# Formatting instructions for NIPS 2018

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### **Abstract**

The abstract paragraph should be indented ½ inch (3 picas) on both the left- and 2 right-hand margins. Use 10 point type, with a vertical spacing (leading) of 11 points. The word **Abstract** must be centered, bold, and in point size 12. Two line spaces 3 precede the abstract. The abstract must be limited to one paragraph.

# Introduction

## **Preliminaries**

We define a Markov decision process (MDP) as a tuple  $\mathcal{M} = \langle \mathcal{S}, \mathcal{A}, \mathcal{P}, \mathcal{R}, p_0, \gamma \rangle$ , where  $\mathcal{S}$  is the state-space,  $\mathcal{A}$  is a finite set of actions,  $\mathcal{P}(\cdot|s,a)$  is the distribution of the next state s' given that action a is taken in state  $s, \mathcal{R}: \mathcal{S} \times \mathcal{A} \to \mathbb{R}$  is the reward function,  $p_0$  is the initial-state 9 distribution, and  $\gamma \in [0,1)$  is the discount factor. We assume the reward function to be uniformly 10 bounded by a constant  $R_{max} > 0$ . A deterministic policy  $\pi : \mathcal{S} \to \mathcal{A}$  is a mapping from states 11 to actions. At the beginning of each episode of interaction, the initial state  $s_0$  is drawn from  $p_0$ . 12 Then, the agent takes the action  $a_0 = \pi(s_0)$ , receives a reward  $\mathcal{R}(s_0, a_0)$ , transitions to the next 13 state  $s_1 \sim \mathcal{P}(\cdot|s_0, a_0)$ , and the process is repeated. The goal is to find the policy maximizing the 14 long-term return over a possibly infinite horizon:  $\max_{\pi} J(\pi) \triangleq \mathbb{E}[\sum_{t=0}^{\infty} \gamma^t r_t \mid \mathcal{M}, \pi]$ . To this end, 15 we define the optimal value function  $Q^*(s,a)$  as the expected return obtained by taking action ain state s and following an optimal policy thereafter. Then, an optimal policy  $\pi^*$  is a policy that 17 is greedy with respect to the optimal value function, i.e.,  $\pi^*(s) = \operatorname{argmax}_a Q^*(s, a)$  for all states 18 s. It can be shown (e.g., [1]) that  $Q^*$  is the unique fixed-point of the optimal Bellman operator T19 defined by  $TQ(s,a) = \mathcal{R}(s,a) + \gamma \mathbb{E}_{\mathcal{P}}[\max_{a'} Q(s',a')]$  for any value function Q. From now on, we 20 adopt the term Q-function to denote any plausible value function, i.e., any function  $Q: \mathcal{S} \times \mathcal{A} \to \mathbb{R}$ 21 uniformly bounded by  $\frac{R_{max}}{1-\gamma}$ . 22 When learning the optimal value function, a quantity of interest is how close a given Q-function 23

is to the fixed-point of the Bellman operator. This is given by its Bellman residual, defined by 24  $B(Q) \triangleq TQ - Q$ . Notice that Q is optimal if, and only if, B(Q)(s,a) = 0 for all s, a. Furthermore, 25 if we assume the existence of a distribution  $\nu$  over  $\mathcal{S} \times \mathcal{A}$ , the squared Bellman error of Q is defined as the expected squared Bellman residual of Q under  $\nu$ ,  $||B(Q)||_{\nu}^2 = \mathbb{E}_{\mu}[B^2(Q)]$ . Although 27 minimizing the empirical Bellman error is an appealing objective, it is well-known that an unbiased 28 estimator requires two independent samples of the next state s' of each s, a (e.g., []). In practice,

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the empirical Bellman error is typically replaced by the TD error, which approximates the former 30 31

using a single transition sample. Given a dataset of N samples, the TD error is computed as  $\|B(Q)\|_D^2 = \frac{1}{N} \sum_{i=1}^N (r_i + \gamma \max_{a'} Q(s_i', a') - Q(s_i, a_i))^2$ .

