Study

In this section, we start by defining the experimental set-up in Section 4.1: we detail the problems chosen for the experimentation, the measures employed to evaluate the performance of the algorithms and finally, the statistical tests conducted to contrast the results obtained. Then, Section 4.2 shows the results analysing the different proposed alternatives to perform the final labelling in HMC problems.

4.1. Experimental set-up

To assess the performance of the proposed labelling strategies, we experimentally evaluate them in 10 datasets. We focus on datasets that come from three different domains: text categorisation, image annotation, and

Table 2: Properties of the datasets considered.

Dataset	Samples			Attr.	Classes
	TRA	VAL	TST		
cellcycle_GO	1625	848	1278	77	4125
diatoms	1376	689	1054	371	397
enron	658	330	660	1001	56
expr_FUN	1639	849	1291	551	499
imclef07a	6666	3334	1006	80	96
interpro_ara_FUN	1674	781	1264	2815	263
reuters	2000	1000	3000	47236	102
seq_FUN	1701	879	1339	478	499
struc_ara_GO	5199	2579	3985	14804	629
wipo	901	451	358	74435	188

gene function prediction. These datasets have been collected from freely-available repositories[2][3][4]. Two of the gene function prediction datasets have annotations coming from the gene ontology (GO) [9]. This ontology forms a directed acyclic graph instead of a tree: each node can have multiple parents. We denote them as GO datasets.

All these data sets are originally split into a training and a test set. For those datasets for which no validation set is available, we set aside a random subset of 1/3 of the training set as validation set. Table 2 details the main properties of these datasets. It shows the number of instances in the different partitions, number of attributes (Attr.) and number of classes.

In our experiments, we use the Clus-HMC-Ens algorithm [2] as a representative state-of-the-art HMC classifier. It constructs a random forest of 50 predictive clustering trees. Each individual tree makes a prediction for the complete multi-label. All the predictions provided by this method preserve the hierarchy constraint. In order to optimise the labelling strategies, a random forest is first built on the training set and tested on the validation set. Afterwards, the final model is built on the combination of training and validation sets, and tested on the test set. As a result, we obtain two prediction matrices P_{val} and P_{test}.

The STS and MTS approaches will be investigated under each of the 3

[2]`https://dtai.cs.kuleuven.be/clus/hmcdatasets/`

[3]`https://dtai.cs.kuleuven.be/clus/hmc-ens/`

[4]`http://kt.ijs.si/DragiKocev/PhD/resources/doku.php?id=hmc_classification`

different schemes presented before: optimising an error measure (EM), class distribution (CD) and label cardinalities (LC). We will denote these approaches as EM(), CD() and LC(), indicating STS or MTS versions between brackets. We will use three error measures: normalised H-loss, HMC-loss and the micro-averaged F-measure with $\beta = 1$ (F_1^m). For the HMC-loss, as in [25], we set $\alpha = \lambda \cdot \beta$ while keeping $\alpha + \beta = 2$, where λ becomes the parameter that balances the misclassification cost between positive and negative examples and it is set to the ratio of negative examples in relation to the positive ones: $\lambda = \#negatives/\#positives$. We also test two different settings for the STS approach, either using all available threshold values (optimal solution) or using a binning procedure. For the approximate STS approach, we use 100 values equally distributed in [0,1], which is the output range of Clus-HMC-Ens. Moreover, we compute the run time spent by the different analysed approaches in order to compare their complexity in practice. Ten executions of each algorithm have been performed and their run time has been averaged. All the experiments have been carried out on an Intel(R) Xeon(R) CPU E5-1650 v2 at 3.50GHz without any kind of parallellization.

To provide statistical support for the analysis of results performed, we will apply hypothesis testing techniques. More specifically, we make use of non-parametric tests that were suggested in the studies presented in [36, 37] for machine learning applications. The Wilcoxon test [38] will be used to perform pairwise comparisons between the STS and MTS labelling schemes. It will be adopted considering a level of significance of $\alpha = 0.05$.

Furthermore, in order to perform an all-versus-all comparison of our proposed schemes, we will use the Friedman test [39] and the post hoc Nemenyi test as recommend by [36], to find out which algorithms are distinctive. The Friedman test ranks the algorithms in terms of their performance, so that, the lower the rank is for an algorithm, the better it is. If the Friedman test detects significant differences in the performance of the algorithms, we apply the Nemenyi post hoc test. In this test, the performance of two classifiers is significantly different only if their average ranks differ by a certain critical distance. The critical distance depends on the number of algorithms, the number of datasets, and the critical value for a significance level provided by a Studentized range statistic. The result from the Nemenyi post hoc test is plotted with an average ranks diagram. The ranks are depicted on the axis, so that the best algorithms are at the right side of the diagram. A line with the length of the critical distance is drawn between those algorithms that do not differ significantly (in performance) for a significance level of 0.05. More information about these tests and other statistical procedures can be found at `http://sci2s.ugr.es/sicidm/`.

