Abstract—Heterogeneous ensembles that can aggregate an unrestricted number and variety of base predictors can effectively address challenging prediction problems. In particular, accurate ensembles that are also parsimonious, i.e., consist of as few base predictors as possible, can help reveal potentially useful knowledge about the target problem domain. Although ensemble selection offers a potential approach to achieving these goals, the currently available algorithms are limited in their abilities. In this paper, we present several algorithms that incorporate ensemble diversity into a reinforcement learning (RL)-based ensemble selection framework to build accurate and parsimonious ensembles. These algorithms, as well as several baselines, are rigorously evaluated on datasets from diverse domains in terms of the predictive performance and parsimony of their ensembles. This evaluation demonstrates that our diversity-incorporated RL-based algorithms perform better than the others for constructing simultaneously accurate and parsimonious ensembles. These algorithms can eventually aid the interpretation or reverse engineering of predictive models assimilated into effective ensembles. To enable such a translation, an implementation of these algorithms, as well as several baselines, are made available at https://github.com/GauravPandeyLab/lens-learning-ensembles-using-reinforcement-learning.

Index Terms—Heterogeneous ensembles, Ensemble selection, Parsimony, Reinforcement learning, Evaluation

I. INTRODUCTION

Ensemble methods that combine the outputs of individual predictive models have been successful in producing accurate predictions for several challenging prediction tasks [1]–[3]. The effectiveness of an ensemble is related to the (degree of) diversity among its constituent base predictors, as complete consensus (lack of diversity) does not provide an advantage over any individual base predictor. Similarly, a lack of consensus (high diversity) is also unlikely to produce useful predictions. Successful ensemble methods aim to strike a balance between diversity and accuracy [4], [5]. For example, popular methods like boosting [6] and random forest [7] generate this diversity by sampling from or assigning weights to training examples. However, they generally utilize a single type of base predictor, such as decision trees, to build the ensemble. Such homogeneous ensembles have limited diversity, and may not be the best choice for difficult classification problems or datasets where the ideal base prediction method is often unclear due to incomplete knowledge and/or data issues.

A more potent approach in this scenario is to build ensembles from an unrestricted variety and number of heterogeneous base predictors, which naturally lends diversity to the resultant ensembles. Two commonly used methods for building such heterogeneous ensembles are stacking [8], [9], and ensemble selection [10], [11]. Stacking learns a higher-level meta-predictor over the base predictors, while ensemble selection uses an iterative strategy to select a subset of the base predictors into the final ensemble. These methods have produced promising results for several challenging prediction problems [12]–[22].

In its basic form, ensemble selection can be posed as a search for the “best” ensemble out of the $2^N$ subsets of the $N$ base predictors being aggregated. This is an especially promising approach, not only for improving prediction performance, but also because of its ability to select parsimonious ensemble constituted of a relatively small number of base predictors. This parsimony can be of great value for gaining domain knowledge, where it is not only important to learn an accurate (ensemble) predictor, but also interpret what novel insights can be inferred about the target problem from the base predictors included in the ensemble. For instance, for the important biomedical problem of predicting functions of proteins [23], it is also beneficial to identify the features or principles on the basis of which accurate predictions are made [24]. It would be easier to reverse engineer a smaller (more parsimonious) ensemble than a much larger one, such as all the base predictors taken together, to identify such features or principles.

However, despite its potential utility, the most well-known algorithms proposed for ensemble selection [10], [11], [25] are generally greedy and ad-hoc in nature. Due to the uncertainties in setting their parameters and components, their performance generally suffers adversely in several directions:

- It is difficult to guarantee their predictive performance on different datasets.
- It is also hard to ensure that the ensembles they select will be parsimonious.

These drawbacks can be partly attributed to an ad-hoc and inexhaustive search of the space of $2^N$ subsets of the $N$ base
predictors. To address this challenge, in previous work [26], we proposed a novel ensemble selection framework based on reinforcement learning (RL) [27]. This framework provides a systematic way of more exhaustively exploring the many possible combinations of base predictors that can be selected into an ensemble. In our initial experiments, the RL-based ensembles turned out to be almost as predictive as the much larger ensembles consisting of all the base predictors, while being substantially more parsimonious [26].

