Discovering General-Purpose Active Learning Strategies

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Abstract—We propose a general-purpose approach to discovering active learning (AL) strategies from data. These strategies are transferable from one domain to another and can be used in conjunction with many machine learning models. To this end, we formalize the annotation process as a Markov decision process, design universal state and action spaces and introduce a new reward function that precisely model the AL objective of minimizing the annotation cost. We seek to find an optimal (non-myopic) AL strategy using reinforcement learning. We evaluated the learned strategies on multiple unrelated domains and show that they consistently outperform state-of-the-art baselines.

Index Terms—Active learning, meta-learning, Markov decision process, reinforcement learning.

1 INTRODUCTION

Modern supervised machine learning (ML) methods require large annotated datasets for training purposes and the cost of producing them can easily become prohibitive. Active learning (AL) mitigates the problem by selecting intelligently and adaptively a subset of the data to be annotated. To do so, AL typically relies on informativeness measures that identify unlabelled data points whose labels are most likely to help to improve the performance of the trained model. As a result, good performance is achieved using far fewer annotations than by randomly labelling data.

Most AL selection strategies are hand-designed either on the basis of researcher’s expertise and intuition or by approximating theoretical criteria [1]. They are often tailored for specific applications and empirical studies show that there is no single strategy that consistently outperforms others in all datasets [2], [3]. Furthermore, they only represent a small subset of all possible strategies.

To overcome these limitations, it has recently been proposed to design the strategies themselves in a data-driven fashion by learning them from prior AL experience [4], [5]. This meta approach makes it possible to go beyond human intuition and potentially to discover completely new strategies by accounting for the state of the trained ML model when selecting the data to annotate. However, many of these methods are still limited to either learning from closely related domains [4], [6], [7], or using a greedy selection that may be suboptimal [7], or relying on properties of specific classifiers [4], [8], [9]. In earlier work [5], we formulated an approach we dubbed Learning Active Learning (LAL) as a regression problem. Given a trained classifier and its output for a specific sample without a label, we predicted the reduction in generalization error that could be expected by adding the label to that point. While effective this approach is still greedy and therefore could be a subject to finding suboptimal solutions.

Our goal is therefore to devise a general-purpose data-driven AL method that is non-myopic and applicable to heterogeneous datasets. To this end, we build on earlier work that showed that AL problems could be naturally reworded in Markov Decision Process (MDP) terms [4], [10]. In a typical MDP, an agent acts in its environment. At each time step \( t \), the agent finds itself in state \( s_t \) and takes an action \( a_t \). It brings a reward \( r_{t+1} \) and takes the agent to a new state \( s_{t+1} \). RL methods, such as Q-learning [11] and policy gradient [12], [13], look for a policy that maximizes the cumulative reward and have a long history in robotics [14], [15], [16]. They have also been extended for tasks, such as active vision [17], [18], [19], learning architectures of neural networks [20], [21], visual question answering [22], [23], image annotation [24], [25], [26], and tracking [27]. In this paper, we demonstrate how this also applies to AL.

To achieve the desired level of generality, we incorporate two innovations. First, we propose an original Q-learning approach for a pool-based AL setting. We rely on deep Q-network (DQN) method [28] and modify it for AL purposes. Second, we define the state and action representations as well as the reward in a new way: We define generic MDP state and action representations that can be computed for arbitrary datasets and without regard to the specific ML model. We then take the AL objective to be minimizing the number of annotations required to achieve a given prediction quality, which is a departure from standard AL approaches that maximize the performance given an annotation budget. We therefore design the MDP reward function to reflect our AL objective and it makes the training and evaluation procedure more transparent.

The resulting approach has several desirable properties. First, we can learn and transfer strategies across various and quite different datasets. Compared to our earlier LAL approach [5], our new formulation produces non-greedy selection strategies. The use of Q-learning instead of policy gradient enables to achieve better data complexity and lower variance, in part thanks to bootstrapping. Our
modifications to DQN procedure help to deal with very large action spaces, to model the dependencies between the actions, and to enforce the AL constraint of selecting each action at most once during an episode. Our state and action formulation makes our approach compatible with most ML models because it does not require model- or dataset-specific features. Furthermore, the simplicity of our state and action representations makes the model conceptually easy to understand and to implement. This is in contrast to an approach such as the one of [10] that also achieves generality by using multiple training datasets, but requires a far more complex state and action embedding. Finally, our reward function allows to optimize what the practitioners truly want, that is, the annotation cost, independently of the specific ML model and performance measure being used.