4.2. Results and analysis

Tables 3 and 4 collect the obtained results in the validation and test set, respectively. In both tables, the best result for each dataset and performance measure has been highlighted in bold-face. We present the validation set results to analyse the generalisation capabilities of the methods. Nevertheless, the conclusions related to the performance of the methods need to be evaluated in the test set.

This study is divided into two parts. We first compare STS and MTS approaches across the proposed optimisation strategies (Section 4.2.1). Afterwards, we perform a global study to determine which is the best alternative according to every performance measure considered (Section 4.2.2). In both studies, we evaluate the resulting threshold selection techniques in terms of predictive performance, influence of the overfitting phenomena and required run time.

Note that for the label cardinality and class distribution approaches we computed the threshold/s once, and then the computed thresholds are used to compute the final performance with the three considered measures. However, for the error measure optimisation process we have independent threshold/s for each measure.

4.2.1. STS vs. MTS

This subsection compares the STS and MTS approaches. As commented before, there is no MTS variant for the label cardinality strategy. Thus, only the error measure and class distribution approaches are included in the following analysis.

To significantly characterise the differences between STS and MTS approaches, the Wilcoxon signed-ranks test has been applied for the possible settings. A total of 12 Wilcoxon tests are conducted to compare STS and MTS approach depending on the performance measure, the optimisation strategy and the considered dataset (validation or test). Table 5 presents the associated p-values for each statistical test conducted. Significant differences ($\alpha = 0.05$) are stressed in bold-face. According to this table we can state that:

- Looking at the EM optimisation techniques, the MTS approach is always statistically better at the validation set, but this not the case at

Table 3: Results obtained at the validation set

.

Measure	Dataset	Error measure		Class distribution		Label cardinality
		STS	MTS	STS	MTS	STS
Normalised H-loss	cellcycle_GO	0.0067	**0.0065**	0.0067	0.0109	0.0088
	diatoms	0.0077	**0.0063**	0.0077	0.0089	0.0117
	enron	0.1382	**0.1325**	0.1400	0.1734	0.1477
	expr_FUN	0.1279	**0.1273**	0.1416	0.1794	0.2870
	imclef07a	0.0395	**0.0366**	0.0397	0.0388	0.0511
	interpro_ara_FUN	0.0667	**0.0655**	0.0671	0.0956	0.1210
	reuters	0.2382	**0.1646**	0.2436	0.1799	0.5233
	seq_FUN	0.1251	**0.1242**	0.1482	0.1735	0.2717
	struc_ara_GO	0.0050	**0.0045**	0.0050	0.0063	0.0061
	wipo	0.1092	**0.0838**	0.1105	0.1050	0.2385
HMC-loss	cellcycle_GO	0.0108	**0.0083**	0.0114	0.0105	0.0112
	diatoms	0.0105	**0.0062**	0.0166	0.0119	0.0124
	enron	0.2087	**0.1738**	0.2093	0.1935	0.2112
	expr_FUN	0.2719	**0.2436**	0.2916	0.2680	0.2740
	imclef07a	0.0600	**0.0440**	0.0779	0.0636	0.0610
	interpro_ara_FUN	0.1276	**0.0991**	0.1312	0.1188	0.1304
	reuters	0.3697	**0.2217**	0.4015	0.2366	0.4412
	seq_FUN	0.2593	**0.2306**	0.2796	0.2589	0.2642
	struc_ara_GO	0.0065	**0.0042**	0.0082	0.0062	0.0072
	wipo	0.2409	**0.1336**	0.2451	0.1683	0.2689
micro-averaged F_1	cellcycle_GO	0.4709	**0.4906**	0.4113	0.3516	0.4615
	diatoms	0.5895	**0.6782**	0.5430	0.6018	0.5784
	enron	0.7006	**0.7198**	0.6893	0.6423	0.6971
	expr_FUN	0.2975	**0.3104**	0.1440	0.2088	0.2913
	imclef07a	0.8110	**0.8254**	0.7957	0.8074	0.8085
	interpro_ara_FUN	0.3560	**0.3746**	0.2486	0.3193	0.3427
	reuters	0.3756	**0.4232**	0.1938	0.3982	0.3727
	seq_FUN	0.2983	**0.3122**	0.1797	0.2190	0.2897
	struc_ara_GO	0.6374	**0.6781**	0.6225	0.6211	0.6322
	wipo	0.5526	**0.6060**	0.5165	0.5831	0.5435

Table 4: Results at the test set

.