However, despite the effectiveness of this initial RL-based framework, it did not explicitly leverage the diversity among the base predictors as a criterion for its ensemble search. Given the close relationship between ensemble performance and diversity discussed above, it is likely that the lack of this consideration deteriorated the performance of the framework. Thus, in the current work, we investigated if explicitly considering the diversity among the base/ensemble predictors within our RL-based framework can help build even more accurate and parsimonious ensemble predictors. In Section II, we describe the algorithms implementing this approach using various measures of ensemble diversity [4], [28], [29]. Section III describes the datasets and experimental setup used to evaluate these algorithms. In Section IV, we examine if, and how well, these algorithms achieve their goal of building accurate and parsimonious ensemble predictors. We conclude with directions for future work in Section V.

II. PROPOSED APPROACH

Here, we describe our proposed ensemble selection approach, starting with basics of reinforcement learning and how it can be utilized to address the ensemble selection problem.

A. Basics of Reinforcement Learning (RL)

RL is a framework in which an agent learns how to behave in its environment using a trial-and-error mechanism [27]. The agent tries to maximize the cumulative reward that it receives from making various decisions. Reinforcement signals are provided by the reward function, which gradually guide the agent towards finding the optimal behavior, or policy, that will maximize its performance.

Q-learning is an RL algorithm that can discover an optimal policy in a theoretically sound way [30]. Here, the Q-table represents the action-value mapping that the agent constructs by searching the environment. Q-learning allows the agent to update the Q-table using a randomized $\epsilon$-greedy approach: with probability $1 - \epsilon$, the agent exploits its accumulated knowledge (best current policy as determined by the Q-table), and with probability $\epsilon$, the agent explores a state in the environment that is different from the one dictated by its current knowledge. This allows the agent to discover better states and actions than the ones it has already assessed.

B. Our previous work on RL-based ensemble learning

In previous work [26], we formulated the ensemble selection problem as a search of the ensemble space and used Q-learning to train an agent, i.e., the ensemble selection algorithm. Specifically, we defined the RL agent’s environment as a lattice, such as the one shown in Figure 1, where the nodes representing the states denote the $2^N$ possible subsets of the $N$ base predictors, and the arrows represent the allowed transitions between states (the “actions” in our setup). We proposed three strategies, namely RL\_greedy, RL\_backtrack and RL\_pessimistic, to search through this environment by defining the possible actions between states. This is done within the Q-learning framework to identify the best possible ensemble for a given search strategy, the corresponding reward function and the value of $\epsilon$. The framework returns the most rewarding path from the root of the lattice to the selected ensemble.

In this work, we focused on the RL\_pessimistic strategy because it achieved the best balance between parsimony and predictive performance in our previous work [26]. The reward function in this strategy is calculated as:

$$R(s_t, a_t, s_{t+1}) = f(s_{t+1}) - f(s_t),$$

where the reward $R(s_t, a_t, s_{t+1})$ received for the transition from the state $s_t$ to the new state $s_{t+1}$ by executing the action $a_t$ is the difference between the values of the predictive performance $f$ of the ensembles represented by the two states.

RL\_pessimistic emulates an agent that resets itself to the empty ensemble state (e.g., START node in Figure 1) as soon as it encounters a negative reward when it moves to a new ensemble state. At that point, the agent starts a new learning episode before it gets to perform a complete traversal of the lattice, i.e., from the START to the FINISH node in Figure 1. For this reason, the pessimistic agent can finish learning episodes relatively quickly, and consequently it tends to evaluate the upper levels of the lattice (where the smaller ensembles reside) more than the lower levels (where the larger ensembles reside). Thus, the lengths of the learning episodes may vary, depending on how soon the agent encounters a “depreciated” state. This strategy is based on the hypothesis that such a depreciated state (negative reward) might indicate
Definition of diversity measure

1. Cosine
   \( 1 - \text{(cosine similarity between prediction vectors)} \)
   Name of RL algorithm: \( \text{RL}_{\text{pessimcos}} \)

2. Correlation
   \( 1 - \text{(Pearson’s correlation coefficient between prediction vectors)} \)
   Name of RL algorithm: \( \text{RL}_{\text{pessimcorr}} \)

3. Euclidean
   Euclidean distance between prediction vectors
   Name of RL algorithm: \( \text{RL}_{\text{pessimeuclid}} \)