Our meta-learning approach to active learning is both easy to deploy and effective. In our experiments we demonstrate its effectiveness for the purpose of binary classification by applying the learned strategies to previously unseen datasets from different domains. We show that this enables us to reach pre-defined quality thresholds with fewer annotations than several baselines, including recent meta-AL algorithms [5], [10], [29]. We also analyse the properties of our strategies to understand their behaviour and how it differs from those of more traditional ones.

2 Related work

Manually-designed AL methods [30], [31], [32] differ in their underlying assumptions, computational costs, theoretical guarantees, and generalization behaviours. However, they all rely on a human designer having decided how the data points should be selected. Representative approaches to doing this are uncertainty sampling [33], which works remarkably well in many cases [31], [34], query-by-committee, which does not require probability estimates [35], [36], and expected model change [37], [38]. However, the performance of any one of these strategies on a never seen before dataset is unpredictable [2], [3], which makes it difficult to choose one over the other. In this section, we review recent methods to addressing this difficulty.

2.1 Combining AL strategies

If a single manually designed method does not consistently outperform all others, it makes sense to adaptively select the best strategy or to combine them. The algorithms that do it can rely on heuristics [39], on bandit algorithms [2], [29], [40], or on RL to find an MDP policy [3], [41]. Still, this approach remains limited to combining existing strategies instead of learning new ones. Furthermore, strategy learning happens during AL and its success depends critically on the ability to estimate the classification performance from scarce annotated data.

2.2 Data-driven AL

Recently, the researchers have therefore turned to so-called data-driven AL approaches that learn AL strategies from annotated data [4], [5], [6], [7], [8], [9], [10]. They learn what kind of datapoints are the most beneficial for training the model given the current state of trained ML model. Then, past experience helps to eventually derive a more effective selection strategy. This has been demonstrated to be effective, but it suffers from a number of limitations. First, this approach is often tailored for learning only from related datasets and domains suitable for transfer or one-shot learning [4], [5], [7], [8], [9]. Second, many of them rely on specific properties of the ML models, be they standard classifiers [5] or few-shot learning models [4], [8], [9], which restricts their generality. Finally, in some approached the resulting strategy is greedy—for example when supervised [5] or imitation learning [7] is used—that might lead to suboptimal data selection.

MDP formulation in data-driven AL is used both for pool-based AL, where datapoints are selected from a large pool of unlabelled data, and for stream-based AL, where datapoints come from a stream and AL decides to annotate a datapoint or not as it appears. In stream-based AL, actions—to annotate or not to—are discrete and Q-learning [11] is the RL method of choice [6], [42]. By contrast, in pool-based AL, the action selection concerns all potential datapoints that can be annotated and it is natural to characterise them by continuous vectors that makes it not suitable for Q-learning. So, policy gradient [12], [13] methods are usually used [4], [8], [9], [10]. In this paper we focus on pool-based AL but we would like to reap the benefits of Q-learning that is, lower variance and better data-complexity thanks to bootstrapping. To this end, we take advantage of the fact that although actions in pool-based AL are continuous, their number is finite. Thus, we can adapt Q-learning for our purposes.

Most data-driven AL methods stipulate a specific objective function that is being maximised. However, the methods are not always evaluated in a way that is consistent with the objective that is optimized. Sometimes, the metric used for evaluation differs from the objective [4], [5], [10]. Sometimes, the learning objective may include additional factors like discounting [6], [10], [42] or may combine several objectives [8], [42]. By contrast, our approach uses our evaluation criterion—minimization of the time spent annotating for a given performance level—directly in the strategy learning process. While the idea of minimising the amount of annotations to reach a given performance has already been explored in theory [43], it has not yet been put into practice or in conjunction with MDP.

Among data-driven AL, the approach of [10] achieves generality by using multiple training datasets to learn strategies, as we do. However, this approach is more complex than ours, relies on policy-gradient RL, and uses a standard AL objective. By contrast, our approach does not require a complex state and action embedding, needs fewer RL episodes for training thanks to using Q-learning, and explicitly maximizes what practitioners care about, that is, reduced annotation cost.

