

# Approximate Bayes Optimal Policy Search using Neural Networks

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**Abstract:** Bayesian Reinforcement Learning (BRL) agents aim to maximise the expected collected rewards obtained when interacting with an unknown Markov Decision Process (MDP) while using some prior knowledge. State-of-the-art BRL agents rely on frequent updates of the belief on the MDP, as new observations of the environment are made. This offers theoretical guarantees to converge to an optimum, but is computationally intractable, even on small-scale problems. In this paper, we present a method that circumvents this issue by training a parametric policy able to recommend an action directly from raw observations. Artificial Neural Networks (ANNs) are used to represent this policy, and are trained on the trajectories sampled from the prior. The trained model is then used online, and is able to act on the real MDP at a very low computational cost. Our new algorithm shows strong empirical performance, on a wide range of test problems, and is robust to inaccuracies of the prior distribution.

## 1 INTRODUCTION

Bayes-Adaptive Markov Decision Processes (BAMDP) (Silver, 1963; Martin, 1967) form a natural framework to deal with sequential decision-making problems when some of the information is hidden. In these problems, an agent navigates in an initially unknown environment and receives a numerical reward according to its actions. However, actions that yield the highest instant reward and actions that maximise the gathering of knowledge about the environment are often different. The BAMDP framework leads to a rigorous definition of an optimal solution to this learning problem, which is based on finding a policy that reaches an optimal balance between exploration and exploitation.

In this research, the case where prior knowledge is available about the environment is studied. More specifically, this knowledge is represented as a random distribution over possible environments, and can be updated as the agent makes new observations. In practice, this happens for example when training a drone to fly in a safe environment before sending it on the operation field (Zhang et al., 2015). This is called offline training and can be beneficial to the online performance in the real environment, even if prior knowledge is inaccurate (Castronovo et al., 2014).

State-of-the-art Bayesian algorithms generally do not use offline training. Instead, they rely on Bayes updates and sampling techniques during the interaction, which may be too computationally expensive, even on very small MDPs (Castronovo et al., 2015). In order to reduce significantly this cost, we propose a new practical algorithm to solve BAMDPs: Artificial Neural Networks for Bayesian Reinforcement Learning (ANN-BRL). Our algorithm aims at finding an optimal policy, i.e. a mapping from observations to actions, which maximises the rewards in a certain environment. This policy is trained to act optimally on some MDPs sampled from the prior distribution, and then it is used in the test environment. By design, our approach does not use any Bayes update, and is thus computationally inexpensive during online interactions. Our policy is modelled as an ensemble of ANNs, combined by using SAMME (Zhu et al., 2009), a boosting algorithm.

Artificial Neural Networks offer many advantages for the needed purpose. First, they are able to learn complex functions and are, thus, capable of encoding almost any policy. Second, ANNs can be trained very efficiently, using the backpropagation method, even on a large dataset. Lastly, ANNs' forward pass is fast, which makes them ideal to perform predictions during the online phase, when the computation time con-

straints are tight.

In our experiments, we used a benchmark recently introduced in (Castronovo et al., 2015). It compares all the major state-of-the-art BRL algorithms on a wide array of test problems, and provides a detailed computation time analysis. Since most state-of-the-art agents found in the literature are not any time algorithms, this last feature is very useful to compare solvers that have different time constraints.

This paper is organised as follows: Section 2 gives an overview of the state-of-the-art in Bayesian Reinforcement Learning. Section 3 presents the problem statement. Section 4 describes the algorithm. Section 5 shows a comparison between our algorithm and state-of-the-art algorithms of the domain. Section 6 offers a conclusion and discusses future work.

## 2 STATE-OF-THE-ART

Bayesian Reinforcement Learning (BRL) algorithms rely on Bayesian updates of the prior knowledge on the environment as new observations are made.

Model-based approaches maintain explicitly a posterior distribution, given the prior and the transitions observed so far. Bayes-adaptive Monte Carlo Planning (BAMCP) (Guez et al., 2012) and Bayesian Forward Search Sparse Sampling (BFS3) (Asmuth and Littman, 2011) rely on the exploration of the belief state space with a belief-lookahead (BL) approach. In this case, the posterior is used to explore efficiently the look-ahead tree and estimate the Q-values of the current belief-state. The accuracy is depending on the number of nodes those algorithms are able to visit, which is limited by an on-line computation time budget. Despite theoretical guarantees to reach Bayesian optimality offered by BL approaches<sup>1</sup>, they may not be applicable when the time budget that can be allocated for on-line decision making is short (Castronovo et al., 2015). Another method, Smarter Best of Sampled Set (SBOSS) (Castro and Precup, 2010), samples several MDPs from the posterior distribution, builds a merged MDP, and computes its Q-function. The number of MDPs to sample and the frequency at which a merged MDP has to be built is determined by uncertainty bounds on the Q-values. As a consequence, the online computation time of SBOSS may vary at each time-step. However, the number of samples and the frequency are depending on two parameters, which are used to fix the online computation time *on average*. More computa-

<sup>1</sup>e.g. BAMCP (Guez et al., 2012).

tion time improves the accuracy of the computed Q-values. However, on the downside, this approach remains computationally expensive (Castronovo et al., 2015).

On the other hand, model-free approaches only maintain a list of the transitions observed, and compute value functions. In this case, the prior distribution is used to initialise this list (e.g.: a uniform distribution consisting to assume each transition has been observed once). Bayesian Exploration Bonus (BEB) (Kolter and Ng, 2009a) builds the expected MDP given the current history at each time-step. The reward function of this MDP is slightly modified to give an exploration bonus to transitions which have been observed less frequently. The optimal Q-function of this MDP is then used to determine which action to perform. BEB is a simple, but efficient algorithm that remains computationally inexpensive for accurate prior distributions. Nevertheless, BEB’s performance drops significantly for inaccurate prior distributions (Castronovo et al., 2015).

Another approach was proposed a few years ago with Offline Prior-based Policy Search (OPPS) (Castronovo et al., 2012; Castronovo et al., 2014). During an offline phase, OPPS builds a discrete set of E/E strategies, and identifies which strategy of the set is the most efficient on average, to address any MDP drawn from the prior distribution. Instead of evaluating the performance of each strategy with the same accuracy, OPPS uses a multi-armed bandit strategy to discard gradually the worst strategies. This idea allows OPPS to consider a strategy space large enough to contain good candidates for many problems. Besides, the E/E strategies considered are computationally inexpensive for on-line decision making, but the approach lacks theoretical guarantees (Castronovo et al., 2015).

A more detailed description of each algorithm is available in the Appendix 6.1.