4. Yule’s Q \([31]\)
   \( 1 - Q_{i,k} = \frac{N_{10}N_{01} - N_{11}N_{00}}{N_{11} + N_{00} + N_{10} + N_{01}} \)
   Name of RL algorithm: \( \text{RL}_{\text{pessimyule}} \)

5. Kappa \((\kappa)\) \([5]\)
   \( 1 - \kappa_{i,k} = \frac{2(N_{11}N_{00} - N_{10}N_{01})}{(N_{11} + N_{00})(N_{10} + N_{01})(N_{11} + N_{01})(N_{00} + N_{10})} \)
   Name of RL algorithm: \( \text{RL}_{\text{pessimkappa}} \)

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**TABLE I**

| Name           | Definition of diversity measure                                                                 | Name of RL algorithm |
|----------------|-------------------------------------------------------------------------------------------------|----------------------|
| Cosine         | \( 1 - \text{(cosine similarity between prediction vectors)} \)                               | \( \text{RL}_{\text{pessimcos}} \) |
| Correlation    | \( 1 - \text{(Pearson’s correlation coefficient between prediction vectors)} \)               | \( \text{RL}_{\text{pessimcorr}} \) |
| Euclidean      | Euclidean distance between prediction vectors                                                  | \( \text{RL}_{\text{pessimeuclid}} \) |
| Yule’s Q \([31]\) | \( 1 - Q_{i,k} = \frac{N_{10}N_{01} - N_{11}N_{00}}{N_{11} + N_{00} + N_{10} + N_{01}} \)       | \( \text{RL}_{\text{pessimyule}} \) |
| Kappa \((\kappa)\) \([5]\) | \( 1 - \kappa_{i,k} = \frac{2(N_{11}N_{00} - N_{10}N_{01})}{(N_{11} + N_{00})(N_{10} + N_{01})(N_{11} + N_{01})(N_{00} + N_{10})} \) | \( \text{RL}_{\text{pessimkappa}} \) |

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A path of overfit and/or under-performing ensembles. It is also one of the reasons why RL_pessimistic was able to identify smaller ensembles than the other strategies from our previous work \([26]\). Finally, with all the episodes completed, and the optimal policy returned, RL_pessimistic picks the final ensemble as the one on the policy path that produces the highest individual performance (on the validation set).

**C. Incorporating ensemble diversity into our RL framework**

Our previously proposed RL strategies didn’t explicitly consider diversity among predictors, as shown by the fact that their reward functions (e.g., Equation \([1]\)), were only based on ensemble performance. In this work, we incorporated diversity into this framework to enable the selection of more accurate and parsimonious ensembles.

The RL_pessimistic strategy offers an avenue towards a diversity-incorporated version of the RL framework. Specifically, note that the native form of Q-learning enables exploration of randomly chosen states with probability \( \epsilon \). Thus, instead of random exploration, we can change the exploration strategy to explicitly visit the state that is the most diverse with respect to the ensemble represented by the current state. We adopted this approach and explain its implementation in terms of its two main components below.

1) **Diversity calculation and incorporation method:** Ensemble diversity has long been studied as a factor influencing ensemble performance, and several measures have been proposed to quantify it \([4]\), \([28]\), \([29]\). However, most of these measures are only defined for a pair of classifiers/predictors, which doesn’t lend them naturally to calculating diversity involving at least one ensemble consisting of multiple base predictors. Specifically, in our case, diversity needs to be calculated between candidate ensembles at the two ends of various transitions/actions in the RL environment, such as those denoted by green nodes and connected by solid arrows in Figure \([1]\). Thus, we used a simple method where the ensemble at the current state, as well as those at the neighboring states in the lattice, are used to generate their respective prediction vectors on the validation set. The diversity measure is then calculated between these all the pairs of current and potential future state ensembles (Figure \([2]\)). Finally, the potential future ensemble that has the highest value of this measure, i.e., is the most diverse with respect to the current ensemble, is the next state of the agent during the exploration phase of the RL process. The rest of algorithm runs the same as the RL_pessimistic strategy \([26]\). The stopping point of the algorithm is reached when it produces the same ensemble for ten consecutive RL episodes.

2) **Ensemble diversity measures:** As mentioned before, a variety of diversity measures have been proposed for studying ensembles \([4]\), \([28]\). To test the effectiveness of incorporating diversity into our RL framework, we chose some representative measures of two types, unsupervised and supervised. These measures, defined in Table \([I]\) and described below, were used in combination with the diversity incorporation method described above in our proposed RL-based algorithms.