Measure	Dataset	Error measure STS	Error measure MTS	Class distribution STS	Class distribution MTS	Label cardinality STS
Normalised H-loss	cellcycle_GO	**0.0071**	0.0366	**0.0071**	0.0112	0.0088
	diatoms	**0.0082**	0.0087	**0.0082**	0.0101	0.0119
	enron	0.1980	0.1991	**0.1929**	0.2856	0.1955
	expr_FUN	**0.1325**	0.1328	0.1418	0.1755	0.2799
	imclef07a	0.0423	**0.0397**	0.0420	0.0420	0.0552
	interpro_ara_FUN	**0.0650**	0.0667	0.0653	0.1060	0.1039
	reuters	0.2382	**0.1830**	0.2324	0.1952	0.5189
	seq_FUN	**0.1274**	0.1316	0.1505	0.1806	0.2665
	struc_ara_GO	**0.0049**	0.0067	**0.0049**	0.0062	0.0058
	wipo	0.1166	**0.0811**	0.1186	0.0995	0.2324
HMC-loss	cellcycle_GO	0.0113	**0.0099**	0.0120	0.0110	0.0118
	diatoms	0.0098	**0.0086**	0.0162	0.0114	0.0117
	enron	0.2761	0.2550	0.2767	**0.2538**	0.2870
	expr_FUN	0.2773	**0.2597**	0.2975	0.2733	0.2780
	imclef07a	0.0656	**0.0477**	0.0821	0.0704	0.0666
	interpro_ara_FUN	0.1272	**0.1080**	0.1333	0.1174	0.1268
	reuters	0.3420	0.2346	0.3911	**0.2246**	0.4448
	seq_FUN	0.2705	**0.2537**	0.2875	0.2704	0.2703
	struc_ara_GO	0.0062	**0.0045**	0.0080	0.0058	0.0068
	wipo	0.2362	**0.1405**	0.2319	0.1526	0.2627
micro-averaged F_1	cellcycle_GO	**0.4744**	0.4621	0.4070	0.3569	0.4740
	diatoms	**0.5856**	0.5789	0.5228	0.5679	0.5731
	enron	0.6574	0.6511	0.6256	0.5494	**0.6643**
	expr_FUN	**0.3156**	0.3119	0.1532	0.2163	0.3088
	imclef07a	0.7955	**0.8080**	0.7887	0.7943	0.7960
	interpro_ara_FUN	0.3601	**0.3662**	0.2770	0.3177	0.3573
	reuters	0.3777	**0.4139**	0.1864	0.3950	0.3734
	seq_FUN	**0.3070**	0.3061	0.1903	0.2221	0.3018
	struc_ara_GO	**0.6566**	0.5959	0.6357	0.6366	0.6521
	wipo	0.5378	**0.5989**	0.5043	0.5958	0.5191

Table 5: Wilcoxon tests: MTS vs. STS for each strategy. The obtained p-values are presented.

	Error measure		Class distribution	
MTS vs STS	Validation	Test	Validation	Test
Normalised H-loss	**0.0020**	>= 0.2	>= 0.2	>= 0.2
HMC-loss	**0.0020**	**0.0020**	**0.0020**	**0.0020**
micro-averaged F_1	**0.0020**	>= 0.2	0.1055	0.1934

Table 6: Run time spent by the different optimisation techniques (in seconds).

	Normalised H-loss		HMC-loss		micro-averaged F_1		CD		LC
Dataset	STS	MTS	STS	MTS	STS	MTS	STS	MTS	STS
cellcycle_GO	18413.4500	90945.4850	21105.3310	10.0470	65620.1360	15.8070	17274.2500	**0.4670**	12712.0640
diatoms	2.0410	26.0260	1.8660	0.1990	5.0070	0.5170	1.5510	**0.0550**	0.9910
enron	2.2040	1.5810	6.1030	0.1290	2.6640	0.5080	1.6030	**0.0160**	1.3950
expr_FUN	1028.9220	172.0720	19802.5300	0.2500	1443.8400	124.0440	817.0490	**0.0690**	699.4520
imclef07a	9.7390	64.2910	8.0860	1.4930	15.0000	4.3880	5.9010	**0.0560**	3.0510
interpro_ara_FUN	85.5010	21.4660	1310.2190	0.1640	149.3200	14.0550	66.8650	**0.0460**	47.3820
reuters	78.7760	4.6170	489.3710	0.0760	126.1640	26.0440	61.7710	**0.0270**	36.8200
seq_FUN	15.9250	105.2940	102.2760	0.2000	30.3710	5.1530	14.2220	**0.0590**	9.2590
struc_ara_GO	432.4320	3466.8010	515.4660	3.2180	2309.8120	4.8010	621.4390	**0.0980**	277.2230
wipo	66.5090	3.3330	586.1680	0.2840	83.0170	15.6270	45.8270	**0.0390**	35.6880

