KFHE-HOMER: Kalman Filter-based Heuristic Ensemble of HOMER for Multi-Label Classification

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Abstract. Multi-label classification allows a datapoint to be labelled with more than one class at the same time. Ensemble methods generally perform much better than single classifiers. Except bagging style ensembles like ECC, RAkEL, in multi-label classification, other ensemble methods have not been explored much. KFHE (Kalman Filter-based Heuristic Ensemble), is a recent ensemble method which uses the Kalman filter to combine several models. KFHE views the final ensemble to be learned as a state to be estimated which it estimates using multiple noisy "measurements". These "measurements" are essentially component classifiers trained under different settings. This work extends KFHE to multi-label domain by proposing KFHE-HOMER which enhances the performance of HOMER using the KFHE framework. KFHE-HOMER sequentially trains multiple HOMER classifiers using weighted training datapoints and random hyperparameters. These models are considered as measurements and their related error as the uncertainty of the measurements. Then the Kalman filter framework is used to combine these measurements to get a more accurate estimate. The method was tested on 10 multi-label datasets and compared with other multi-label classification algorithms. Results show that KFHE-HOMER performs consistently better than similar multi-label ensemble methods.

1 Introduction

In multi-label classification problems a datapoint can be assigned to more than one class, or label, simultaneously [9]. For example, an image can be classified as containing multiple different objects, or a document can be labelled with more than one topic. In multi-class classification problems, objects can only belong to a single class, which makes multi-label classification a more general classification approach. Multi-label classification algorithms either break the multi-label
problem down into smaller multi-class classification problems—for example *ensemble classifier chains* [16] known as *problem transformation* methods—or modify multi-class algorithms to directly train on multi-label datasets—for example BPMLL [25] known as *algorithm adaptation* methods.

Ensemble classification methods train multiple component classifiers and aggregate them. Generally, ensemble methods perform better than the single component classifiers [10]. In multi-label classification literature, several methods are proposed which combine multiple multi-label models to form an ensemble.

Ensemble classifier chains (ECC) [16] trains a classifier chain (CC) [16] model at each iteration with a subset of the training dataset and a random chain order of the labels and then combines the results. Random k-Label sets (RAkEL) [21] first partitions the labels into random overlapping subsets, and for each subset trains a label powerset classifier [1] and aggregates the results. Ensemble of binary relevance (EBR) [16] simply bags multiple binary relevance models [1]. Ensemble of pruned set (EPS) [15] is a bagged version of pruned set method, which is similar to label powerset, but removes the infrequently occurring labelsets (unique combination of labels) and focuses on the more important label relationships. AdaBoost.M1 [15] uses boosting in multi-label context. Hierarchy of multi-label classifiers (HOMER) [22] partitions the dataset hierarchically in a tree format, where each node in the hierarchy only predicts if a datapoint has at least one relevant of a group. Then it further splits the group of labels into smaller groups to form child nodes. The prediction task starts from the root, and at any given internal node $v$, the datapoint is passed down to a child based on the prediction of the model at $v$. The final label predictions are done at the leaves.

Although, except AdaBoost.M1 most of these methods essentially combines multiple multi-label classification methods using simple bagging. AdaBoost.M1 performs boosting, but the performance was previously found to be poor [12].

Kalman filter-based Heuristic Ensemble (KFHE) [14] is a multi-class ensemble algorithm which takes a new approach. Unlike the existing boosting or bagging methods, KFHE imagines the ensemble to be trained as a hypothesis to be estimated in the hypothesis space. Then it takes noisy measurements in the hypothesis space, which is essentially trained classifiers, which it then combines using a Kalman filter. In effect, KFHE behaves like a combination of boosting and bagging.

As ensembles generally outperforms the individual classifiers and the multi-label literature lacks non-bagging style ensemble classifiers, this leaves an opportunity to improve a multi-label classification using the KFHE framework. The main contributions of this work are:

- To propose a multi-label ensemble classification method, KFHE-HOMER, which combines multiple HOMER classifier models using the KFHE framework.
- Extensive experiment demonstrating the effectiveness of KFHE-HOMER.
- Introduction of E-HOMER, a simple bagged ensemble version of HOMER.
The remainder of the paper is structured as follows. Section 2 presents the relevant aspects of HOMER and KFHE. Section 3 introduces the proposed method KFHE-HOMER and E-HOMER. The experimental setup is described in Section 4 and the results are discussed in detail in Section 5. Finally, Section 6 discusses future works and concludes the paper.