**Unsupervised measures:** The simplest measures of the diversity of two prediction vectors are standard similarity or distance measures. These are unsupervised as they don’t involve using the actual labels of the examples the predictions are generated from. In this work, we tested diversity measures based on Pearson’s correlation coefficient, cosine similarity and Euclidean distance.

**Supervised measures:** The more established ensemble diversity measures are supervised in nature. These measures don’t only quantify how similar or different a pair of set of predictions are, but also use the true label information of the examples to measure how similar or different their classification errors are. Given the predicted labels produced by a pair of predictors \( D_i \) and \( D_k \), we generated a contingency table counting how often each predictor produced the correct label in relation to the other:

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Fig. 2. Calculation of diversity between a pair of ensembles being assessed for exploration during the ensemble process. The prediction vectors are generated by applying the respective ensembles to the validation set.
Using this information, we calculated Yule’s $Q$ \cite{31} and Fleiss’ $\kappa$ \cite{5} (defined in Table I) as the representative supervised diversity measures tested in our study. These measures have the same range as the correlation coefficient, i.e., they produce values tending towards 1 when $D_i$ and $D_k$ correctly classify the same instances, 0 when they do not, and −1 when they are negatively correlated. So, we used one minus their respective values to quantify diversity, just as for the unsupervised correlation measure.

The conjunction of the above components with the RL pessimistic algorithm yielded the diversity-incorporated algorithms listed in Table II.

### III. Evaluation Methodology

We evaluated our proposed diversity-enabled RL-based ensemble selection algorithms, as well as several other baseline algorithms, on diverse datasets from genomics, healthcare and non-biological areas. These datasets and baseline algorithms, as well as the experimental setup used in our evaluations, are described below. All the non-numeric features in these datasets were removed from our analyses because they were not readily amenable to the base prediction algorithms we used. Also, any features with missing values in more than 50% of the examples in the dataset were eliminated. For the remaining numeric features, we imputed the missing values with the mean of the available values.

#### A. Datasets used for the evaluation

**Protein function prediction from genomic data.** Prediction of protein function is an important problem in biology \cite{23,24}. The most common source of data used for this task are the proteins’ amino acid sequences. These sequences can be represented as strings constructed from an alphabet of twenty amino acids. In this study, we evaluated the ability of the tested algorithms to predict the functions of several thousand proteins from 19 clinically relevant bacterial pathogens that were also studied in our previous work \cite{18}. We chose normalized 3-mer frequencies, extracted using the khmer package \cite{32}, as our feature set to represent the information contained in these proteins’ amino acid sequences. Specifically, we extracted the frequencies of 8,000 3-mers, which are all the possible strings of length three that can be constructed from the twenty amino acids, throughout a given protein’s sequence. We then normalized these frequencies by the length of the sequence to reduce the potential bias due to the variation of the lengths among the proteins. These steps yielded a feature matrix that served as input to all the algorithms evaluated in this study.

Gene Ontology (GO) is the most commonly used definition and source of functions of proteins \cite{23,24}. Thus, as the class labels to be predicted, we chose the three GO terms with the most proteins annotated to them in our previous study \cite{18}. Since GO is a hierarchy of terms/labels, it is often difficult to define the negative examples associated to a given label. Thus, for each GO term, we followed the commonly used approach of assigning any proteins that are neither annotated to the GO term nor its ancestors or descendants as its negative examples \cite{33}. The resultant datasets and prediction problems are referred to as PFP1, PFP2, and PFP3 respectively (details in Table II).

**Predicting a patient’s hospital readmission.** A patient’s likelihood of readmission to a hospital, especially within 30 days, is an important consideration in healthcare, and can potentially be reduced by changing the patient’s treatment in the course of the initial admission \cite{34}. Thus, we evaluated the performance of the algorithms under consideration in predicting hospital readmission using a dataset that represents 10 years (1999-2008) worth of clinical care at 130 US hospitals and integrated delivery networks \cite{35}. The clinically relevant features used for this prediction were the patient’s race, gender, age, admission type, and time in hospital, the medical specialty of admitting physician, the number of lab tests performed, HbA1c test result, diagnosis, number of medications, and the number of outpatient, inpatient, and emergency visits in the year before the hospitalization.