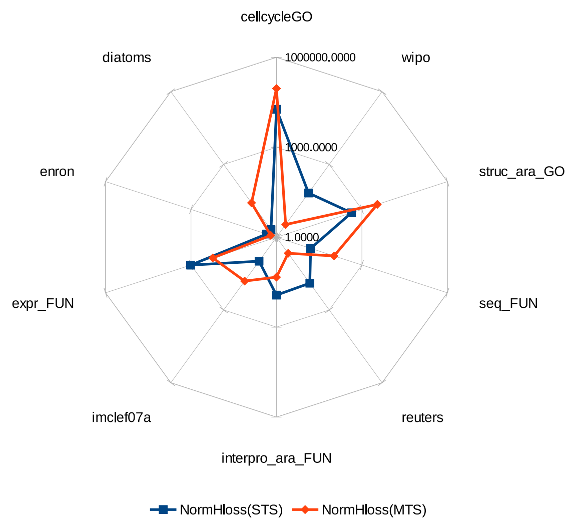
the test set. This fact shows that the generalisation capabilities of the MTS with F-measure and normalised H-loss are rather limited. Nevertheless, for the HMC-loss we can state that the MTS approach is the most suitable approach.

- When the CD optimisation is considered, no significant differences are found between the methods in both validation and test phase, except for the HMC-loss, in which the MTS class distribution optimisation has provided statistically better results.

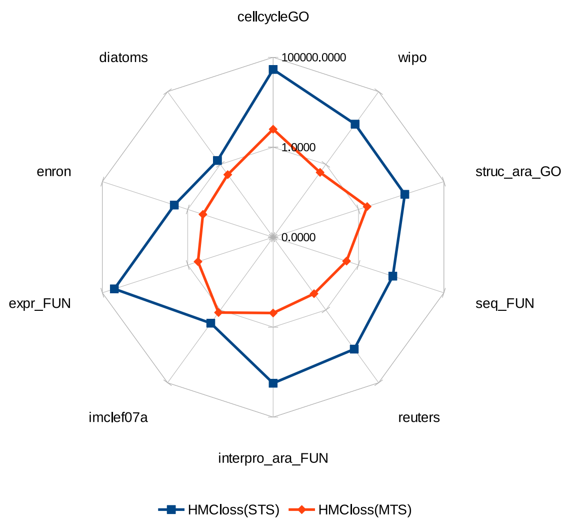
To compare both STS and MTS in terms of efficiency, Figure 2 depicts star plots representing the average run time obtained in each dataset for the four STS vs. MTS comparisons considered (note that ClassDistribution is only run once). This star plot presents the run time as the distance from the center; thus, a lower area determines the most efficient methods. For sake of clarity, logarithm scale has been used to counter the skewness between the run times in the different datasets. Table 6 collects the complete list of run time values in seconds. The fastest technique for each dataset is highlighted in bold-face.

In 3 out of the 4 plots, we can observe that STS requires more time to compute a single threshold than MTS to compute often hundreds of thresholds. To fully understand these results, several points must be clarified:

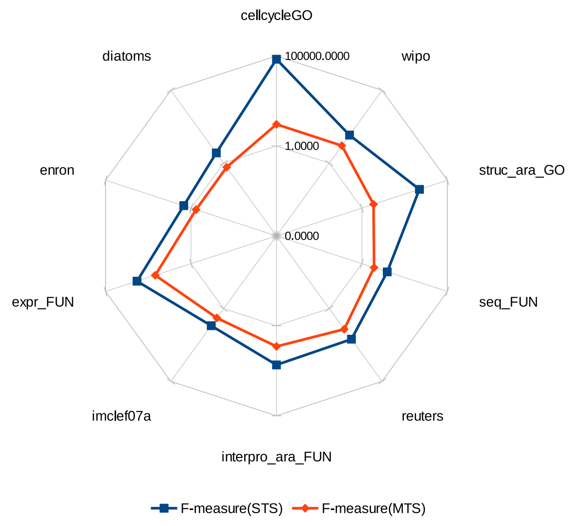
- STS approaches have obtained an optimal threshold for the validation set, while MTS approaches have not been designed to be optimal, but efficient and effective. Therefore, despite the linear complexity of STS