## 3 PRELIMINARIES

### 3.1 Bayes Adaptive Markov Decision Process (BAMDP)

We, hereafter, describe the formulation of optimal decision-making in a BAMDP. Let  $M = (X, U, f(\cdot), \rho_M, \gamma)$  be a given unknown MDP, where

- $X = \{x^{(1)}, \dots, x^{(nx)}\}$  denotes its finite state space
- $U = \{u^{(1)}, \dots, u^{(nu)}\}$  denotes its finite action space

- $r_t = \rho_M(x_t, u_t, x_{t+1}) \in [R_{\min}, R_{\max}]$  denotes an instantaneous deterministic, bounded reward
- $\gamma > 0$  its discount factor

When the MDP is in state  $x_t$  at time  $t$  and action  $u_t$  is selected, the agent moves instantaneously to a next state  $x_{t+1}$  with a probability  $P(x_{t+1}|x_t, u_t) = f(x_t, u_t, x_{t+1})$ . In the BAMDP setting, the dynamics are unknown, and we assume that  $f$  is drawn according to a known distribution  $P(f)$ . Such a probability distribution is called a prior distribution; it represents what the MDP is believed to be before interacting with it. Let  $h_t = (x_0, u_0, r_0, x_1, \dots, x_{t-1}, u_{t-1}, r_{t-1}, x_t)$  denote the history observed until time  $t$ . Given the current history  $h_t$ , a policy  $\pi$  returns an action  $u_t = \pi(h_t)$ . Given an MDP  $M$  and a policy  $\pi$ , we define the cost  $\mathfrak{J}_M^\pi = \mathbb{E}_M^\pi [\sum_t \gamma^t r_t]$  as the expected cumulated discounted reward on  $M$ , when applying policy  $\pi$ . Given a prior distribution  $p_{\mathcal{M}}^0(\cdot)$ , the goal is to find a policy  $\pi^*$ , called *Bayes optimal* that maximises the expected cost with respect to the prior distribution:

$$\pi^* = \arg \max_{\pi} \mathbb{E}_{M \sim p_{\mathcal{M}}^0(\cdot)} \mathfrak{J}_M^\pi \quad (1)$$

It is important to note that although this policy is good on average, with respect to the prior, it does not necessarily perform efficiently on each MDP sampled from the prior. Conversely, given a fixed and fully known MDP  $M$ , a policy that is optimal on  $M$  is likely to be very different from  $\pi^*$ .

### 3.2 Solving BAMDP

Though solving a BAMDP exactly is theoretically well defined, it is intractable in practice (Guez et al., 2013) for two reasons. First, sampling possible transition probabilities, based on past observations, relies on the computation of  $P(f|h_t) \propto P(h_t|f)P(f)$ , which is intractable for most probabilistic models (Duff, 2002; Kaelbling et al., 1998; Kolter and Ng, 2009b). Second, the BAMDP state space is actually made of all possible histories and is infinite. Therefore, all known tractable algorithms rely on some form of approximation. They can be divided in two main classes: online methods, and offline methods. The former group (Fonteneau et al., 2013; Asmuth and Littman, 2011; Walsh et al., 2010; Kolter and Ng, 2009a) relies on sparse sampling of possible models based on the current observations, to reduce the number of transition probabilities computations. The latter group (Wang et al., 2012) uses the prior knowledge to train an agent able to act on all possible sequences of observations. Our approach belongs to this group, and is described in Section 4.

## 4 ALGORITHM DESCRIPTION

A Bayes optimal policy  $\pi^*$ , as defined by Eq. 1, maps histories to Bayes actions. Although  $\pi^*$  is unknown, an approximation may be computed. Let  $\pi_\theta$  be a parametric policy whose model parameters are  $\theta$ . The model is fed up with the current history  $h_t$ , and computes an output vector, associating a confidence score to each action in return. The agent simply selects the action with the highest score.

Our model is composed of several ANNs, where the model parameters, denoted by  $\theta$ , are the weights of all the networks. All ANNs are fed up with the same inputs, and build several output vectors which are merged by using a weighted linear combination.

The training of this model requires a training dataset, whose generation is described in Section 4.1. It consists in performing simulations on MDPs drawn from the prior distribution to generate a training set. To each history observed during these simulations, we recommend an optimal action. Each  $\langle$  history, recommended action  $\rangle$  pair is a sample of the training dataset.

A history is a series of transitions whose size is unbounded, but ANNs can only be fed up with input vectors of a fixed size. To address this issue, histories are processed into fixed-size input vectors prior to training our model. This procedure is described in Section 4.2.

More specifically, the ANNs are built iteratively by using SAMME — an Adaboosting algorithm. It consists in modifying the training dataset in order to increase the weights of the samples misclassified by the ANNs built previously. Section 4.3 details the SAMME algorithm and the necessary changes to fit the BRL setting.

Moreover, we also pseudo-code descriptions in both offline and online phases (Algorithm 1 and Algorithm 2 respectively) along with UML diagrams (Figure 1 and Figure 2 respectively).