Using these features, we made a binary prediction of if the patient was readmitted within 30 days after leaving the hospital the first time (positive class), or if they never returned or were readmitted after 30 days (negative class). The details of this readmission dataset are provided in Table II.

**Predicting default payments on credit cards.** This problem/dataset focuses on the prediction of default payments (yes/no) by credit card clients, based on their demographic factors, credit data, history of payment, and past bill statements \cite{36,37}. This dataset, described in Table II was collected in Taiwan between April-September 2005.

**Santander customer transaction prediction.** The goal of this dataset, available from a Kaggle challenge \cite{38}, is to predict if a Banco Santander customer will make a transaction based on their numeric features. Note that we only used that training
data of this challenge for our evaluation (details in Table [I]), since the true labels for the test set were not available.

Vehicle type prediction. This dataset was obtained from the Kaggle Classified Ads for Cars Challenge [39]. The dataset is a collection of car attributes, such as engine power, engine displacement, type of transmission, etc. The prediction problem we addressed using this dataset was classifying whether a vehicle was electric-driven (positive class) or fuel-based (negative class).

B. Baseline algorithms

In addition to examining the performances of the diversity-incorporated RL-based ensemble selection algorithms, we also compared them to several baseline algorithms:

- Best base predictor: Among all the base predictors evaluated and used to construct ensembles, we identified the one with the best performance. Comparison with this base predictor indicated if, and by how much, the ensembles improved performance.

- Stacking with all base predictors: Stacking [8], [9] is one of the most commonly used heterogeneous ensemble approaches. Thus, we also considered two implementations of stacking applied to the full set of base predictors as baselines:
  - Stacking with $L_2$-regularized logistic regression, which produced the best ensemble results in our and others’ previous studies [2], [18], [22], [40].
  - Stacking with $L_1$-regularized logistic regression. Due to the sparse regularization property of the $L_1$ norm, this baseline selects a subset of all the base predictors into the final ensemble, thus offering an alternative approach to ensemble selection.

- RL-based ensemble selection with random exploration: We also evaluated the RL-pessimistic strategy proposed in our previous work [26] and described in Section [I-B] as a baseline.

Finally, note that one of the steps of all our RL-based algorithms is the aggregation of the base predictors at a state of the exploration lattice (e.g. Figure 1) into an ensemble. Instead of the weighted average method used in our previous work [26], we used the stacking with $L_2$-regularized logistic regression method for this task in this study. This further improved the RL-based algorithms’ prediction performance, and made them more comparable with the stacking baselines. Also, we set $\epsilon$ to 0.01 in all our RL executions, since this value produced the best results in our previous work [26].

C. Experimental Setup

We used the same experimental setup (Figure 3), as our previous work [25], to evaluate all the baseline and diversity-incorporated algorithms tested in this study. Also, as in that work, in all our RL-based experiments, the parameters of the Q-learning algorithm, namely $\alpha$ and $\gamma$, were set to the commonly used values of 0.1 and 0.9 respectively [27]. The iterative nature of Q-learning requires the initialization of its parameters (values in the Q-table). We initialized the Q-table as a zero matrix, and updated the values as states and rewards were observed by the agent.

We used a 5-fold cross validation (CV) setup to estimate the performances of all the algorithms (Figure 3). All the base predictors were learned from the training set (60% of the original dataset). To reduce the adverse effects of class imbalance, which is an issue with the datasets in Table II, we randomly undersampled the majority class in the training set to be of the same size as the minority one [41]. The validation set (20% of the dataset) was used for calculating the rewards of the nodes in the RL environment, the diversity measures, and train the baseline ensemble methods described earlier.

![Fig. 3. Experimental setup used to evaluate all the algorithms tested in this work on all the datasets listed in Table II.](image-url)
The test set (the remaining 20% of the dataset) was used to assess the performance of the predictive models learned by all studied algorithms from the training and validation sets. An experiment for an algorithm being tested consisted of the concatenation of its prediction scores over all five test folds, and the evaluation of the resultant prediction vector of the same size as the original dataset.