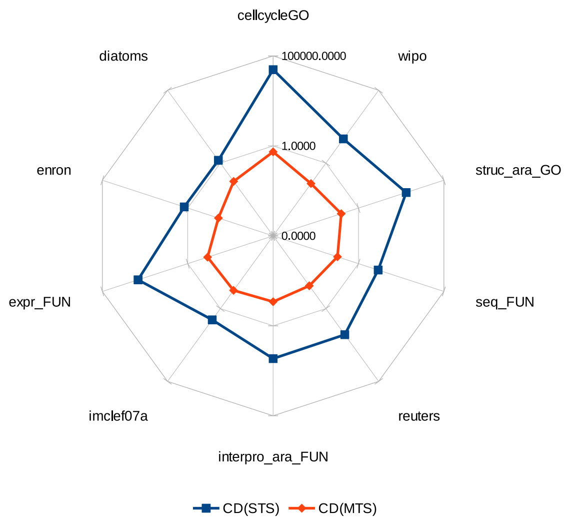
(a) Normalised H-loss comparison



(b) HMC-loss comparison



(c) micro-averaged F_1 comparison



(d) ClassDistribution comparison

Figure 2: Run time comparison between STS and MTS approaches

approaches, they must analyse all the possible thresholds $N_v \times k$, independently of the relation between classes.

- MTS approaches have the advantage that they can prune many of the cut points, due to the followed top-down approach and the hierarchy constraint checks.

- Nevertheless, as stated before, the complexity of the STS approach could be further reduced by using a sub-optimal approach. Figure 3 presents a comparison of the run time required between a non-optimal STS approach, the optimal STS and the proposed MTS model. This figure considers the EM optimisation of the micro-averaged F_1 measure as an example. We can see that such kind of sub-optimal approach (fixing 100 thresholds) provides a reduced run time. However, the micro-averaged F_1 obtained by the sub-optimal STS is always less than the optimal approach, and a statistical comparison with Wilcoxon test results in a p-value=0.0039.

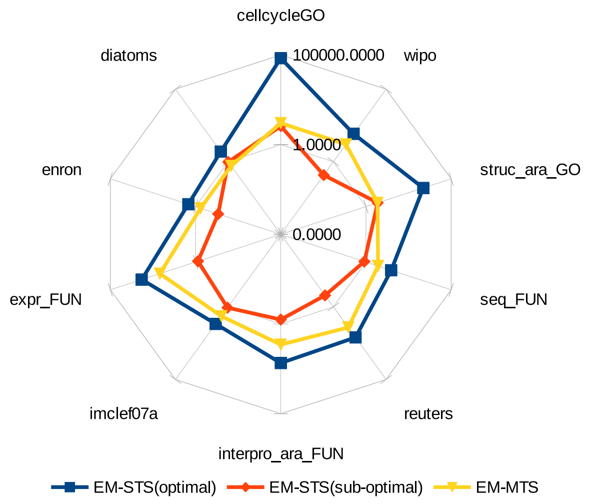


Figure 3: micro-averaged F_1 run time comparison for STS sub-optimal approach. Log scale is utilised.

4.2.2. Global analysis

This subsection is devoted to perform a global analysis of all the proposed approaches. Table 7 presents the results of the Friedman test for each

Table 7: Average Friedman Rankings sorted from the best to the worst

	Validation set		Test set	
Normalised H-loss	EM(MTS)	1.0000	EM(STS)	2.1500
	EM(STS)	2.4500	CD(STS)	2.3000
	CD(STS)	3.1500	EM(MTS)	2.7000
	CD(MTS)	3.7000	CD(MTS)	3.6500
	LC(STS)	4.7000	LC(STS)	4.2000
HMC-loss	EM(MTS)	1.0000	EM(MTS)	1.2000
	CD(MTS)	2.3000	CD(MTS)	2.2000
	EM(STS)	2.8000	EM(STS)	3.1000
	LC(STS)	4.2000	LC(STS)	3.9000
	CD(STS)	4.7000	CD(STS)	4.6000
micro-averaged F_1	EM(MTS)	1.0000	EM(STS)	1.8000
	EM(STS)	2.3000	EM(MTS)	2.1000
	LC(STS)	3.3000	LC(STS)	2.7000
	CD(MTS)	3.7000	CD(MTS)	3.7000
	CD(STS)	4.7000	CD(STS)	4.7000

performance measure. In this table, algorithms are ordered from the best (lowest) to the worst (highest) ranking.