2 Related Work

In this section, first the HOMER method will be discussed, followed by a basic introduction of Kalman filter required to describe KFHE. Next the KFHE method will be briefly explained.

2.1 HOMER

Hierarchy of multi-label classifiers (HOMER) [22] is a problem transformation method which divides the multi-label dataset into smaller subsets, but hierarchically. This method divides the dataset based on the labels, but establishes a hierarchical relationship between the partitions.

It starts with the entire dataset $D(x_i, l_i)\forall 1 \leq i \leq n$ at the root node of the hierarchy which has all the labels $L = \{\lambda_1, \ldots, \lambda_q\}$. Here $x_i$ is the datapoint, $l_i = [l_{i1}, \ldots, l_{iq}]$ is the vector or labels assigned to the corresponding datapoint. If a label $\lambda_q$ is applicable to $x_i$ then $l_{iq} = 1$, otherwise $l_{iq} = 0$.

Every leaf node has one associated label $\lambda_l$. Any internal node $v$ have only a subset of labels $L_v \subset L$ associated with itself, which is a union of the label subsets associated to its children. Therefore, $L_v = \cup_{c \in children(v)} L_c$, where $children(v)$ indicates the children of the node $v$ in the hierarchy. Each node only keeps the datapoints which have at least one of the associated labels of the node applicable to them. Therefore, the dataset in node $v$ is $D_v = \{(x_j, l_j) | \forall (x_j, l_j) \in parent(v), \exists \lambda_q \in L_v \wedge l_{jq} = 1\}$.

In each internal node $v$, the original labels of the datapoints are not stored, instead a meta-labels are generated and stored. At node $v$ if the labels are partitioned into $k$ partitions, then $k$ meta-labels are created, where the meta label $\mu_i$ represents the union of the labels in the $i$th partition. A datapoint is labelled with $\mu_i$ if the datapoint is associated to any of the labels in the $i$th partition. The meta labels are generated as $D'_v = \{(x_j, l'_j) | \forall (x_j, l_j) \in parent(v), \exists \lambda_q \in L_v \wedge l_{jq} = 1\}$.

The root node and all the internal nodes $v$ will have a trained model $h_v$ associated to it, which is trained using the dataset $D'_v$ with the target being the meta labels associated with each datapoint in the child nodes. The utility of the meta labels is to indicate which branch or branches in the hierarchy has to be followed to the root for the prediction of the labels. A new datapoint $d$ starts from the root of the hierarchy travels one or more paths from root to leaf. All the labels represented by the leaves which are encountered by the datapoint $d$ are taken as the prediction.

The partition of the labels at each level of the hierarchy is done in such a way that the similar labels stay together, this is to decrease the number of
paths traveled from root to leaf. To keep the similar labels together, at each level a clustering algorithm on the label assignments of $D_v$ is performed on each node to partition the label subset $L_v$ into $k$ disjoint label subsets for the node $v$’s children. A variation of k-Means algorithm, named the balanced $k$-Means is proposed, which attempts to balance the cluster sizes.

### 2.2 Static State Estimation using Kalman filter

The discrete Kalman filter is a mathematical framework to estimate an unobservable state of a linear stochastic discrete time controlled process through noisy measurements \([6]\). In this section a very brief and intuitive overview of the Kalman filter to estimate a static one dimensional state will be given.

Let there be a state, $y$, of a linear stochastic system has to be estimated, where $y$ cannot be observed directly. The state of the system can be estimated in two ways. Firstly, given an estimate of the state $\hat{y}_{t-1}$ at time step $(t-1)$, a linear model is used to make an a priori state estimate $\hat{y}_{t-1}^-$. The variance related to $\hat{y}_{t-1}^-$ is also updated to $p_{t-1}^-$. This variance can be imagined as the uncertainty of state. This is known as the time update step. Secondly, an external sensor can be used to get an estimate through a measurement, $z_t$, of the state with a related variance $r_t$, which can also be seen as the uncertainty of the measurement.

Given these two noisy state estimates, the a priori estimate, $\hat{y}_{t-1}^-$, its related variance $p_{t-1}^-$, and the measurement $z_t$, its related variance $r_t$, the Kalman filter combines them optimally to get an a posteriori state estimate, $\hat{y}_t$, which potentially has a lower uncertainty than the previous two. This is known as the measurement update step. The Kalman filter iterates through the time update and the measurement update steps. At iteration $t$, the a priori estimate is used in the measurement update step to get an a posteriori estimate, which is fed back to the time update in the next iteration as the a priori estimate.