3 Method

One way to approach active learning with meta-learning is to start by formulating the AL process as a Markov decision process (MDP) and then to use reinforcement learning (RL) to find an optimal strategy. In this section, we first outline our design philosophy and then formalize AL in MDP.
Our goal is to advance data-driven AL towards general-purpose learning. Desirable strategies should have two key properties. They should be transferable across unrelated datasets and have sufficient flexibility to be applied in conjunction with different ML models. Our design decisions are therefore geared towards learning such strategies. The iterative structure of AL is naturally suited for an MDP formulation: For every state of an AL problem, an agent takes an action that defines the datapoint to annotate and it receives a reward that depends on the quality of the model that is re-trained using the new label. An AL strategy then becomes an MDP policy that maps a state into an action.

To achieve seamless transferability and flexibility, our task is therefore to design the states, actions, and rewards to be generic. To this end, we represent states and actions as vectors that are independent from specific dataset feature representations and can be computed for a wide variety of ML models. For example, the probability that the classifier assigns to a datapoint suits this purpose because most classifiers estimate this value. By contrast, the number of support vectors in a support vector machine (SVM) or the number of layers of a neural network (NN) are not suitable because they are model-specific. Raw feature representations of data are similarly inappropriate because they are domain specific.

A classical AL objective is to maximize the prediction quality—often expressed in terms of accuracy, AUC, F-score, or negative squared error—for a given annotation budget. For flexibility’s sake, we prefer an objective that is not directly linked to a specific performance measure. We therefore consider the dual objective of minimizing the number of annotations required for a given target quality value. When learning a strategy by optimizing this objective, the AL agent only needs to know if the performance is above or below this target quality, as opposed to its exact value. Therefore, the procedure is less tied to a specific performance measure or setting. Our MDP reward function expresses this objective by penalizing the agent until the target quality is achieved. This motivates the agent to minimize its “suffering” by driving the amount of requested annotations down.

Having formulated the AL problem as a MDP, we can learn a strategy using RL. We simulate the annotation process on data from a collection of unrelated labelled datasets, that ensures the transferability to new unlabelled datasets. Our approach to finding the optimal policy is based on DQN method of [28]. To apply DQN with pool-based AL, we modify it in two ways. First, we make it work with MDP where actions are represented by vectors corresponding to individual datapoints instead of being discrete. Second, we deal with the set of actions \( A_t \) that change between iterations \( t \) as it makes sense to annotate a datapoint only once.

### 3.2 Formulating AL as an MDP

Let us consider an AL problem where we annotate a dataset \( D \). A test dataset \( D' \) is used to evaluate the AL procedure. Then, we iteratively select a datapoint \( x^{(t)} \in D \) to be annotated. Let \( f_t \) be a classifier trained on a subset \( L_t \) that is annotated after iteration \( t \). This classifier assigns a numerical score \( \hat{y}_t(x_i) \in \mathbb{R} \) to a datapoint and then maps it to a label \( y_i \in \{0, 1\} \). For example, if the score \( \hat{y}_t(x_i) \) is the predicted probability \( \hat{y}_t(x_i) = p(y_i = 0|L_t, x_i) \), the mapping function simply thresholds it at 0.5. If we wanted to perform a regression instead, \( \hat{y}_t(x_i) \) could be a predicted label and the mapping function would be the identity. In AL evaluation we measure the quality of classifier \( f_t \) by computing its empirical performance \( \ell_t \) on \( D' \).

Then, we formulate AL procedure as an episodic MDP. Each AL run starts with a small labelled set \( L_0 \subset D \) along with a large unlabelled set \( U_0 = D \setminus L_0 \). The following steps are performed at iteration \( t \):

1. Train a classifier \( f_t \) using \( L_t \).
2. A state \( s_t \) is characterised by \( f_t, L_t \), and \( U_t \).
3. The AL agent selects an action \( a_t \in A_k \) by following a policy \( \pi : s_t \mapsto a_t \) that defines a datapoint \( x^{(t)} \in U_t \) to be annotated.
4. Look up the label \( y^{(t)} \) of \( x^{(t)} \) in \( D \) and set \( L_{t+1} = L_t \cup \{x^{(t)}, y^{(t)}\} \), \( U_{t+1} = U_t \setminus \{x^{(t)}\} \).
5. Give the agent the reward \( r_{t+1} \) linked to empirical performance value \( \ell_t \).