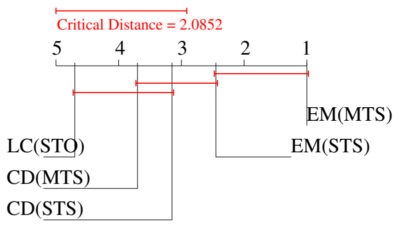
The Friedman test has detected statistically significant differences between the performance of all the labelling schemes. Thus, the Nemenyi post hoc test is applied to characterise the significant differences. Figure 4 plots the corresponding average ranks diagrams.

Finally, Figure 5 establishes a global comparison in terms of run time with all the considered methods.

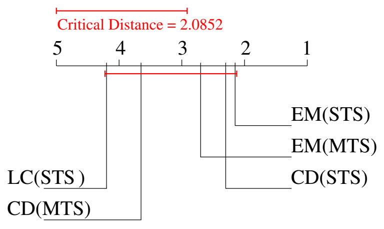
From these figures and Table 7, we can conclude that:

- For normalised H-loss, EM techniques together with CD(STS) rank in the first positions. The difference between EM techniques and the rest of alternatives is more accentuated in the validation phase than in the test phase. It may indicate that, for the considered datasets, EM techniques have suffered from overfitting.

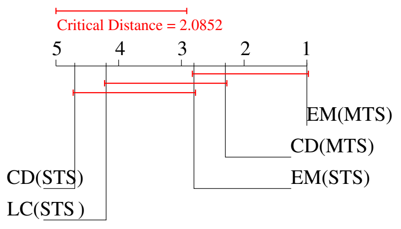
- In the case of the HMC-loss, EM(MTS) is ranked in the first position in both validation and test sets. Thus, no overfitting seems to occur for this measure. It is also noteworthy that the CD(MTS) has ranked second in this study, without statistically significant differences with the first one. As we can observe in Table 6 and Figure 5, it corresponds to the fastest technique we have defined.



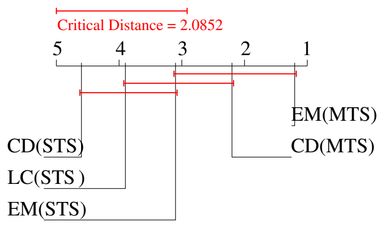
(a) Normalised H-loss validation



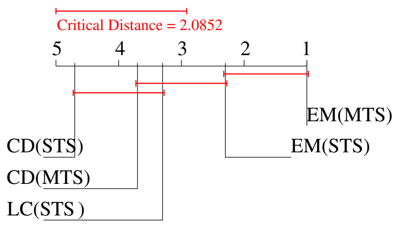
(b) Normalised H-loss test



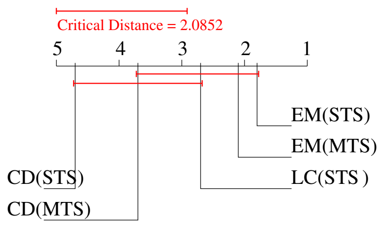
(c) HMC-loss validation



(d) HMC-loss test



(e) micro-averaged F_1 validation



(f) micro-averaged F_1 test

Figure 4: Average ranks diagrams for the different performance measures in validation and test sets. Better algorithms are located on the right side of the plot (rank closer to 1). Those that differ by less than the critical distance computed for a p-value=0.05 are linked by a red line.