If the state to be estimated is assumed to be static then the time update step is considered to be non-existent, hence it becomes $\hat{y}_t^- = \hat{y}_{t-1}$ and $p_t^- = p_{t-1}^-$. This kind of scenario can occur in cases when, say, the voltage level of a DC battery or the altitude of a cruising aircraft is being estimated. In both of the cases, the DC voltage and the altitude of the aircraft is supposed to be constant, but unknown. In such cases, the measurement of the static state from a noisy sensor is repeatedly combined using the measurement update step. After considering $\hat{y}_t^- = \hat{y}_{t-1}$ and $p_t^- = p_{t-1}^-$ the measurement update steps are as follows

$$\hat{y}_t = \hat{y}_{t-1} + k_t(z_t - \hat{y}_{t-1})$$  \hspace{1cm} (1)

$$k_t = p_{t-1}^-/(p_{t-1}^- + r_t)$$  \hspace{1cm} (2)

$$p_t = (1 - k_t)p_{t-1}^-$$  \hspace{1cm} (3)
Here \( z_t \), the measurement, can be an external source or sensor (voltage or altitude sensor), \( r_t \) is the related measurement variance indicating the uncertainty of the estimate. The \( k_t \) is the \textit{Kalman gain}, which optimally combines the \textit{a priori} estimate and the measurement. A complete and detailed explanation of Kalman filters can be found in [6,23].

2.3 KFHE

Kalman filter-based heuristic ensemble (KFHE) [14] is a multi-class ensemble algorithm proposed by Pakrashi and Mac Namee, which takes a different approach by viewing the ideal hypothesis for a specific classification problem as the static state to be estimated in the hypothesis space [5].

A classifier training task can be seen as searching for a hypothesis for a given problem in the hypothesis space, where a training algorithm navigates through the hypothesis space toward the ideal hypothesis\(^1\) For a specific learning problem the target of a learning algorithm is to learn the ideal hypothesis, which can be assumed to be stationary within the hypothesis space. In KFHE, estimation of this stationary hypothesis is modelled as a static state estimation problem and is then estimated by multiple noisy measurements as explained above.

Two Kalman filters interact with each other in KFHE. The Kalman filter which estimates the ideal hypothesis is called the model Kalman filter, abbreviated as kf-m. The kf-m estimates the final model or hypothesis by combining multiple noisy measurements. The measurement in this case is defined as

\[
z^{(y)}_t = (h_t(D) + \hat{y}_{t-1})/2
\]

Where \( h_t = \mathcal{H}(D, \hat{w}_{t-1}) \) is a classifier model trained using algorithm \( \mathcal{H} \) (decision tree, SVM, etc.) trained using different weights updated in the previous iteration, \( \hat{w}_{t-1} \), assigned to different datapoints. A datapoint is weighted more if it was misclassified previously. Although, unlike AdaBoost [8], the weight for

\(^1\) In this text hypothesis and classifier model are used interchangeably.
Table 1: Intermediate representation of a state for KFHE and KFHE-HOMER. A trained model is represented using the prediction scores of a given set of datapoints. This representation is used with \( \hat{y}_t, z_t \) and \( h_t(D) \).

| \( x \) | \( c_1 \) | \( c_2 \) | \( c_3 \) |
|---|---|---|---|
| \( x_1 \) | 0.10 | 0.89 | 0.01 |
| \( x_2 \) | 0.08 | 0.27 | 0.65 |
| ... | ... | ... | ... |
| \( x_n \) | 0.77 | 0.20 | 0.03 |

The datapoints are determined by the weight Kalman filter or kf-w. The intuition of averaging the \( h_t \) and \( \hat{y}_t \) is to estimate the impact \( h_t \) will be induced on \( y_t \). Although, other measurement heuristics can be used, Eq. (4) will be used in this work.

Note that, the ensemble model \( h_t \) cannot directly be used with the equations in Section 2.2, therefore an intermediate proxy representation is used for the states in kf-m. The intermediate representation of a trained model is the label-wise prediction scores of a given dataset by the model of the corresponding state, as shown in. Therefore, the intermediate representation of a model (individual or ensemble) would be the prediction \( \hat{y}_t \) as shown in Figure 1. All arithmetic operations on this representation are done element wise, as it represents one single state as in Section 2.2. This representation is used for \( \hat{y}_t \) and \( z_t \). In the final estimated state the class assignment is done by taking the class with the highest score.