All predictive performance evaluation, whether internal (on the validation set) or external (on the test set), was conducted using the $F_{\text{max}}$ measure \[24\] for the positive class in a dataset. $F_{\text{max}}$ is the maximum value of the F-measure across all the values of precision and recall obtained from all the thresholds applied to the prediction scores generated by the base predictors and their resultant ensembles. This measure is appropriate for our study due to the skewed class distributions of the datasets used (Table II). We also used the recommended Friedman and Nemenyi tests \[43\] to assess the statistical significance of the comparative performance of all the evaluated algorithms across all the datasets.

As described in the Introduction, one of the goals of ensemble selection algorithms is the selection of a parsimonious subset of the base predictors into the final ensemble. This parsimony can itself be an advantage for interpretation purposes. Thus, we also evaluated the performance of all the ensemble algorithms in terms of relative size, which is defined as the ratio of the size of the final ensemble to the original number of base predictors. The lower the value of this metric, the more parsimonious an ensemble is. This metric was analyzed alongside, and in exactly the same way as the predictive performance measured in terms of $F_{\text{max}}$.

We trained 18 representative base classification algorithms from Weka \[44\], including Naïve Bayes, Multilayer Perceptron, SVM with a polynomial kernel, AdaBoost, Logistic Regression, and Random Forest. Each CV training set was resampled with replacement 10 times to balance the classes, as described above. Applying the 18 algorithms to these resampled training sets yielded in 180 base predictors.

Each ensemble/baseline algorithm was presented with a pool of base predictors. We started all our experiments with ten randomly selected base predictors in this pool. This pool was increased in steps of ten randomly selected base predictors for each experiment, until we reached the entire set of 180 base predictors. This setup was designed to address the question of how the various methods, including our diversity-incorporated ones, behaved with an increasingly larger set of initial base predictors to build ensemble or baseline predictors from. The performances of the predictors resulting from all these methods were evaluated across all these sets, yielding curves such as the ones shown in Figure 4. To account for variation, each set of experiments was repeated ten times for all the datasets, and average scores and standard errors were reported in the results shown in the next section.

Finally, an implementation of our RL-based and baseline ensemble algorithms, as well the above experimental setup, is available at https://github.com/GauravPandeyLab/lens-learning-ensembles-using-reinforcement-learning.

IV. RESULTS

In this section, we describe several aspects of the performance of the different algorithms and baselines evaluated in this study.

A. Variation of performance with growing number of base predictors

We first examined the performance of all the baseline and ensemble algorithms in terms of their predictive and parsimony performance as the number of initial base predictors increased from 10 to 180. These results are shown in Figure 4 for the representative PFP1, vehicle, and credit datasets (Table II).

Several trends can be observed from these results:

- In terms of predictive ability ($F_{\text{max}}$ values shown in the left panel of Figure 4), all the ensemble methods performed substantially better than the best base predictor, validating the utility of these methods.
- The predictive performance of all the ensemble methods improved with an increasing number of base predictors, although this growth saturated at higher numbers (close to 180). However, their performance was relatively similar to that of the others.
- The differences among the ensemble methods were most evident in their parsimony performance (Relative size values shown in the right panel of Figure 4). Stacking with $L_2$-regularized logistic regression had the expected value of 1, since all the base predictors were used in the resultant ensemble. $L_1$ regularization, an alternative ensemble selection algorithm, produced more parsimonious ensembles, with the lowest value being around 0.7.
- The RL-based ensemble selection algorithms produced even more parsimonious ensembles than the stacking ones. For instance, their relative size values were lower than 0.5, often substantially so, at the highest number of base predictors (180).

Collectively, the above observations indicate that the RL-based ensemble selection algorithms, including the diversity-incorporated ones, produced ensembles that were as predictive as the stacking baselines, but substantially more parsimonious. This supports the original hypothesis that RL-based algorithms are able to search the space of possible ensembles more effectively than several other alternative algorithms.