These steps repeat until a terminal state \( s_T \) is reached. In the case of target quality objective of Sec. 3.1, we reach the terminal state \( s_T \) when \( \ell_T \geq \eta \), where \( \eta \) is fixed by the user, or when \( T = |U_0| \). The agent only observes \( s_t, r_{t+1} \) and a set of possible actions \( A_t \), while \( f_t, D' \) and \( \eta \) are the parts of the environment. The agent aims to maximize the return of the AL run: \( R_0 = r_1 + \ldots + r_{T-1} \) by following policy \( \pi \) that intelligently chooses the actions, that is, the datapoints to annotate. We now turn to specifying our choice for states, actions, and rewards that reflect the AL objective of minimizing the number of annotations while providing flexibility and transferability.

#### 3.2.1 States

It only makes sense to perform AL when there is a lot of unlabelled data. Without loss of generality, we can therefore set aside at the start of each AL run a subset \( V \subset U_0 \) and replace \( U_0 \) by \( U_0 \setminus V \). We use the classifier’s score \( \hat{y}_t \) on \( V \) as a means to keep track of the state of the learning procedure. Then, we take the state representation to be a vector \( s_t \) of sorted values \( \hat{y}_t(x_i) \) for all \( x_i \in V \). Intuitively, the state representation is rich in information on, for example, the average prediction score or the uncertainty of a classifier. Besides, it is just the simplest representation that can be obtained given a classifier and a dataset. In Fig. [1] we plot the evolution of this vector for \( t \) using a policy defined by random sampling, uncertainty sampling, or our learnt strategy, on the same dataset and all starting from the same initial state \( s_0 \). Note that the statistics
of the vectors are clearly different. Although their structure is difficult to interpret for a human, it is something RL can exploit to learn a policy.

3.2.2 Actions

We design our MDP so that taking an action \(a_t\) amounts to selecting a datapoint \(x_t^{(i)}\) to be annotated. We characterize a potential action of choosing a datapoint \(x_t\) by a vector \(a_t\) which consists of the score \(\hat{y}_t(x_t)\) of the current classifier \(f_t\) on \(x_t\) and the average distances from \(x_t\) to \(L_t\) and \(U_t\), that is \(g(x_t, L_t) = \sum_{x_j \in L_t} d(x_t, x_j)/|L_t|\) and \(g(x_t, U_t) = \sum_{x_j \in U_t} d(x_t, x_j)/|U_t|\), where \(d\) is a distance measure. So, at iteration \(t\) we choose an action \(a_t\) from a set \(A_t = \{a_i\}\), where \(a_i = [\hat{y}_t(x_i), g(x_t, L_t), g(x_t, U_t)]\) and \(x_i \in U_t\). Notice, that \(a_i\) is represented by the quantities that are not specific neither for the datasets nor for the classifiers.

Again this is just the simplest representation that relates three components of AL problem: Classifier, labelled and unlabelled datasets. In addition to the classification score, two of these statistics are related to the sparsity of data and they represent the heuristic approximation for density.

3.2.3 Rewards

To model our target quality objective of reaching the quality \(q\) in as few MDP iterations as possible, we choose our reward function to be \(r_t = -1\). This makes the return \(R_0\) of an AL run that terminates after \(T\) iterations to be \(r_1 + \ldots + r_{T-1} = -T + 1\). The fewer iterations, the larger the reward, thus the optimal policy of MDP matches the best AL strategy according to our objective. This reward structure is not greedy because it does not restrict the choices of the agent as long as the terminal condition is met after a small number of iterations.

3.3 Policy learning using RL

Thanks to our reward structure, learning an AL strategy accounts to finding an optimal (with the highest return) policy \(\pi^*\) of MDP that maps a state \(s_t\) into an action \(a_t\) to take, i.e. \(\pi^* : s_t \rightarrow a_t\). To find this optimal policy \(\pi^*\) we use DQN [28] method on the data that is already annotated. In our case, \(Q^\pi(s_t, a_t)\) aims to predict \(-T + t\): a negative amount of iterations that are remaining before a target quality is reached from state \(s_t\) after taking action \(a_t\) and following the policy \(\pi\) afterwards. Note that it is challenging to learn from our reward function because the positive feedback is only received at the end of the run, thus the credit assignment is difficult.