The kf-w estimates \( \hat{w}_t \), which is a vector of weights to be used by the measurement step of kf-m. kf-w is identical to kf-m, but it estimates the weights. The measurement for the kf-w, \( z_t^{(w)} \) is a function \( f \) of weighted per datapoint error:

\[
z_t^{(w)} = [z_{ti}^{(w)} | z_{ti}^{(w)} = \hat{w}_{ti} \times f(\text{class}(c_i) \neq \text{class}(z_{ti}^{(y)})) \] \quad 1 \leq i \leq n \tag{5}
\]

Here, class indicates the class assignment of the prediction and \( c_i \) indicates the class assigned to the datapoint \( x_i \). There are two variants discussed in [14] where \( f \) can be either the exponential function or the linear function in Eq. (5). The use of exponential function is similar to AdaBoost, but the final combination in \( \hat{w}_t \) is done using the kf-w filter in the measurement update step using equation similar to Eq. (1).

The related noise is set same as the measurement noise taken in kf-m, which makes an assumption that weight measurement will induce an error no more than what the kf-m had in the previous iteration.

The training step stores the component classifiers \( h_t \) and the Kalman gains \( k_t^{(y)} \). When a new datapoint is encountered during the prediction step the equation Eq. (1) is repeatedly used using the component classifiers \( h_t \) and the Kalman gains \( k_t^{(y)} \) found during the training stage.
The setting of the measurements and the related errors are the heuristic components of the method, which are set by making assumptions.

An overall interaction of the $kf-m$ and $kf-w$ is shown in Figure 1. The superscript $(y)$ indicates that the variables are related to $kf-m$, and the superscript $(w)$ indicates these variables are related to $kf-w$. $\hat{y}$ is the state estimate by $kf-m$, and $\hat{w}_t$ is estimated by $kf-w$.

The detailed derivation and explanation of KFHE can be found in [14].

3 KFHE-HOMER

In this work, KFHE-HOMER extends KFHE to multi-label domain by combining multiple HOMER models. Also, a bagged ensemble version of HOMER, named E-HOMER, is introduced. HOMER is a method which has competitive performance [11,13] also with relatively faster training times.

As explained in Section 2.2, there are two components of KFHE, the $kf-m$ which estimates the hypothesis, and the $kf-w$, which computes the weights of the training datapoints during each measurement. To make KFHE work in a multi-label setting, the measurements of the $kf-m$ and $kf-w$ steps were adapted in this work.

For KFHE-HOMER, the measurement at each step is considered as the average of a trained HOMER classifier and the previous estimate of the ensemble as shown in Eq. (4). The related measurement uncertainty $r_t^{(w)}$ is considered as the hamming loss ($\text{hloss}$) [26] of the trained model. Each HOMER model at every step is trained on different weights, $\hat{w}_t$, assigned to different datapoints, where the weights are determined by the $kf-w$ component. The $kf-w$ estimates one single vector of weights $\hat{w}_t$ using which a sampling with replacement of the training dataset is done. The measurement $z_t^{(w)}$ for $kf-w$ is taken as per-datapoint weighted hamming loss can be defined as follows

$$z_t^{(w)} = [z_t^{(w)} | z_t^{(w)} = \hat{w}_{ti} \times \exp(\text{hloss}(x_i, l_i)) \ 1 \leq i \leq n] \quad (6)$$

Eq. (6) is similar to Eq. (5) but uses hamming loss and exponential function to highlight misclassified datapoint in the measurement which will later be used by the measurement update step to get the weights $\hat{w}_t$ to be used in $kf-m$ in the next iteration. In this case the related uncertainty is kept as in KFHE.

The model $h_t$ in this case is a trained HOMER classifier model $\mathcal{H}(D, \hat{w}_{t-1}, C, k, \phi)$. To weight the datapoints for training, the HOMER classifiers are trained using samples using the distribution $\hat{w}_{t-1}$, the last updated weights, here the sample size is twice the size is $2n$, or twice the size of original number of datapoints. Also, while training, the clustering algorithm $C$ used by HOMER is randomly selected from \{random, k-means, balanced k-means\}, the number of cluster $k$ is randomly selected too. Also, the kernel $\phi$ of the underlying SVM used by HOMER, is also selected randomly. Next the measurement is done using Eq. (4). The intuition of averaging is to estimate how much impact $h_t$ will be induced on $\hat{y}_{t-1}$.