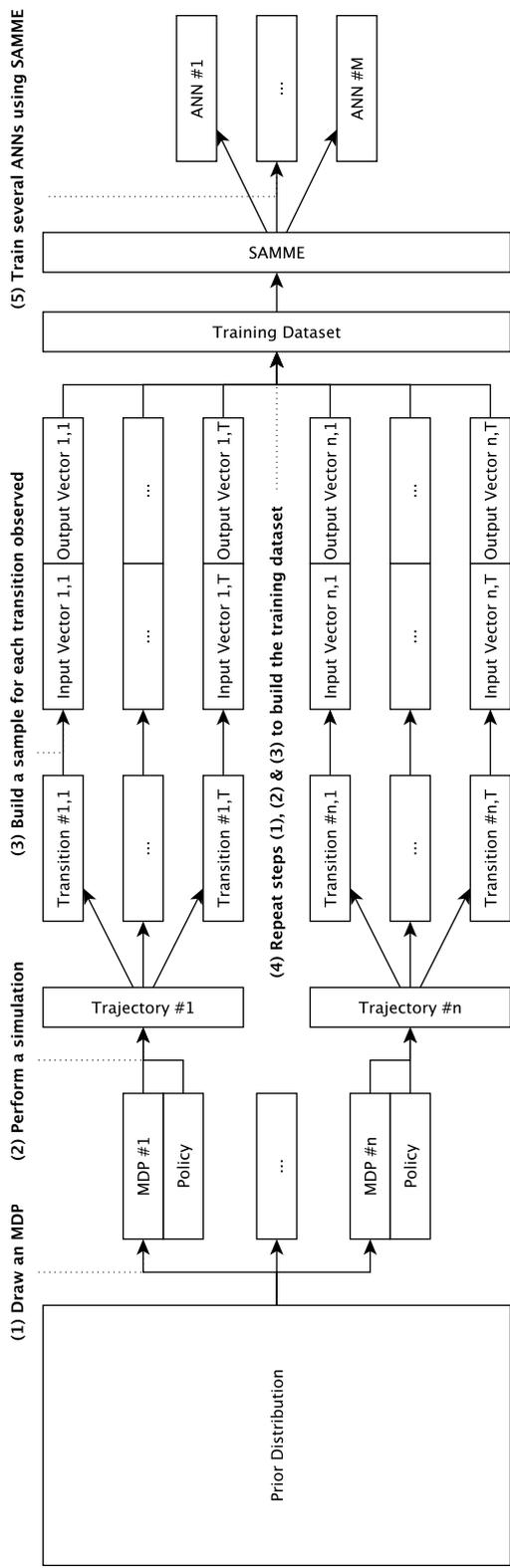


Figure 1: ANN-BRL - Offline phase

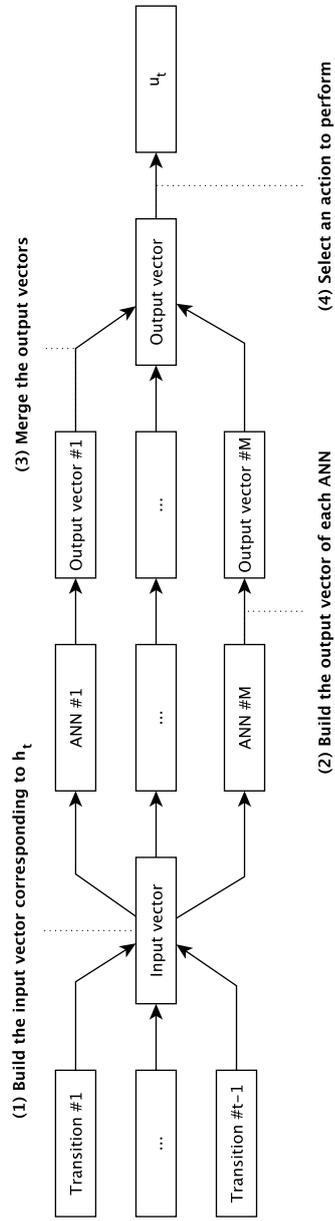


Figure 2: ANN-BRL - Online phase

## 4.1 Generation of the Training Dataset

During the offline phase, we use the prior knowledge to generate samples which will compose the training dataset. For a given series of observations  $h_t$ , we consider the optimal action w.r.t. the MDP from which  $h_t$  has been generated. In other words, we give a label of 1 to actions that are optimal when the transition function  $f(\cdot)$  is known, and  $-1$  to the others.

Our dataset is, thus, filled with suboptimal recommendations, from the Bayes optimal perspective. However, our samples are generated from multiple MDPs which are themselves sampled from the prior distribution. As a consequence, a history  $h$  can appear multiple times in our dataset but with different output vectors, because it has been generated from different

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### Algorithm 1 ANN-BRL - Offline phase

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**Input:** Time horizon  $T$ , prior distribution  $p_{\mathcal{M}}^0(\cdot)$   
**Output:** A classifier  $C(\cdot)$

{Generate transitions}  
**for**  $i = 1$  **to**  $n$  **do**  
 $M^{(i)} \sim p_{\mathcal{M}}^0(\cdot)$   
 $H^{(i)} \leftarrow$  Simulate 1 trajectory of length  $T$  on  $M^{(i)}$   
**end for**

{Compute input/output vectors for each transition}  
**for**  $i = 1$  **to**  $n$  **do**  
 $h_T \leftarrow H^{(i)}$   
**for**  $j = 1$  **to**  $T$  **do**  
 {Compute the input vector of sample  $(i, j)$ }  
 $h_j \leftarrow (h_T^{(1)}, \dots, h_T^{(j)})$   
 $\phi_{i,j} \leftarrow$  Reprocess  $h_j$

{Compute the output vector of sample  $(i, j)$ }  
 $Q_{i,j}^* \leftarrow$  Q-Iteration( $M^{(i)}, T$ )  
**for**  $k = 1$  **to**  $n_U$  **do**  
**if**  $k$  maximises  $Q_{i,j}^*(x, u^{(\cdot)})$  **then**  
 $output_{i,j}^{(k)} = 1$   
**else**  
 $output_{i,j}^{(k)} = -1$   
**end if**  
**end for**

$DataSet^{(i,j)} \leftarrow \{\phi_{i,j}, output_{i,j}\}$   
**end for**  
**end for**

{Train a model and compute a policy}  
 $C(\cdot) \leftarrow$  Run SAMME on  $DataSet$

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MDPs for which the labels were different. The average output vector for a history  $h$  approximates the probability of each action  $u$  to be the optimal response to  $h$  when  $f_M(\cdot)$  is known, where  $M \sim p_{\mathcal{M}}^0(\cdot)$ . To a certain extent, it is similar to what is done by other BRL algorithms, such as BAMCP (Guez et al., 2012) when it explores a specific part of the belief-states space using Tree-Search techniques.

During the data generation phase, it is necessary to choose which parts of the state space to explore. Generating samples by following what is believed to be an optimal policy is likely to provide examples in rewarding areas of the state space, but only for the current MDP. Since it is not possible to know in advance which MDPs our agent will encounter during the online phase, we choose to induce some random exploration in the data generation process. More precisely, we define an  $\epsilon$ -Optimal agent, which makes optimal decisions<sup>2</sup> w.r.t. to the MDP with a probability  $1 - \epsilon$ , and random decisions otherwise. By varying the value of  $0 < \epsilon < 1$  from one simulation to another, we are able to cover the belief-states space more efficiently than using a random agent.

## 4.2 Reprocess of a History

The raw input fed to our model is  $h_t$ , an ordered series of observations up to time  $t$ . In order to simplify the problem and reduce training time, a data preprocessing step is applied to reduce  $h_t$  to a fixed number of features  $\phi_{h_t} = [\phi_{h_t}^{(1)}, \dots, \phi_{h_t}^{(N)}]$ ,  $N \in \mathbb{N}$ . There are two types of features that are considered in this paper: Q-values and transition counters.

<sup>2</sup>By optimal we mean the agent knows the transition matrix of the MDP, and solve it in advance.