B. Aggregate performance of ensemble algorithms across all the datasets

Although the results in Figure 4 are informative, it is difficult to quantitatively compare the aggregate performances of all the ensemble algorithms from them. Thus, in this part of the analysis, we quantified the algorithms’ predictive and parsimony performances across all the datasets, and compared them. Specifically, we calculated the area under the curve of each algorithm as the initial number of base predictors increased from 10 to 180. These areas/scores were denoted by $auEPC$ (area under Ensemble Prediction Curve) and $auESC$ (area under Ensemble Size Curve) for the prediction ($F_{\text{max}}$) and parsimony (relative size) performances respectively, and
calculated for all the algorithms for each dataset individually. These scores were translated to a range of $[0, 1]$ by linearly normalizing the X-axes of the prediction and parsimony performance plots to $[0, 1]$ (the Y-axis ($F_{max}$ and relative size) ranges was already $[0, 1]$). Next, we analyzed the auEPC and auESC scores as global ensemble performance metrics. Specifically, we statistically compared the performance of all the ensemble algorithms across all the datasets in terms of their respective auEPC and auESC scores. We assessed the statistical significance of these comparisons using the recommended Friedman and Nemenyi tests [43]. The results are shown as Critical Different (CD) plots in Figure 5 (details of these plots are in the figure’s caption).

The trends in these CD plots were generally consistent with those shown in Figure 4. Although all the ensemble algorithms were statistically tied in terms of predictive performance, there was substantial variation in their relative performance in terms of average ranks across the datasets (Figure 5(a)). There was substantially more statistical variation in the parsimony performance of the algorithms (Figure 5(b)). Specifically, although stacking with $L_1$-regularized logistic regression performed the best in terms of predictive performance, its parsimony was substantially worse. The more commonly used stacking with $L_2$-regularized logistic regression algorithm didn’t perform well in either of these aspects.

The variations among the RL-based ensemble selection algorithms were more interesting. While RL_pessimistic produced the most parsimonious ensembles (Figure 5(b)), its predictive performance was ranked the lowest among all the ensemble algorithms (Figure 5(a)). In contrast, the diversity-incorporated algorithms performed well, i.e., were generally towards the left of in terms of both predictive and parsimony performances. The algorithms based on supervised diversity measures (Table 1), namely RL_pessimyule and RL_pessimkappa generally performed better than the others based on unsupervised measures.

Collectively, the results presented in this section show that diversity-incorporated RL-based algorithms are an effective approach for producing both accurate and parsimonious heterogeneous ensembles.

V. CONCLUSIONS AND FUTURE DIRECTIONS

Heterogeneous ensembles that are both accurate and parsimonious can help address challenging prediction problems, as well as reveal potentially useful knowledge about the problem domains. In this paper, we presented several algorithms that incorporated ensemble diversity into a reinforcement learning (RL)-based ensemble selection framework that aimed to achieve these goals. These algorithms were implemented using a variety of established ensemble diversity measures. They, as well as several other baseline algorithms, were rigorously evaluated on datasets from diverse domains in terms of their predictive performance, as well as the parsimony of the resultant ensembles. This evaluation demonstrated that the diversity-incorporated RL-based ensemble selection algorithms performed better than the others for constructing simultaneously accurate and parsimonious ensembles. Our proposed algorithms can eventually aid the interpretation or reverse engineering of predictive models assimilated into effective ensembles.

Our algorithms can be improved by considering other RL frameworks, as well as other ensemble diversity measures. Also, it will be beneficial to objectively assess if and how the parsimonious nature of our ensembles can actually aid interpretation, as we hypothesize. Finally, as with several other applications of RL, computational efficiency was a challenge for us as well. This can be addressed using several approaches, such as more efficient RL algorithms and implementations, and parallelizing the algorithms for high-performance computing platforms.

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Fig. 4. Predictive and parsimony performances of all the evaluated algorithms on the representative PFP1 (SubFigs. a & b), Vehicle (SubFigs. c & d) and Credit (SubFigs. e & f) datasets (Table II). These performances were measured in terms of the $F_{\text{max}}$ and relative size metrics respectively, as defined in Section III-C. The values shown are averages of the corresponding metrics over ten experiments of each algorithm on each dataset. Also shown are standard error bars for each value, although these are too small to be visible here for the relative size results.
Fig. 5. Critical Difference (CD) plots [43] representing the comparative (a) predictive (auEPC) and (b) parsimony (auESC) performances of all the ensemble algorithms across all the datasets in Table II. These plots show the results of the statistical significance of the comparative performances, assessed using the recommended Friedman and Nemenyi tests [43]. In each plot, the X-axis represents rank order, and the vertical lines connected to it illustrate where the associated algorithm (denoted by abbreviations to the side) falls in rank. Thus, the more left the vertical line for an algorithm, the better its overall performance was. Furthermore, algorithms that are grouped by thick horizontal lines are considered statistically tied in their performance.