Given the different HOMER models trained using different hyperparameters, many of them may lead to a poor measurement. The KFHE framework combines
the measurements based on the measurement errors. If the measurement uncertainty $r_t^{(y)}$ is higher than the uncertainty of the ensemble found up to $t$th iteration $p_t^{(y)}$, then the measurement is weighted less and the Kalman gain is lower than 0.5, and when the measurement error is lower the measurement is incorporated more, as a result of the Kalman gain being greater than 0.5. Therefore, based on this property, the HOMER models which have a poor performance will have a much less impact on the entire ensemble, whereas a more accurate HOMER model will have more impact on the entire ensemble.

A simple bagged version of HOMER, E-HOMER, is also introduced and compared with KFHE-HOMER. In E-HOMER, at each iteration a HOMER classifier is trained on a bootstrap sample of the dataset of size $2n$ along with random HOMER cluster type, random number of clusters and selecting the type of underlying SVM kernel randomly, as done in the case of KFHE-HOMER.

The values of $\hat{y}_0$, $p_0^{(y)}$ and $\hat{w}_0$, $p_0^{(w)}$ has to be initialised. $\hat{y}_0$ is initialised using a single HOMER classifier model $h_0$. The value of $p_0^{(y)}$ is set to 1 indicating maximum uncertainty. Equal weights to every point is given in $\hat{w}_0$ and $p_0^{(w)}$ is also initialised with 1.

The KFHE-HOMER training algorithm is given in Algorithm 1. Here, all the lowercase symbols corresponds to symbols in Eq. (1), (2) and (3). The superscript $(y)$ and $(w)$ indicates that the corresponding variables are related to $kf-m$ and $kf-w$ respectively. In line 5-8 the different hyperparameter of HOMER is selected randomly. Next, the HOMER model is trained in line 9, and the measurement is done in line 10. Line 12 computes the Kalman gain $k_t^{(y)}$ for $kf-m$ and line 13 computes the proxy representation of the ensemble $\hat{y}_t$, which indicates the KFHE-HOMER ensemble predictions on the training dataset. The $kf-w$ steps are similar and are performed from line 16-20. The process runs until a maximum number of ensemble iterations $T$.

The prediction algorithm is same as in KFHE and is shown in Algorithm 2. Here the trained models and the Kalman gain values learned during the training along with the new datapoint is given. Using the models in line 5 the Kalman gain is repeatedly used to combine the measurements in line 4. After $T$ iterations the predicted labels for the new datapoint $d$, the estimate $\hat{y}_T^{(y)}$ is returned. To find the label assignments, these scores are thresholded at 0.5.

4 Experiment

To evaluate the effectiveness of KFHE-HOMER, experiments were performed on ten well-known multi-label benchmark datasets listed in Table 2. In Table 2 the different properties of the multi-label datasets are summarised. *Instances*, *Inputs* and *Labels* are the number of datapoints, the dimension of the datapoints and the number of labels, respectively. *Labelsets* indicates the number of unique combinations of labels. *Cardinality* measures the average number of labels assigned to each datapoint and *MeanIR* [2] indicates the degree of imbalance of the labels, where higher values indicate higher imbalance.
Algorithm 1 KFHE-HOMER training

1: procedure TRAIN($D = \{(x_i, l_i) | 1 \leq i \leq n\}, T$)  
2: \[ p_0^{(w)} = 1, \quad \hat{w}_0 = \frac{1}{n}, \ldots, \frac{1}{n} \]  
3: \[ h_t = \mathcal{H}(D, \hat{w}_0, C, k, \phi), \quad \hat{y}_0 = h_0(D) \]  
4: \[ t = 1 \]  
5: for \( t \leq T \) do  
6: \[ \triangleright \text{ kf-m Section} \]  
7: Randomly select $C$, $k$ and $\phi$  
8: \[ C \in \{\text{k-means, balanced k-means, random}\}, \]  
9: \[ k \in \{2, \ldots, \lceil \sqrt{\|C\|} \rceil\}, \]  
10: \[ \phi \in \{\text{linear, radial}\} \]  
11: \[ h_t = \mathcal{H}(D, \hat{w}_{t-1}, C, k, \phi) \]  
12: \[ z_t^{(y)} = (h_t(D) + \hat{y}_{t-1})/2 \] \( \triangleright \text{ Measurement} \)  
13: \[ r_t^{(y)} = hloss(D, z_t^{(y)}) \]  
14: \[ k_t^{(y)} = p_{t-1}^{(y)}/(p_{t-1}^{(y)} + r_t^{(y)}) \] \( \triangleright \text{ Kalman gain} \)  
15: \[ \hat{y}_t = \hat{y}_{t-1} + k_t^{(y)}(z_t^{(y)} - \hat{y}_{t-1}) \] \( \triangleright \text{ Measurement update} \)  
16: \[ p_t^{(y)} = (1 - k_t^{(y)})p_{t-1}^{(y)} \]  
17: \[ \triangleright \text{ kf-w Section} \]  
18: \[ z_t^{(w)} = [z_t^{(w)} | z_t^{(w)} = \hat{w}_t \times \exp(hloss(x_i, l_i)) \ 1 \leq i \leq n] \]  
19: \[ r_t^{(w)} = r_t^{(m)} \]  
20: \[ k_t^{(w)} = p_{t-1}^{(w)}/(p_{t-1}^{(w)} + r_t^{(w)}) \] \( \triangleright \text{ Kalman gain} \)  
21: \[ \hat{w}_t = \hat{w}_{t-1} + k_t^{(w)}(z_t^{(w)} - \hat{w}_{t-1}) \] \( \triangleright \text{ Measurement update} \)  
22: \[ p_t^{(w)} = (1 - k_t^{(w)})p_{t-1}^{(w)} \]  
23: \[ t = t + 1 \]  
24: end for  
25: return $\{(h_t, k_t^{(y)}) | \forall 1 \leq t \leq T\}$  
26: end procedure