3.3.1 Procedure

To account for the diversity of AL experiences we use a collection of \(Z\) annotated datasets \(\{Z_t\}_{t \leq T}\) to simulate AL episodes. We start from a random policy \(\pi\). Then, learning is performed by repeating the following steps:

1) Pick a labelled dataset \(Z \in \{Z_t\}\) and split it into subsets \(D\) and \(D'\).

2) Use \(\pi\) to simulate AL episodes on \(Z\) by initially hiding the labels in \(D\) and following an MDP as described in Sec. 3.2.

3) Keep the experience in the form of transitions \((s_t, a_t, r_{t+1}, s_{t+1})\).

3) Update policy \(\pi\) according to the experience with the DQN update rule.

Even though the features are specific for every \(Z\), the experience in the form of transitions \((s_t, a_t, r_{t+1}, s_{t+1})\) is of the same nature for all datasets, thus a single strategy is learned for the whole collection. When the training is completed, we obtain an optimal policy \(\pi^*\).

In the standard DQN implementation, the Q-function takes a state representation \(s_t\) as input and outputs several values corresponding to discrete actions [28], as shown in Fig. 2(a). However, we represent actions by vectors \(a_t\) and each of them can be chosen only once per episode as it does not make sense to annotate the same point twice. To account for this, we treat actions as inputs to the Q-function along with states and adapt the standard DQN architecture accordingly, as shown in Fig. 2(b). Then, Q-values for the required actions are computed on demand for \(a_t \in A_t\) through a feed-forward pass through the network. As our modified architecture is still suitable for Q-learning [11], [44], and the same optimization procedure as in a standard DQN can be used. Finding \(\max_{a_t} Q^\pi(s_t, a_t)\) still is possible because our set of actions is finite and the procedure has the same computational complexity as an AL iteration.

3.3.2 DQN implementation details

RL with non-linear Q-function approximation is not guaranteed to converge, but in practice it finds a good policy with the following heuristics. We incorporate the following techniques: First, we use separate target network [28] to deal with non-stationary targets (the update rate is set to 0.01). Second, the replay buffer [28] (of size 10 000) is employed to...
avoid correlated updates of neural network. Then, double DQN \cite{Hasselt2016} help to avoid the overestimation bias. Finally, the prioritized replay \cite{Schaul2015} uses the experience from the replay buffer with the highest temporal-difference errors more often (the exponent parameter is 3). Besides, we use a non-conventional technique instead of reward normalisation: We initialise the bias of the last layer to the average of all negative rewards. Our experiments have shown the procedure to be not sensitive to most of these parameters except exponent in prioritized experience replay that influences the speed of convergence.

To compute $Q^\pi(s_t, a_t)$ we use NN where first $s_t$ goes in and a compact representation of it is learnt. Recall that the scores in the state representation were sorted. Now it becomes clear that this is needed because it serves as an input to a fully connected layer of neural network that does not allow for permutations. Then, $a_t$ is added to a learnt representation and $Q^\pi(s_t, a_t)$ is the output. We use fully connected layers with sigmoid activations except for the final layer that is linear. As $y_i(x_i)$ we use $p(y_i = 0 \mid L_t, x_i)$.

## 4 Experimental Evaluation

In this section, we demonstrate the transferability and flexibility of our method, as defined in Sec. 3.3 and analyse its behaviour. The corresponding code is publicly available\footnote{https://github.com/ksenia-konyushkova/LAL-RL}.

### 4.1 Baselines and Parameters

#### 4.1.1 Baselines

We will refer to our method as LAL-RL, that is, a natural continuation of LAL approach \cite{Konyushkova2019} by using reinforcement learning for finding an AL strategy. We compare LAL-RL against the following 7 baselines. The first 3 are manually-designed. The next 3 are meta-AL algorithms with open source implementations. The final approach is similar in spirit to ours but no code is available on-line.

Rand, random sampling. The datapoint to be annotated is picked at random.

Uncert, uncertainty sampling \cite{Settles2013}, selects a datapoint that maximizes the Shannon entropy $H$ over the probability of predictions:

\[ x^{(i)} = \arg \max_{x_i \in U_t} H[p(y_i = y \mid L_t, x_i)]. \]

QUIRE \cite{Kobyzev2017}, a query selection strategy that uses the topology of the feature space. This strategy accounts for both the informativeness and representativeness of datapoints. The vector that characterizes our actions is in the spirit of this representativeness measure.