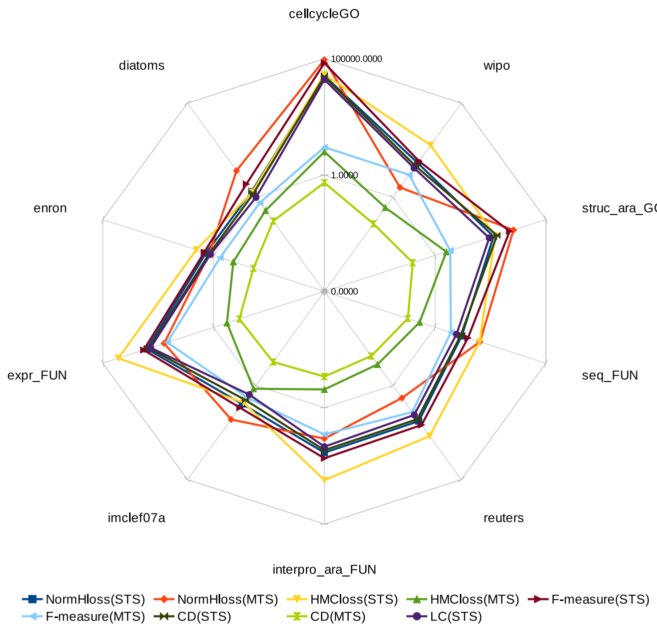


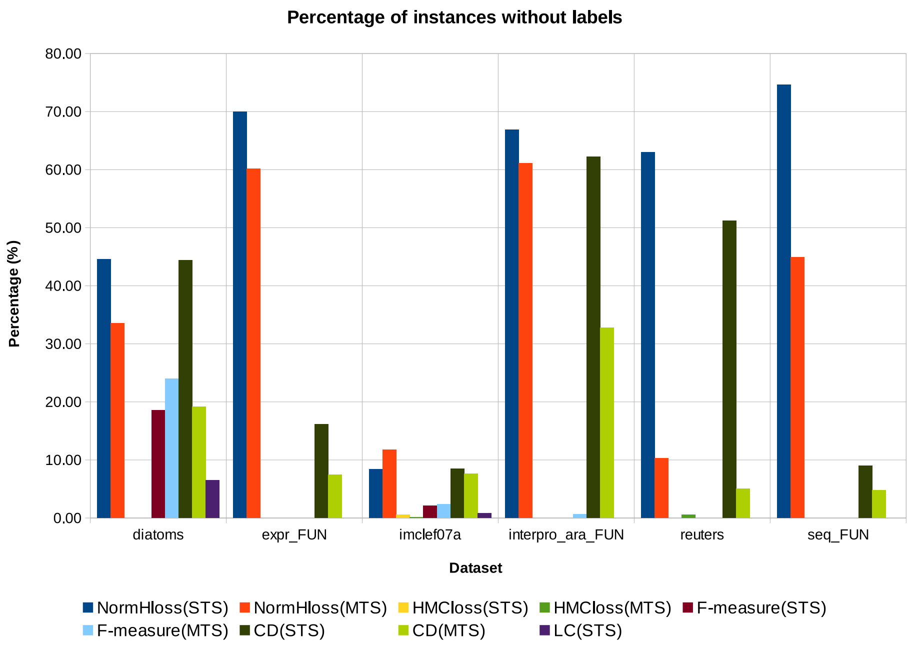
Figure 5: Global run time comparison. Note that log scale has been used.

- In terms of the micro-averaged F-measure, the EM optimisation is the best alternative. However, there is no significant difference between STS or MTS approaches. Thus, the choice of using one or another may rely on the run time needed to obtain the threshold/s. In this way, the MTS approach would be preferred over STS.

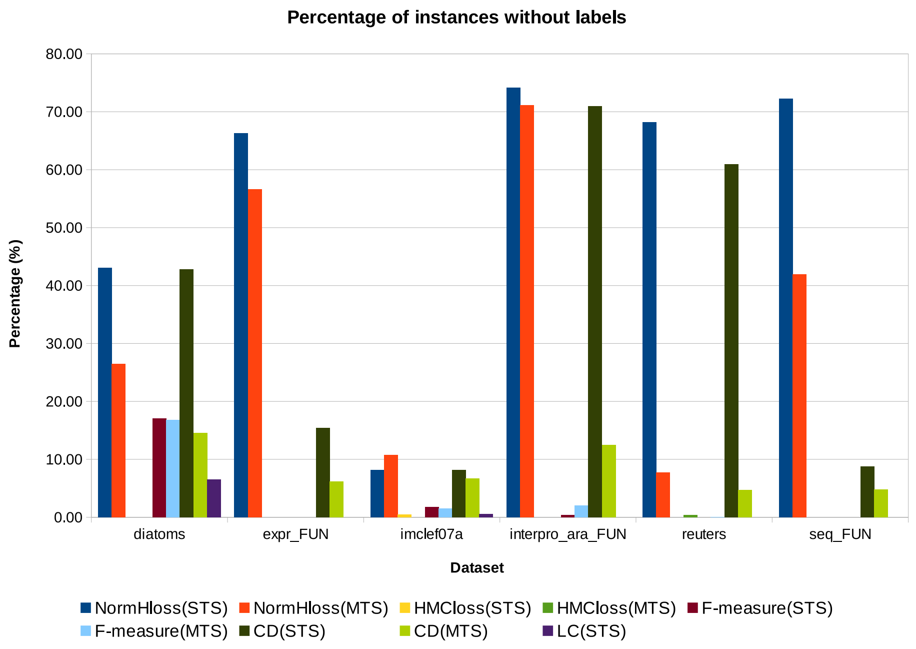
- In general, EM techniques (either STS or MTS) always rank first in all the performed experiments. The LC alternative does not seem to provide very accurate thresholds for any of the measures. However, the CD schemes provide a nice trade-off between performance and required run time in most of the cases, especially the MTS version.