Algorithm 2 KFHE-HOMER prediction

1: procedure PREDICT($d, \{h_t, k_t^{(y)} | \forall 1 \leq t \leq T\}, T$)  
2: \[ \hat{y}_0^{(y)} = h_0(x), \quad t = 1 \]  
3: for \( t \leq T \) do  
4: \[ \triangleright \text{ Measurement} \]  
5: \[ \hat{y}_t^{(y)} = (h_t(d) + \hat{y}_{t-1})/2 \]  
6: \[ \hat{y}_t = \hat{y}_{t-1} + k_t^{(y)}(z_t^{(y)} - \hat{y}_{t-1}) \] \( \triangleright \text{ Measurement update} \)  
7: \[ t = t + 1 \]  
8: return $\hat{y}_T^{(y)}$  
9: end procedure
Table 2: Multi-label datasets

| Dataset | Instances | Inputs | Labels | Labelsets | Cardinality | MeanIR |
|---------|-----------|--------|--------|-----------|-------------|--------|
| flags   | 194       | 26     | 7      | 24        | 3.392       | 2.255  |
| yeast   | 2417      | 103    | 14     | 77        | 4.237       | 7.197  |
| scene   | 2407      | 294    | 6      | 3         | 1.074       | 1.254  |
| emotions| 593       | 72     | 6      | 4         | 1.869       | 1.478  |
| medical | 978       | 1449   | 45     | 33        | 1.245       | 89.501 |
| enron   | 1702      | 1001   | 53     | 573       | 3.378       | 73.953 |
| birds   | 322       | 260    | 20     | 55        | 1.503       | 13.004 |
| genbase | 662       | 1186   | 27     | 10        | 1.252       | 37.315 |
| cal500  | 502       | 68     | 174    | 502       | 26.044      | 20.578 |
| llog    | 1460      | 1004   | 75     | 189       | 1.180       | 39.267 |

The label-based macro-averaged F-Score \[26\] was used to measure the performance of models in these evaluations. This was chosen over Hamming loss, which has been used in several previous studies (e.g. \[3,20,24\]). This is because with the highly imbalanced multi-label datasets used in this study (see the high MeanIR scores for several datasets in Table 2) when Hamming loss is used the majority classes may overwhelm the performance of the minority class. The label-based macro-averaged F-Score is defined as follows

\[
F = \frac{1}{q} \sum_{l=1}^{q} \frac{2 \times \text{Precision}_l \times \text{Recall}_l}{\text{Precision}_l + \text{Recall}_l}
\]

For all evaluations 2 times 5 cross-validation experiments were performed. The iterative stratification method \[19\] was used to generate the folds in the cross validation experiment.

Performance of KFHE-HOMER was compared with ECC, a state-of-the-art ensemble based multi-label classifier, and E-HOMER, a bagging-based ensemble using HOMER as the base model. Also, individual CC model, HOMER-K (using k-means clustering) and HOMER-B (using balanced clustering) models were included to understand how much the ensembles led to improved performance over single base models. The cluster size for HOMER was selected using the best values found in the benchmark experiments in \[13\]. The HOMER and CC models used support vector machines (SVM) as their underlying learner, as they have proved to perform very well \[11,13\]. At each iteration of E-HOMER and KFHE-HOMER the type of HOMER clustering \(C\) was selected randomly from \{balanced k-means, k-means, random\}. The number of clusters \(k\) was selected randomly from the range \(k \in \{2, \ldots, \lceil \sqrt{\|L\|} \rceil \}\). The kernel types \(\phi\) for each of the base SVM models used by the component HOMER models were also selected randomly, from \{linear, radial\}.