ALBE \cite{Bordes2017}, a recent meta-AL algorithm that adaptively combines strategies, including Uncert, Rand and QUIRE.

LAL-indep \cite{Konyushkova2019}, a recent approach that formulates AL as a regression task and learns a greedy strategy that is transferable between datasets.

LAL-iterat \cite{Konyushkova2019}, a variation of LAL-indep that tries to better account for the bias caused by AL selection.

MLP-GAL(\text{Te}) \cite{Kim2017}, a recent method that learns a strategy from multiple datasets with a policy gradient RL method.

### 4.1.2 Parameters

We use logistic regression (LogReg) or support vector machines (SVM) as our base classifiers for AL. We make no effort to tune them and use their sklearn python implementations with default parameters. For LogReg, they include an $\ell^1$ penalty with regularization strength $1$ and a maximum of 100 iterations. For SVM the most important parameters include rbf kernel and penalty parameter of 1. This corresponds to a realistic scenario where there is no obvious way to choose parameters.

Recall from Sec. 3.2 that our strategy is trained to reach the target quality $q$. For each dataset, we take $q$ to be 98% of the maximum quality of the classifier trained on 100 randomly drawn datapoints, which is the maximum number of annotations we allow. We allow for a slight decrease in performance (98% instead of 100%) because AL learning curves usually flatten and our choice enables AL agents to reach the desired quality much quicker during the episode. Our stopping criterion is motivated by a practical scenario where achieving 98% of prediction quality (for example, accuracy, f-score, AUC) is enough for a final user if it results in significant cost savings. We varied the stopping conditions by changing the size of the total target set in the range between 100 and 500 datapoints.

The parameters needed to define the state representation are the distance measure between datapoints and the number of datapoints in set $V$. The distance measure $d$ between datapoints is the cosine distance. Other distance measures yield similar performance, but they might require some scaling as the input to a neural network. We used 30 datapoints in validation set and the procedure shows itself to be insensitive to the choice of this parameter in the tested range between 20 and 100. One choice of this parameter value is suitable across all datasets.

We use the same RL parameters in all the experiments. The RL procedure starts with 100 “warm start” episodes with random actions and 100 Q-function updates. While learning an RL policy, the Adam optimizer is used with learning rate 0.0001 and a batch size 32. To force exploration during the course of learning, we use $\epsilon$-greedy policy $\pi$, which means that with probability $1 - \epsilon$ the action $a_t = \arg \max_a Q^\pi_T(s_t, a)$ is performed and with probability $\epsilon$ a random one is. The parameter $\epsilon$ decays from 1 to 0 in 1000 training iterations. We perform 1000 RL iterations, each of which comprise 10 AL episodes and 60 updates of the Q-function. 1000 iterations were chosen by tracking the performance of RL policy on a validation set and stopping the training when the rewards stops growing. In the vast majority of cases it happens before 1000 iterations and thus we set a rule to stop the execution at this point.

The baselines LAL-iterat and LAL-indep are not as flexible as LAL-RL. They were originally designed to deal with Random Forest classifiers. To use them within our experimental setup with LogReg, we let them train 2 classifiers in parallel and use the hand-crafted by RF in AL policy.
4.2 Transferability

We tested the transferability of LAL-RL on 10 widely-used standard benchmark datasets from the UCI repository [48]: 0-adult, 1-australian, 2-breast cancer, 3-diabetes, 4-flare solar, 5-heart, 6-german, 7-mushrooms, 8-waveform, 9-attribute. We use LogReg and ran 500 trials where AL episodes run up to 100 iterations.

In Table 1 we report the average number of annotations required to achieve the desired target accuracy using either our method or the baselines. In the 9 columns marked as leave-one-out, we test out method using a leave-one-out procedure, that is, training on 8 of the datasets selected from number 1 to number 9, and evaluating on the remaining one. In the course of this procedure, we never use dataset 0-adult for training purposes. Instead, we show in the column labelled as test the average number of annotations needed by all 9 strategies learnt in the leave-one-out procedure (the standard deviation is 2.34). In each column, the best number appears in bold, the second is underlined, and the third is printed in italics. We consider a difference of less than 1 to be insignificant and the corresponding methods to be ex-aequo.