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### Algorithm 2 ANN-BRL - Online phase

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**Input:** Prior distribution  $p_{\mathcal{M}}^0(\cdot)$ , current history  $h_t = (x_0, u_0, r_0, x_1, \dots, x_{t-1}, u_{t-1}, r_{t-1}, x_t)$ , classifier  $C(\cdot)$   
**Output:**  $u_t$ , the action to perform at time-step  $t$

{Compute the input vector}  
 $\phi_t \leftarrow$  Reprocess  $h_t$   
 $input \leftarrow \phi_t$

{Compute the output vector}  
 $output \leftarrow C(input)$

{Choose action  $u_t$  w.r.t. the output vector}  
 $k \leftarrow k$  maximising  $output^{(\cdot)}$   
 $u_t \leftarrow u^{(k)}$

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Q-values are obtained by building an approximation of the current MDP from  $h_t$  and computing its Q-function, thanks to the well-known Q-Iteration algorithm (Sutton and Barto, 1998). Each Q-value defines a different feature:

$$\varphi_{h_t} = [ Q_{h_t}(x^{(1)}, u^{(1)}), \dots, Q_{h_t}(x^{(n_X)}, u^{(n_U)}) ]$$

A transition counter represents the number of occurrences of specific transition in  $h_t$ . Let  $C_{h_t}(<x, u, x'>)$  be the transition counter of transition  $<x, u, x'>$ . The number of occurrences of all transitions defines the following features:

$$\varphi_{h_t} = [ C_{h_t}(<x^{(1)}, u^{(1)}, x^{(1)}>), \dots, C_{h_t}(<x^{(n_X)}, u^{(n_U)}, x^{(n_X)}>) ] \quad (2)$$

At this stage, we computed a set of features which do not take into account the order of appearance of each transition. We consider that this order is not necessary as long as the current state  $x_t$  is known. In this paper, two different cases have been studied:

1. **Q-values:** We consider the set of all Q-values defined above. However, in order to take  $x_t$  into account, those which are not related to  $x_t$  are discarded.

$$\varphi_{h_t} = [ Q_{h_t}(x_t, u^{(1)}), \dots, Q_{h_t}(x_t, u^{(n_U)}) ]$$

2. **Transition counters:** We consider the set of all transition counters defined above to which we add  $x_t$  as an extra feature.

$$\varphi_{h_t} = [ C_{h_t}(<x^{(1)}, u^{(1)}, x^{(1)}>), \dots, C_{h_t}(<x^{(n_X)}, u^{(n_U)}, x^{(n_X)}>), x_t ] \quad (3)$$

### 4.3 Model Definition and Training

The policy is now built from the training dataset by supervised learning on the multi-class classification problem where the classes  $c$  are the actions, and the vectors  $v$  are the histories. SAMME has been chosen to address this problem. It is a boosting algorithm which directly extends Adaboost from the two-class classification problem to the multi-class case. As a reminder, a full description of SAMME is provided in Appendix 6.2.

SAMME builds iteratively a set of weak classifiers in order to build a strong one. In this paper, the weak classifiers are neural networks in the form of multi-layer perceptrons (MLPs). SAMME algorithm aims to allow the training of a weak classifier to focus on

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#### Algorithm 3 Resampling algorithm

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**Input:** The original training dataset *DataSet* (size =  $N$ ), a set of weights  $w_1, \dots, w_N$

**Output:** A new training dataset *DataSet'* (size =  $p$ )

{Normalise  $w_k$  such that  $0 \leq \bar{w}_k \leq 1$  and  $\sum_k \bar{w}_k = 1$ }

**for**  $i = 1$  **to**  $N$  **do**

$$\bar{w}_k \leftarrow \frac{w_k}{\sum_{k'} w_{k'}}$$

**end for**

{Resample *DataSet*}

**for**  $i = 1$  **to**  $p$  **do**

*DataSet'*( $i$ )  $\leftarrow$  Draw a sample  $s$  from *DataSet*

{ $P(s = \text{DataSet}(k))$  is equal to  $\bar{w}_k, \forall k$ }

**end for**

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the samples misclassified by the previous weak classifiers. This results in associating weights to the samples which reflect how bad the previous weak classifiers are for this sample.

MLPs are trained by backpropagation<sup>3</sup>, which does not support weighted samples. Schwenk et al. presented different resampling approaches to address this issue with neural networks in (Schwenk and Bengio, 2000). The approach we have chosen samples from the dataset by interpreting the (normalised) weights as probabilities. Algorithm 3 describes it formally.

One of the specificities of the BRL formalisation lies in the definition of the classification error  $\delta$  of a specific sample. This value is critical for SAMME in the evaluation of the performances of an MLP and the tuning of the sample weights. Our MLPs do not recommend specific actions, but rather give a confidence score to each one. As a consequence, different actions can receive the same level of confidence by our MLP(s), in which case the agent will break the tie by selecting one of those actions randomly. Therefore, we define the classification error  $\delta$  as the probability for an agent following a weak classifier  $C'(\cdot)$  (= an MLP) to select the class  $c$  associated to a sample  $v$  ( $<v, c>$  being an  $<$  history, recommended action  $>$  pair):

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<sup>3</sup>In order to avoid overfitting, the dataset is divided into two sets: a learning set (LS) and a validation set (VS). The training is terminated once it begins to be less efficient on VS. The samples are distributed 2/3 for LS and 1/3 for VS.

$$\begin{aligned}
u^* &= u^{(c)}, \hat{p} = C'(v) \\
\hat{U} &= \{u \in U \mid u = \arg \max_u \hat{p}_u\} \\
\delta &= \frac{|\hat{U} \setminus \{u^*\}|}{|\hat{U}|}
\end{aligned}$$

## 5 EXPERIMENTS

### 5.1 Experimental Protocol

In order to empirically evaluate our algorithm, it is necessary to measure its expected return on a test distribution  $p_{\mathcal{M}}$ , after an offline training on a prior distribution  $p_{\mathcal{M}}^0$ . Given a policy  $\pi$ , we denote this expected return  $\mathfrak{J}_{p_{\mathcal{M}}}^{\pi(p_{\mathcal{M}}^0)} = \mathbb{E}_{M \sim p_{\mathcal{M}}(\cdot)} \left[ \mathfrak{J}_M^{\pi(p_{\mathcal{M}}^0)} \right]$ . In practice, we can only approximate this value. The steps to evaluate an agent  $\pi$  are defined as follows:

1. Train  $\pi$  offline on  $p_{\mathcal{M}}^0$
2. Sample  $N$  MDPs from the test distribution  $p_{\mathcal{M}}^4$
3. For each sampled MDP  $M$ , compute estimate of  $\mathfrak{J}_M^{\pi(p_{\mathcal{M}}^0)}$
4. Use these values to compute an empirical estimate of  $\mathfrak{J}_{p_{\mathcal{M}}}^{\pi(p_{\mathcal{M}}^0)}$

To estimate  $\mathfrak{J}_M^{\pi(p_{\mathcal{M}}^0)}$ , the expected return of agent  $\pi$  trained offline on  $p_{\mathcal{M}}^0$ , we sample one trajectory on the MDP  $M$ , and compute the truncated cumulated return up to time  $T$ . The constant  $T$  is chosen so that the approximation error is bounded by  $\varepsilon = 0.01$ .