For ECC and E-HOMER the bootstrap sample was selected to be twice the size of the training dataset, to keep it consistent with KFHE-HOMER. For ECC, E-HOMER and KFHE-HOMER 100 component classifiers were trained.
Table 3: Experimental results. Values in cells are mean label-based macro-averaged F-Scores from the crossvalidation experiments, and their standard deviations. The rank of each score for a dataset across the algorithms compared is shown in parenthesis. The last row shows the average rank of each algorithms. The "\(\downarrow\)" and "\(\uparrow\)" symbols indicate the significance level at which the performance of an algorithm is shown to be worse than the performance of KFHE-HOMER for a dataset, "\(\downarrow\)" = 0.01, "\(\downarrow\)" = 0.05 and "\(\downarrow\)" = 0.1. The "\(\uparrow\)" symbol indicates that the corresponding method is better than KFHE-HOMER at a significance level of 0.1.

|        | KFHE-HOMER | E-HOMER | ECC     | CC      | HOMER-B   | HOMER-K   |
|--------|------------|---------|---------|---------|-----------|-----------|
| flags  | 0.6862 ± 0.02 (1) | 0.6710 ± 0.05 (2) | 0.6387 ± 0.04 (5) | \(\downarrow\) | 0.5957 ± 0.05 (6) | \(\downarrow\) |
| yeast  | 0.4959 ± 0.01 (1) | 0.4400 ± 0.04 (4) | \(\downarrow\) | 0.4403 ± 0.02 (3) | \(\downarrow\) | \(\downarrow\) |
| scene  | 0.8090 ± 0.02 (1) | 0.7806 ± 0.02 (4) | \(\downarrow\) | 0.7818 ± 0.02 (3) | \(\downarrow\) | \(\downarrow\) |
| emotions | 0.7046 ± 0.03 (1) | 0.6991 ± 0.03 (5) | \(\downarrow\) | 0.6955 ± 0.04 (6) | \(\downarrow\) | \(\downarrow\) |
| medical | 0.6387 ± 0.03 (1) | 0.6374 ± 0.02 (2) | \(\downarrow\) | 0.6114 ± 0.02 (4) | \(\downarrow\) | \(\downarrow\) |
|厨师    | 0.2612 ± 0.02 (1) | 0.2587 ± 0.02 (2) | \(\downarrow\) | 0.2435 ± 0.03 (3) | \(\downarrow\) | \(\downarrow\) |
| birds  | 0.3928 ± 0.03 (1) | 0.3834 ± 0.04 (2) | \(\downarrow\) | 0.3297 ± 0.04 (4) | \(\downarrow\) | \(\downarrow\) |
| geobase | 0.5402 ± 0.03 (1) | 0.5374 ± 0.03 (4) | \(\downarrow\) | 0.5024 ± 0.02 (3) | \(\downarrow\) | \(\downarrow\) |
| cas500 | 0.438 ± 0.03 (1) | 0.4152 ± 0.01 (2) | \(\downarrow\) | 0.3679 ± 0.01 (4) | \(\downarrow\) | \(\downarrow\) |
| llog   | 0.2315 ± 0.01 (2) | 0.2308 ± 0.01 (3) | \(\downarrow\) | 0.2286 ± 0.01 (5) | \(\downarrow\) | \(\downarrow\) |
| Avg. rank | 1.1 | 2.7 | 3.5 | 3.8 | 4.7 | 5.2 |

Therefore, the experimental environment were kept identical for all ensemble methods for a fair comparison. KFHE-HOMER and E-HOMER is implemented in R\(^2\) and the \textit{utiml} library \cite{17} is used for the multi-label classifiers.

### 5 Results

Table 3 shows the results of the experiments performed. The columns indicate the algorithms and the rows indicate the datasets. In each cell, the mean and standard deviation label-based macro-averaged F-Score (higher values are better) across the crossvalidation performed are shown. The values in the parenthesis indicate the relative ranking (lower values are better) of the algorithm with respect to the corresponding dataset. The last row of Table 3 indicates the overall average ranks of the algorithms compared.