LAL-RL comes out on top in 8 cases out of 10, second and third in the two remaining cases. As it has been noticed in the literature, Uncert is good in a wide range of problems [11]. In our experiments as well, it comes second overall and, for the same level of performance, it saves 29.80% over Rand while LAL-RL, saves 34.71%. Table 2 reports similar results reaching 98% of the quality of a classifier trained with 200 and 500 random datapoints instead.

In Table 1 we report the average duration and variance of the episodes of 9 learned strategies LAL-RL on dataset 0-adult. The individual durations for all strategies are 38.80, 37.72, 36.74, 33.95, 34.58, 38.76, 37.46, 41.84, and 37.85. Fig. 3 shows the learning curves with standard errors for all the baselines and for the 9 strategies. Some variability is present, but in 8 out of 9 cases LAL-RL outperforms all others baseline and once it shares the first rank with Uncert in terms of average episode duration.

Unfortunately, we cannot compare LAL-RL to MLP-GAL(Te) in the same fashion for lack of publicly available code. They report results for 20 annotations, we therefore check that even if we also stop all our episodes that early, LAL-RL still outperforms the strongest baseline Uncert in 90% of cases whereas MLP-GAL(Te) does so in 71% of the cases. Besides, we learn a policy using 5 times less data: 10,000 AL episodes instead of 50,000.

4.3 Flexibility

To demonstrate the flexibility of our approach now we repeat the experiments of Sec. 4.2 with our method, best baseline and random sampling using an SVM instead of LogReg and report the results in the last row of Table 2. Note that Uncert saves only 8% with respect to Rand, which is much less than in the experiments of Sec. 4.2 shown in rows 1 to 3. This stems from the fact that the sklearn implementation of SVMs relies on Platt scaling [49] to estimate probabilities, which biases the probability estimates when using limited amounts of training data. By contrast, LAL-RL is much less affected by this problem and delivers a 28% cost saving when being transferred across datasets.

Note that our state representation is universal for various types of classifiers. With this property we conduct the following experiment: We learn a LAL-RL strategy using classifier of type X and then apply it in an AL experiment with classifier Y. LAL-RL trained with SVM applied with LogReg results in 31.68% of cost saving and LAL-RL trained with LogReg applied with SVM results in 22.18% of cost saving. Although these cost saving are smaller than those of LAL-RL optimised with classifier X (34.71 and 28.35 correspondingly), it is still better that the Uncert.
4.4 Analysis

We now turn to analysing the behaviour of LAL-RL and its evolution over time. To this end, we ran additional experiments to answer the following questions.

4.4.1 Non-myopic behaviour

As described in Section 4.3, predicted probabilities of SVM are unreliable during early AL iterations. Thus, greedy performance maximization is unlikely to result in good performance. It makes setting a perfect task for validating the non-myopic strategies that can be learned by LAL-RL. In Fig. 4, we plot the percentage of the target quality reached by Rand and LAL-RL as a function of the number of annotated datapoints on one of the UCI datasets. The curve for LAL-RL demonstrates a non-myopic behaviour. It is worse than Rand at the beginning for approximately 15 iterations but almost reaches the target quality after 25 iterations, while it takes Rand 75 iteration to catch up.

4.4.2 What do we select?

While performing the experiments of Sec. 4.2, we record $p_t = p(y(t) = 0|L_t, x(t))$. We show the resulting normalized histograms in Fig. 3(a) for Rand, Uncert, and LAL-RL. The one for Rand is very broad and it simply represents the distribution of available $p_t$ in our data, while the one for Uncert is very peaked as it selects $p_t$ closest to 0.5 by construction. Figs. 3(b,c) depict the evolution of $p_t$ for Rand and LAL-RL for the time intervals $0 \leq t \leq 19, 20 \leq t \leq 39, 40 \leq t \leq 59, 60 \leq t \leq 79, 80 \leq t \leq 99$. The area of all histograms decreases over time as episodes terminate after reaching the target quality. However, while their shape remains roughly Gaussian in the Rand case, the shape changes significantly over time in case of LAL-RL strategy. Evidently, LAL-RL starts by annotating highly uncertain datapoints, then switches to uniform sampling, and finally exhibits a preference for $p_t$ values close to 0 or 1. In other words, the LAL-RL demonstrates a structured behaviour.