Finally, to estimate our comparison criterion  $\mathfrak{J}_{p_{\mathcal{M}}}^{\pi(p_{\mathcal{M}}^0)}$ , we compute the empirical average of the algorithm performance over  $N$  different MDPs, sampled from  $p_{\mathcal{M}}$ . For all our experiments, we report the measured values along with the corresponding 0.95 confidence interval.

The results will allow us to identify, for each experiment, the most suitable algorithm(s) depending on the constraints the agents must satisfy. Note that this protocol has been first presented in more details in (Castronovo et al., 2015).

<sup>4</sup>In practice, we can only sample a finite number of trajectories, and must rely on estimators to compare algorithms.

### 5.2 Algorithms Comparison

In our experiment, the following algorithms have been tested, from the most elementary to the state-of-the-art BRL algorithms: Random,  $\varepsilon$ -Greedy, Softmax, OPDS (Castronovo et al., 2012; Castronovo et al., 2014), BAMCP (Guez et al., 2012), BFS3 (Asmuth and Littman, 2011), SBOSS (Castro and Precup, 2010), and BEB (Kolter and Ng, 2009a). For detailed information on an algorithm and its parameters, please refer to the Appendix 6.1.

Most of the above algorithms are not any-time methods, i.e. they cannot be interrupted at an arbitrary time and yield a sensible result. Given an arbitrary time constraint, some algorithms may just be unable to yield anything. And out of those that do yield a result, some might use longer time than others. To give a fair representation of the results, we simply report, for each algorithm and each test problem, the recorded score (along with confidence interval), and the computation time needed. We can then say, for a given time constraint, what the best algorithms to solve any problem from the benchmark are.

### 5.3 Benchmarks

In our setting, the transition matrix is the only element which differs between two MDPs drawn from the same distribution. Generating a random MDP is, therefore, equivalent to generating a random transition matrix. In the BRL community, a common distribution used to generate such matrices is the Flat Dirichlet Multinomial distribution (FDM). It is chosen for the ease of its Bayesian updates. A FDM is defined by a parameter vector that we call  $\theta$ .

We study two different cases: when the prior knowledge is accurate, and when it is not. In the former, the prior distribution over MDPs, called  $p_{\mathcal{M}}^{\theta_0}(\cdot)$ , is exactly equal to the test distribution that is used during online training,  $p_{\mathcal{M}}^{\theta}(\cdot)$ . In the latter, the inaccuracy of the prior means that  $p_{\mathcal{M}}^{\theta_0}(\cdot) \neq p_{\mathcal{M}}^{\theta}(\cdot)$ .

Sections 5.3.1, 5.3.2 and 5.3.3 describes the three distributions considered for this study.

#### 5.3.1 Generalised Chain Distribution

The Generalised Chain (GC) distribution is inspired from the 5-states chain problem (5 states, 3 actions) (Dearden et al., 1998). The agent starts at state 1, and has to go through state 2, 3 and 4 in order to reach the last state, state 5, where the best rewards are. This cycle is illustrated in Figure 3(a).

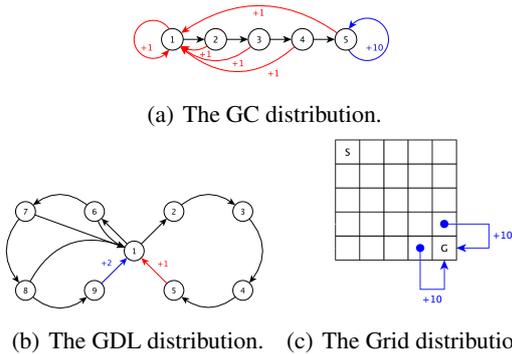


Figure 3: Studied distributions for benchmarking.

### 5.3.2 Generalised Double-Loop Distribution

The Generalised Double-Loop (GDL) distribution is inspired from the double-loop problem (9 states, 2 actions) (Dearden et al., 1998). Two loops of 5 states are crossing at state 1 (where the agent starts) and one loop yields more rewards than the other. This problem is represented in Figure 3(b).

### 5.3.3 Grid Distribution

The Grid distribution is inspired from the Dearden’s maze problem (25 states, 4 actions) (Dearden et al., 1998). The agent is placed at a corner of a 5x5 grid (the **S** cell), and has to reach the goal corner (the **G** cell). The agent can perform 4 different actions, corresponding to the 4 directions (up, down, left, right), but the actual transition probabilities are conditioned by the underlying transition matrix. This benchmark is illustrated in Figure 3(c).

## 5.4 Results

For each experiment, we tested each algorithm with several values for their parameter(s). The values considered in this paper are detailed in Appendix 6.1. Three pieces of information have been measured for each test: (i) an empirical score, obtained by testing the agent on 500 MDPs drawn from the test distribution<sup>5</sup>; (ii) a mean online computation time, corresponding to the mean time taken by the agent for performing an action; (iii) an offline computation time, corresponding to the time consumed by the agent while training on the prior distribution<sup>6</sup>.

<sup>5</sup>The same MDPs are used for comparing the agents. This choice has been made to reduce drastically the variance of the mean score.

<sup>6</sup>Notice that some agents do not require an offline training phase.

Each of the plots in Fig. 4 and Fig. 5 present a 2-D graph, where the X-axis represents a mean online computation time constraint, while the Y-axis represents an offline computation time constraint. For each point of the graph: (i) all agents that do not satisfy the constraints are discarded; (ii) for each algorithm, the agent leading to the best performance in average is selected; (iii) the list of agents whose performances are not significantly different is built. For this purpose, a paired sampled Z-test (with a confidence level of 95%) has been used to discard the agents which are significantly worse than the best one. Since several algorithms can be associated to a single point, several boxes have been drawn to gather the points which share the same set of algorithms.

### 5.4.1 Accurate Case

In Table 1, it is noted that ANN-BRL (Q)<sup>7</sup> gets extremely good scores on the two first benchmarks. When taking into account time constraints, ANN-BRL (Q) requires a slightly higher offline time bound to be on par with OPPS, and can even surpass it on the last benchmark as shown in Fig. 4.

ANN-BRL (C)<sup>8</sup> is significantly less efficient than ANN-BRL (Q) on the first and last benchmarks. The difference is less noticeable in the second one.

### 5.4.2 Inaccurate Case

Similar results have been observed for the inaccurate case and can be shown in Fig. 5 and Table 2 except for the last benchmark : ANN-BRL (Q) obtained a very high score, 4 times larger than the one measured for OPPS-DS. It is even more noteworthy that such a difference is observed on the most difficult benchmark. In terms of time constraints, ANN-BRL (Q) is still very close to OPPS-DS except for the last benchmark, where ANN-BRL (Q) is significantly better than the others above certain offline/online time periods.