Table 3 shows that KFHE-HOMER attains the best average rank of 1.1. KFHE-HOMER attained the top rank for all the datasets, except for llog where KFHE-HOMER got the second rank. E-HOMER attained the second best overall average rank of 2.7, whereas ECC attained the third best overall average rank of 3.5. The classifiers, CC, HOMER-B and HOMER-K attained average ranks of 3.8, 4.7 and 5.2 respectively. This shows that for each case the ensemble methods have consistently performed better than the component classifiers. The E-HOMER method has performed better in almost all cases compared to a single HOMER model, as well as have performed better than ECC, which

\(^2\) A version of KFHE-HOMER and E-HOMER is available at: https://github.com/phoxis/kfhe-homer
demonstrates the effectiveness of ensembling the HOMER method. The difference between E-HOMER and KFHE-HOMER is the aggregation method of the component HOMER classifier models and KFHE-HOMER has performed better than E-HOMER in all the cases. This demonstrates that KFHE-HOMER performs better than a bagged version of HOMER.

To understand if KFHE-HOMER did attain significantly different (better or worse) results than the other methods per dataset, a two-tailed paired Wilcoxon's signed rank sum test [4] was performed over the folds of each crossvalidation experiment. KFHE-HOMER was set as the control method and compared to the other methods. The different significance levels at which the differences were found are indicated in the table. The symbols "\(\downarrow\)", "\(\downarrow\)" and "\(\uparrow\)" beside the values in Table 3 indicates that the method was significantly worse than KFHE-HOMER at a significance level of 0.01, 0.05 and 0.1, respectively. "\(\uparrow\)" symbol indicates that a method was significantly better than KFHE-HOMER with a significance level of 0.1. From Table 3 it is clear that for almost all the datasets, KFHE-HOMER was significantly better than both the single HOMER-K and HOMER-B models. Also, KFHE-HOMER is significantly better than CC for most of the datasets. Interestingly, CC was better than KFHE-HOMER in the case of llog dataset.

To further analyse the overall difference of the methods over the different datasets, a multiple classifier comparison was performed following the recommendations of García et al. [7]. A post-hoc Friedman aligned rank test was performed with the Finner p-value correction. The results of this evaluation is summarised in Figure 2, where the scale indicates the average ranks and if the methods are not connected with a horizontal line then they are significantly different over different datasets with a significance level of 0.05. This shows that KFHE-HOMER was significantly better than all the methods except E-HOMER in which case the null hypothesis of Friedman aligned rank test could not be rejected with a significance level of 0.05. Although, KFHE-HOMER attained better ranks in all the datasets.

An overall pairwise table of the p-values of the post-hoc Friedman test is shown in Table 4. The lower diagonal of Table 4 a value in a cell is the p-values of the post-hoc Friedman aligned rank test with the Finner p-value correction for of the corresponding pair of algorithms in the rows and columns. Also, in the upper diagonal of the Table 4 each cell has the win/lost/tie count of the algorithm in the corresponding row, over the algorithms in the corresponding column.

To summarise, the results indicate that

- KFHE-HOMER was able to perform consistently better than its component classifiers.
- The aggregation method of KFHE-HOMER using the Kalman filter is more effective than E-HOMER, a simple bagged version of HOMER.
- KFHE-HOMER performed significantly better than ECC.
6 Conclusion and Future Work

This work introduces a multi-label classification method, KFHE-HOMER, by extending the Kalman filter-based Heuristic Ensemble (KFHE). The method KFHE views the ensemble classifier model to be trained as a state to be estimated in the hypothesis space. Then the state is estimated using a Kalman filter by using multiple noisy measurements, where each measurement is a trained classifier and the noise is its related classification error.

In KFHE-HOMER, the KFHE framework to aggregate multiple HOMER models. The method combines multiple HOMER models trained on weighted samples and different hyperparameter settings. The KFHE framework combines these models based on the classification error of the HOMER models. Experiments showed that KFHE-HOMER performed consistently the best compared to ECC and other state-of-the-art multi-label classifiers as HOMER and classifier chains. Also, KFHE-HOMER performed better than a simple ensemble of bagged HOMER named E-HOMER demonstrating the effectiveness of the KFHE framework.

The KFHE framework can be utilised with other methods in future along with improvements to the KFHE methods. Some research directions for future can be as follows:
A per-label KFHE can be studied, where instead of the combination of multiple labels using one Kalman gain, per-label Kalman gains will be maintained.

The present algorithm does not have a time update step, which can introduced and studied.

To stop the method converging to fast, process noise or a slowdown mechanism can be introduced, which may improve performance in some cases where the Kalman gain becomes 1.

Instead of one single measurement per iteration, multiple measurements can be performed and combined to achieve a better performance.

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