4.4.3 Transfer or not?

To separate the benefits of learning a strategy and the difficulties of transferring it, we introduce an artificial scenario LAL-RL-transfer in which we learn on one-half of a dataset and transfer to the other half. In Table 1 LAL-RL-transfer is better than LAL-RL in 3 cases, much better in 2 and equal in 3 (we skip one small dataset). This shows that having access to the underlying data distribution confers a modest advantage to LAL-RL. Therefore, our approach still enables to learn a strategy that is competitive to having access to the underlying distribution thanks to its experience on other AL tasks. We also check how LAL-RL-transfer performs on unrelated datasets, for example, learning the strategy on dataset 1 and testing it on datasets 2-9. The success rate in this case drops to around 40% on average, which again confirms the importance of using multiple datasets. As learning on one dataset to apply to another does not work well in general, we conclude that LAL-RL learns to distinguish between datasets to be successful across datasets.

### Table 1: Average number of annotations required to reach a predefined quality level.

| Scenario | Dataset | test | 1-austr | 2-breast | 3-diab | 4-flare | 5-germ | 6-heart | 7-mush | 8-wave | 9-wdbc |
|----------|---------|------|---------|----------|--------|---------|--------|---------|--------|--------|--------|
| Rand     | 0-adult | 50.78| 25.31   | 25.65    | 30.33  | 15.57   | 44.83  | 20.80   | 42.81  | 45.28  | 19.36  |
| Uncert   | 41.83   | 13.53| 27.07   | 27.84    | 15.50  | 37.10   | 15.60  | 15.60   | 23.83  | 7.25   |
| QUIRE    | 58.33   | 30.02| 33.33   | 37.12    | 9.02   | 57.58   | 20.30  | 42.9    | 36.49  | 15.45  |
| ALBE     | 55.66   | 29.79| 31.84   | 33.62    | 10.91  | 50.71   | 21.02  | 39.12   | 41.23  | 16.16  |
| LAL-indep| 59.39   | 20.88| 20.85   | 26.63    | 15.31  | 44.14   | 18.16  | 24.15   | 39.13  | 11.22  |
| LAL-iterat| 63.29  | 20.24| 21.79   | 28.03    | 14.84  | 40.38   | 19.90  | 25.2    | 36.97  | 10.39  |
| LAL-RL   | 37.52   | 14.15| 18.79   | 26.77    | 14.67  | 32.16   | 15.06  | 21.94   | 20.91  | 7.09   |
| notransf| —       | 15.01| 16.14   | 24.40    | —      | 23.26   | 14.65  | 16.47   | 18.06  | 7.14   |

| Baseline | Rand    | Uncert | LAL-RL |
|----------|---------|--------|--------|
| LogReg-100| 32.07  | −28.80%| −34.71%|
| LogReg-200| 80.06  | −29.61%| −39.96%|
| LogReg-500| 51.59  | −31.49%| −37.75%|
| SVM      | 30.87  | −7.81% | −28.35%|

Fig. 4: Example of non-greedy behaviour of a learnt RL strategy. The progress of the classifier is indicated along with the standard error. LAL-RL looses to Rand at the beginning, but reaches full quality faster.
5 Conclusion

We have presented a data-driven approach to AL that is transferable and flexible. It can learn strategies from a collection of datasets and then successfully use them on completely unrelated data. It can also be used in conjunction with different base classifiers without having to take their specificities into account. The resulting AL strategies outperform state-of-the-art approaches. Our AL formulation is oblivious to the quality metric. In this paper, we have focused on the accuracy for binary classification tasks, but nothing in our formulation is specific to it. It should therefore be equally applicable to multi-class classification and regression problems. In future work, we plan to generalize it to these additional ML models. Another interesting direction is to combine learning before the annotation using meta-AL on unrelated data and during the annotation to adapt to specificities of the dataset.

Appendix A

Figs. 5 and 6 show additional learning curves that depict the performance of our baselines with LogReg and SVM. The LogReg experiment shows the curves for all the methods and SVM show the curves for the 2 methods that delivered the best performance on average in the experiments of Sec. 4.2 and random sampling. Note that the SVM curve with dataset 5-flare solar also clearly exhibits non-myopic behaviour.
Fig. 7: Results of experiment from Sec. 4.3. Performance of 3 top strategies from experiment of Sec. 4.2 and a random sampling on the next 3 datasets.

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