Another difference is that even though ANN-BRL (C) is still outperformed by ANN-BRL (Q), Fig. 5 reveals some cases where ANN-BRL (C) outperforms (or is on par with) all other algorithms considered. This occurs because ANN-BRL (C) is faster than ANN-BRL (Q) during the online phase, which allows it to comply with smaller online time bounds.

<sup>7</sup>Refers to ANN-BRL using Q-values as its features.

<sup>8</sup>Refers to ANN-BRL using transition counters as its features.

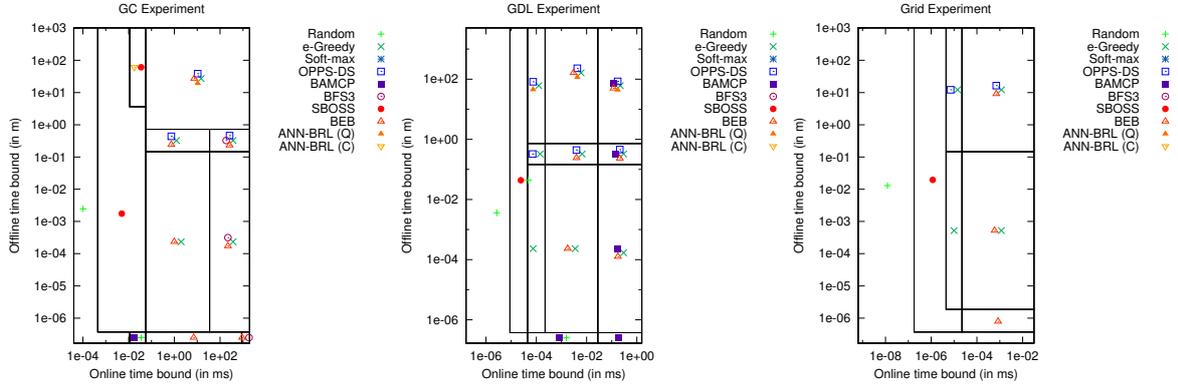


Figure 4: Best algorithms w.r.t offline/online periods (accurate case)

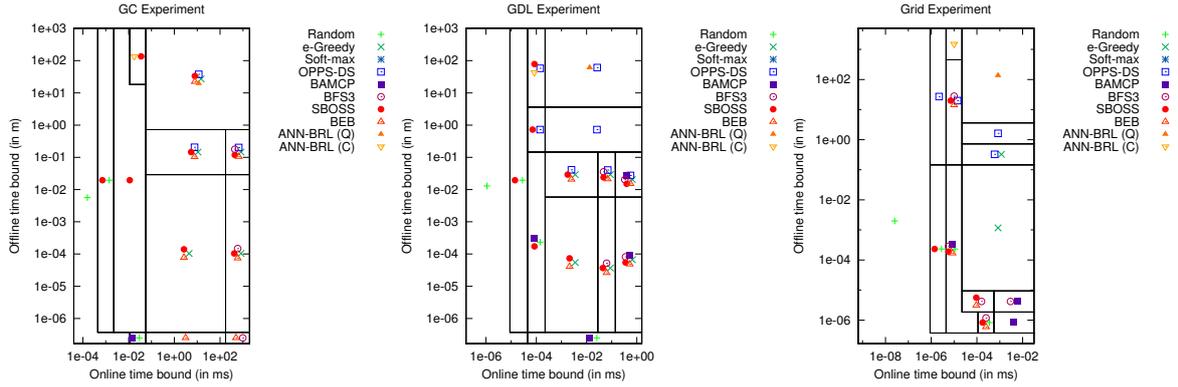


Figure 5: Best algorithms w.r.t offline/online time (inaccurate case)

Table 1: Best algorithms w.r.t Performance (accurate case)

Agent	Score on GC	Score on GDL	Score on Grid
Random	31.12 ± 0.90	2.79 ± 0.07	0.22 ± 0.06
e-Greedy	40.62 ± 1.55	3.05 ± 0.07	6.90 ± 0.31
Soft-Max	34.73 ± 1.74	2.79 ± 0.10	0.00 ± 0.00
OPPS-DS	42.47 ± 1.91	3.10 ± 0.07	7.03 ± 0.30
BAMCP	35.56 ± 1.27	3.11 ± 0.07	6.43 ± 0.30
BFS3	39.84 ± 1.74	2.90 ± 0.07	3.46 ± 0.23
SBOSS	35.90 ± 1.89	2.81 ± 0.10	4.50 ± 0.33
BEB	41.72 ± 1.63	3.09 ± 0.07	6.76 ± 0.30
ANN-BRL (Q)	42.01 ± 1.80	3.11 ± 0.08	6.15 ± 0.31
ANN-BRL (C)	35.95 ± 1.90	2.81 ± 0.09	4.09 ± 0.31

Table 2: Best algorithms w.r.t Performance (inaccurate case)

Agent	Score on GC	Score on GDL	Score on Grid
Random	31.67 ± 1.05	2.76 ± 0.08	0.23 ± 0.06
e-Greedy	37.69 ± 1.75	2.88 ± 0.07	0.63 ± 0.09
Soft-Max	34.75 ± 1.64	2.76 ± 0.10	0.00 ± 0.00
OPPS-DS	39.29 ± 1.71	2.99 ± 0.08	1.09 ± 0.17
BAMCP	33.87 ± 1.26	2.85 ± 0.07	0.51 ± 0.09
BFS3	36.87 ± 1.82	2.85 ± 0.07	0.42 ± 0.09
SBOSS	38.77 ± 1.89	2.86 ± 0.07	0.29 ± 0.07
BEB	38.34 ± 1.62	2.88 ± 0.07	0.29 ± 0.05
ANN-BRL (Q)	38.76 ± 1.71	2.92 ± 0.07	4.29 ± 0.22
ANN-BRL (C)	36.30 ± 1.82	2.84 ± 0.08	0.91 ± 0.15

## 6 CONCLUSION AND FUTURE WORK

We developed ANN-BRL, an offline policy-search algorithm for addressing BAMDPs. As shown by our experiments, ANN-BRL obtained state-of-the-art performance on all benchmarks considered in this paper. In particular, on the most challenging benchmark<sup>9</sup>, a score 4 times higher than the one measured for the second best algorithm has been observed. Moreover, ANN-BRL is able to make online decisions faster than most BRL algorithms.