When establishing threshold values to determine the final labelling, there is a risk of leaving instances without any labels. This occurs when the probabilities of belonging to any class are lower than the computed threshold/s. Next, we analyse to what extent this issue is present in the selected datasets and the different threshold selection models.

Figure 6 plots the percentage of instances that have not been labelled according to the threshold/s established by the different techniques in both



(a) Percentage of unlabeled instances in the validation set



(b) Percentage of unlabeled instances in the test set

Figure 6: Percentage of examples that have not been labeled according to the established threshold/s

validation (Fig. 6a) and test (Fig. 6b) set. The datasets not reported in the figure did not experience the issue of unlabeled instances after applying the threshold/s.

According to these figures, we can make the following observations:

- The optimisation of the normalised H-loss has resulted in very high percentages of non-labelled instances in most of the data sets. This result is particularly surprising at the validation set. Note that the resulting normalised H-loss is computed as the average of all the losses in the validation set. Thus, it means that according to this measure, it is often better to provide many non-classified examples to achieve a lower total loss in the whole set.

  We can explain this as follows. Remember that for uniform H-loss, making zero predictions results in the second best H-loss value for the instances with target labels that all belong to a single level1 class (see Section 2.1). For normalised H-loss, it is not the second best value, as long as we do not predict more than the correct class at the first level. Referring back to Fig. 1, where the correct label belongs to B's subtree, it is easy to see that correctly predicting B, and not C and D at the first level, results in a normalised H-loss $\leq 1/3$. Including also C or D results in a H-loss $\geq 1/3$. Making zero predictions yields a H-loss $= 1/3$. Thus, for difficult classification tasks, where classes at the first level are already hard to separate, the optimal result may come from a high threshold that leaves many instances without prediction.

- On the contrary, the HMC-loss and the micro-averaged F-measure report very low percentages of non-labelled instances for most of the datasets. In contrast to the normalised H-loss, these measures add losses from all classes, what prevents them to incur in this issue.

- For the CD optimisation, we can observe that this issue is also present in some datasets, especially for the STS approach. In many datasets, the CD of many classes (bottom classes) may be close to 0. Higher thresholds may result in higher number of 0's in the CD' vector. As this approach gives the same importance to every class, high thresholds may result in lower Euclidean distances.

The issue discussed above also reflects the intrinsic complexity of HMC problems, in which a high number of instances are very difficult to be classified properly.

5. Conclusions and further work

In this work we have proposed and investigated several alternatives to perform the final labelling for hierarchical multi-label classification (HMC). These alternatives consist of selecting single or multiple thresholds that transform the real valued prediction scores provided by a HMC classifier into actual classes. To determine the threshold/s, two main approaches have been proposed: optimisation of a given error measure of interest or simulating some training set properties in the test set predictions. We have focused on three well-known measures to evaluate the labelling performed: H-loss, HMC-loss and micro-averaged F-measure. Training set properties were reflected by using thresholds yielding a similar class distribution or label cardinality. An experimental comparison on 10 HMC dataset has resulted in the following conclusions:

- Optimizing H-loss has a tendency to favour empty predictions. Especially the uniform H-loss suffers from this, but also the normalised variant resulted in empty predictions for more than 60 percent of the test instances in four datasets.

- In the optimisation of the HMC-loss, selecting multiple thresholds is significantly better than a single threshold. In addition, the multiple threshold scheme is also faster than the optimal single threshold version.

- When the micro-averaged F-measure is considered, both single and multiple threshold selection methods perform similarly. However, the multiple threshold approach again requires a smaller computation cost.

- When evaluated using HMC-loss, selecting multiple thresholds by imitating the class distribution has become a competitive alternative, especially when the run time matters.

We conclude that, although selecting different thresholds per class has not been considered before in HMC, it provides a valid alternative, often resulting in better label sets than the single-threshold variant, and always resulting in smaller computation time, because of the hierarchy constraint.

As future work we plan the application of these strategies to perform the labelling of HMC predictions within a self-training semi-supervised learning context [40]. Another direction for future work is to compute macro- and micro-averaged precision-recall curves for HMC in the multiple-threshold setting.

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