Our idea is to define a parametric policy as an ANN, and train it using backpropagation algorithm. This requires a training set made of observations-action pairs and in order to generate this dataset, several simulations have been performed on MDPs drawn from prior distribution. In theory, we should label each example with a Bayes optimal action. However, those are too expensive to compute for the whole dataset. Instead, we chose to use optimal actions under full observability hypothesis. Due to the modularity of our approach, a better labelling technique could easily be integrated in ANN-BRL, and may bring stronger empirical results.

Moreover, two types of features have been considered for representing the current history: Q-values and transition counters. The use of Q-values allows to reach state-of-the-art performance on most benchmarks and outperform all other algorithms on the most difficult one. On the contrary, computing a good policy from transition counters only is a difficult task to achieve, even for Artificial Neural Networks. Nevertheless, we found that the difference between this approach and state-of-the-art algorithms was much less noticeable when prior distribution differs from test distribution, which means that at least in some cases, it is possible to compute efficient policies without relying on online computationally expensive tools such as Q-values.

An important future contribution would be to provide theoretical error bounds in simple problems classes, and to evaluate the performance of ANN-BRL on larger domains that other BRL algorithms might not be able to address.

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<sup>9</sup>Grid benchmark with a uniform prior.

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## APPENDIX

### 6.1 BRL Algorithms

Each algorithm considered in our experiments is detailed precisely. For each algorithm, a list of “reasonable” values is provided to test each of their parameters. When an algorithm has more than one parameter, all possible parameter combinations are tested.

#### 6.1.1 Random

At each time-step  $t$ , the action  $u_t$  is drawn uniformly from  $U$ .

#### 6.1.2 $\epsilon$ -Greedy

The  $\epsilon$ -Greedy agent maintains an approximation of the current MDP and computes, at each time-step, its associated Q-function. The selected action is either selected randomly (with a probability of  $\epsilon$  ( $1 \geq \epsilon \geq 0$ )), or greedily (with a probability of  $1 - \epsilon$ ) with respect to the approximated model.

##### Tested values:

$$\epsilon \in \{0.0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0\}.$$

#### 6.1.3 Soft-max

The Soft-max agent maintains an approximation of the current MDP and computes, at each time-step, its associated Q-function. The selected action is selected randomly, where the probability to draw an action  $u$  is proportional to  $Q(x_t, u)$ . The temperature parameter  $\tau$  allows to control the impact of the Q-function on these probabilities ( $\tau \rightarrow 0^+$ : greedy selection;  $\tau \rightarrow +\infty$ : random selection).

##### Tested values:

$$\tau \in \{0.05, 0.10, 0.20, 0.33, 0.50, 1.0, 2.0, 3.0, 5.0, 25.0\}.$$

#### 6.1.4 OPPS

Given a prior distribution  $p_{\mathcal{M}}^0(\cdot)$  and an E/E strategy space  $\mathcal{S}$ , the Offline, Prior-based Policy Search algorithm (OPPS) identify a strategy  $\pi^* \in \mathcal{S}$  which maximises the expected discounted sum of returns over MDPs drawn from the prior. The OPPS for Discrete Strategy spaces algorithm (OPPS-DS) (Castronovo et al., 2012; Castronovo et al., 2014) formalises the strategy selection problem for a discrete strategy space of index-based strategies. The E/E strategy spaces tested are the ones introduced in (Castronovo et al., 2015) and are denoted by  $\mathbb{F}_2, \mathbb{F}_3, \mathbb{F}_4, \mathbb{F}_5, \mathbb{F}_6$ .  $\beta$  is a parameter used during the strategy selection.

##### Tested values:

$$\mathcal{S} \in \{\mathbb{F}_2, \mathbb{F}_3, \mathbb{F}_4, \mathbb{F}_5, \mathbb{F}_6\}^{10},$$

$$\beta \in \{50, 500, 1250, 2500, 5000, 10^4, 10^5, 10^6\}.$$

<sup>10</sup>The number of arms  $k$  is always equal to the number of strategies in the given set. For your information:  $|\mathbb{F}_2| = 12$ ,  $|\mathbb{F}_3| = 43$ ,  $|\mathbb{F}_4| = 226$ ,  $|\mathbb{F}_5| = 1210$ ,  $|\mathbb{F}_6| = 7407$

### 6.1.5 BAMCP

Bayes-adaptive Monte Carlo Planning (BAMCP) (Guez et al., 2012) is an evolution of the Upper Confidence Tree algorithm (UCT) (Kocsis and Szepesvári, 2006), where each transition is sampled according to the history of observed transitions. The principle of this algorithm is to adapt the UCT principle for planning in a Bayes-adaptive MDP, also called the belief-augmented MDP, which is an MDP obtained when considering augmented states made of the concatenation of the actual state and the posterior. BAMCP relies on two parameters: (i)  $K$ , which defines the number of nodes created at each time-step, and (ii)  $depth$  defines the depth of the tree.

**Tested values:**

$$K \in \{1, 500, 1250, 2500, 5000, 10000, 25000\},$$

$$depth \in \{15, 25, 50\}.$$

### 6.1.6 BFS3

The Bayesian Forward Search Sparse Sampling (BFS3) (Asmuth and Littman, 2011) is a BRL algorithm whose principle is to apply the principle of the FSSS (Forward Search Sparse Sampling, see (Kearns et al., 2002)) algorithm to belief-augmented MDPs. It first samples one model from the posterior, which is then used to sample transitions. The algorithm then relies on lower and upper bounds on the value of each augmented state to prune the search space.  $K$  defines the number of nodes to develop at each time-step,  $C$  defines the branching factor of the tree, and finally  $depth$  controls its maximal depth.

**Tested values:**

$$K \in \{1, 500, 1250, 2500, 5000, 10000\},$$

$$C \in \{2, 5, 10, 15\}, depth \in \{15, 25, 50\}.$$

### 6.1.7 SBOSS

The Smarter Best of Sampled Set (SBOSS) (Castro and Precup, 2010) is a BRL algorithm which relies on the assumption that the model is sampled from a Dirichlet distribution. Based on this assumption, it derives uncertainty bounds on the value of state action pairs. Following this step, it uses those bounds to decide the number of models to sample from the posterior, and the frequency with which the posterior should be updated in order to reduce the computational cost of Bayesian updates. The sampling technique is then used to build a merged

MDP, as in (Asmuth et al., 2009), and to derive the corresponding optimal action with respect to that MDP. The number of sampled models is determined dynamically with a parameter  $\varepsilon$ , while the re-sampling frequency depends on a parameter  $\delta$ .

**Tested values:**

$$\varepsilon \in \{1.0, 1e-1, 1e-2, 1e-3, 1e-4, 1e-5, 1e-6\},$$

$$\delta \in \{9, 7, 5, 3, 1, 1e-1, 1e-2, 1e-3, 1e-4, 1e-5, 1e-6\}.$$

### 6.1.8 BEB

The Bayesian Exploration Bonus (BEB) (Kolter and Ng, 2009a) is a BRL algorithm that builds, at each time-step  $t$ , the expected MDP given the current posterior. Before solving this MDP, it computes a new reward function  $\rho_{BEB}^{(t)}(x, u, y) = \rho_M(x, u, y) + \frac{\beta}{c_{\langle x, u, y \rangle}^{(t)}}$ , where  $c_{\langle x, u, y \rangle}^{(t)}$  denotes the number of times transition  $\langle x, u, y \rangle$  has been observed at time-step  $t$ . This algorithm solves the mean MDP of the current posterior, in which we replaced  $\rho_M(\cdot, \cdot, \cdot)$  by  $\rho_{BEB}^{(t)}(\cdot, \cdot, \cdot)$ , and applies its optimal policy on the current MDP for one step. The bonus  $\beta$  is a parameter controlling the E/E balance.

**Tested values:**

$$\beta \in \{0.25, 0.5, 1, 1.5, 2, 2.5, 3, 4, 8, 16\}.$$

### 6.1.9 ANN-BRL

The Artificial Neural Network for Bayesian Reinforcement Learning algorithm (ANN-BRL) is fully described in Section 4. It samples  $n$  MDPs from prior distribution, and generates 1 trajectory for each MDP drawn. The transitions are then used to build training data (one SL sample per transition), and several ANNs are trained on this dataset by SAMME and backpropagation<sup>11</sup>. The training is parametrised by  $n_h$ , the number of neurons on the hidden layer of the ANN<sup>12</sup>,  $p$ , the number of samples resampled from the original training set at each epoch,  $\varepsilon$ , the learning rate used during the training,  $r$ , the maximal number of epoch steps during which the error on VS can increase before stopping the backpropagation training, and  $M$ , the maximal number of ANNs built by SAMME. When interacting with an MDP, the

<sup>11</sup>2/3 for the learning set (LS) and 1/3 for the validation set (VS).

<sup>12</sup>In this paper, we only consider 3-layers ANNs in order to build weak classifiers for SAMME.

BRL agent uses the ANN trained during the offline phase to determine which action to perform.

**Fixed parameters:**

$$n = 750, p = 5T^{13}, \varepsilon = 1e-3, r = 1000.$$

**Tested values:**

$$n_h \in \{10, 30, 50\}, M \in \{1, 50, 100\},$$

$$\varphi = \{ \{ \text{Q-values not related to } x_t \}, \\ \{ \text{Transition counters, current state} \} \}.$$

## 6.2 SAMME Algorithm

A multi-class classification problem consists to find a rule  $\mathcal{C}(\cdot)$  which associates a class  $c \in \{1, \dots, K\}$  to any vector  $v \in \mathbb{R}^n$ ,  $n \in \mathbb{N}$ . To achieve this task, we are given a set of training samples  $\langle v^{(1)}, c^{(1)} \rangle, \dots, \langle v^{(N)}, c^{(N)} \rangle$ , from which a classification rule has to be inferred.

SAMME is a boosting algorithm whose goal is to build iteratively a set of weak classifiers  $\mathcal{C}^{(1)}(\cdot), \dots, \mathcal{C}^{(M)} : \mathbb{R}^n \rightarrow \mathbb{R}^K$ , and combine them linearly in order to build a strong classifier  $\mathcal{C}(\cdot)$ . In our case, the weak classifiers are Multilayer Perceptrons (MLPs).

$$\mathcal{C}(h) = \frac{1}{M} \sum_{m=1}^M \alpha^{(m)} \mathcal{C}^{(m)}(h),$$

where  $\alpha^{(1)} \dots \alpha^{(M)}$  are chosen to minimise the classification error.

Given a set of training samples  $\langle v^{(1)}, c^{(1)} \rangle, \dots, \langle v^{(N)}, c^{(N)} \rangle$ , we associate a weight  $w_i$  to each sample. Let  $err(\mathcal{C}'(\cdot))$  be the weighted classification error of a classifier  $\mathcal{C}'(\cdot)$ :

$$err(\mathcal{C}'(\cdot)) = \frac{1}{\sum_{i=1}^N w_i} \sum_{i=1}^N w_i \delta_i^{\mathcal{C}'},$$

where  $\delta_i^{\mathcal{C}'}$  is the classification error of  $\mathcal{C}'(\cdot)$  for  $\langle v^{(i)}, c^{(i)} \rangle$ .

At each iteration  $m$ , a weak classifier is trained to minimise the weighted classification error.

$$\mathcal{C}^{(m)}(\cdot) = \arg \min_{\mathcal{C}''(\cdot)} err(\mathcal{C}''(\cdot)) \\ err^{(m)} = err(\mathcal{C}'(\cdot))$$

If this classifier behaves better than a random classifier ( $err^{(m)} < (n_U - 1)/n_U$ ), we compute its coefficient  $\alpha^{(m)}$ , update the weights of the samples, and build another classifier. Otherwise, we quit.

$$\alpha^{(m)} = \log \left( \frac{1 - err^{(m)}}{err^{(m)}} \right) + \log(n_U - 1) \\ w_i = w_i \exp(\alpha^{(m)} \delta_i^{\mathcal{C}'})$$

In other words, each new classifier will focus on training samples misclassified by the previous classifiers. Algorithm 4 presents the pseudo-code description for SAMME.

---

### Algorithm 4 SAMME

---

**Input:** A training dataset *DataSet*

**Output:** A classifier  $\mathcal{C}(\cdot)$

```
{Initialise the weight of each sample}
N ← |DataSet|
w_i^{(1)} ← 1/N, ∀i ∈ {1, ..., N}

{Train weak classifiers}
m ← 1
repeat
  {Train a weak classifier}
  C^{(m)} ← Train a classifier on DataSet w.r.t. w^{(m)}

  {Compute its weighted error and its coefficient}
  err^{(m)} ← 1 / (∑_i w_i^{(m)}) ∑_i w_i^{(m)} δ_i^{C'}
  α^{(m)} ← log( (1 - err^{(m)}) / err^{(m)} ) + log(n_U - 1)

  {Adjust the weights for the next iteration}
  w_i^{(m+1)} ← w_i^{(m)} exp(α^{(m)} δ_i^{C'}), ∀i
  Normalise the weights w^{(m+1)}

  m ← m + 1
until err^{(m)} ≥ (n_U - 1) / n_U {Stop if C^{(m)} is random}

C(·) ← { < C^{(1)}, α^{(1)} >, ..., < C^{(m)}, α^{(m)} > }
```

---

<sup>13</sup>The number of samples in LS is equal to  $n \times T = 500T$ . We resample 1% of LS at each epoch, which equals to  $5T$ .