# 3 Variational Transfer Learning

In this section, we describe our variational approach to transfer in RL. In Section 3.1, we start by introducing our algorithm from a high-level perspective, in such a way that it can be used for any choice of prior and posterior distributions. Then, in Sections 3.2 and 3.3, we propose practical implementations based on Gaussian prior/posterior and mixture of Gaussian prior/posterior, respectively.

## 3.1 Algorithm

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We begin with a simple consideration: the distribution  $\mathcal{D}$  over tasks clearly induces a distribution over optimal Q-functions. Since, for any MDP, learning its optimal Q-function is sufficient for solving the problem, one can safely replace the distribution over tasks with the distribution over their optimal value functions. Furthermore, assume we know such distribution and we are given a new task  $\tau$  to solve. Our goal is to design an algorithm that efficiently explores  $\tau$  so as to quickly adapt the prior distribution in a Bayesian fashion to put all probability mass over the optimal Q-function of  $\tau$ .

We consider a parametric family of Q-functions,  $Q = \left\{Q_{\boldsymbol{w}} : \mathcal{S} \times \mathcal{A} \to \mathbb{R} \mid \boldsymbol{w} \in \mathbb{R}^K\right\}$ . For simplicity, we assume each function in Q to be uniformly bounded by  $\frac{R_{max}}{1-\gamma}$ . Then, we can reduce our prior

ity, we assume each function in  $\mathcal{Q}$  to be uniformly bounded by  $\frac{R_{max}}{1-\gamma}$ . Then, we can reduce our prior distribution over Q-functions to a prior distribution over weights p(w). Assume that we are given a dataset  $D = \{(s_i, a_i, s_i', r_i) \mid i = 1, 2, \dots N\}$  of samples from some task  $\tau$  that we want to solve. Then, the posterior distribution over weights given such dataset can be computed by applying Bayes theorem as  $p(w|D) \propto p(D|w)p(w)$ . Unfortunately, this cannot be directly used in practice since we do not have a model of the likelihood p(D|w). In such case, it is very common to make strong assumptions on the MDPs or the Q-functions so as to get tractable posteriors []. However, in our transfer settings all distributions involved depend on the family of tasks under consideration, and making such assumptions is likely to limit the applicability of the approach. Thus, we take a different approach to derive a more general and meaningful solution. Recall that our final goal is move all probability mass over the weights minimizing some empirical loss measure, which in our case is the TD error  $\|B(w)\|_D^2$ . Then, given a prior p(w), we know from PAC-Bayesian theory that the optimal Gibbs posterior takes the form []:

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$$q(\boldsymbol{w}) = \frac{e^{-\Lambda \|B(\boldsymbol{w})\|_D^2} p(\boldsymbol{w})}{\int e^{-\Lambda \|B(\boldsymbol{w}')\|_D^2} p(d\boldsymbol{w}')}$$
(1)

for some parameter  $\Lambda>0$ . Since  $\Lambda$  is typically chosen to increase with the number of samples N, in the remaining we set it to  $\lambda^{-1}N$ , for some constant  $\lambda>0$ . Notice that, whenever the term  $e^{-\Lambda\|B(\boldsymbol{w})\|_D^2}$  can be interpreted as the actual likelihood of D, q becomes a classic Bayesian posterior. Although we now have an appealing distribution, the integral at the denominator of (1) is intractable to compute even for simple Q-function models. Thus, we propose a variational approximation  $q_{\boldsymbol{\xi}}$  by considering a simpler family of distributions parameterized by  $\boldsymbol{\xi} \in \Xi$ . Then, our problem reduces to finding the variational parameters  $\boldsymbol{\xi}$  such that  $q_{\boldsymbol{\xi}}$  minimizes the Kullback-Leibler (KL) divergence w.r.t. the Gibbs posterior q. From the theory of variational inference (e.g., []), this can be shown to be equivalent to minimizing the well-known (negative) evidence lower bound (ELBO):

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$$\min_{\boldsymbol{\xi} \in \Xi} \mathcal{L}(\boldsymbol{\xi}) = \mathbb{E}_{\boldsymbol{w} \sim q_{\boldsymbol{\xi}}} \left[ \|B(\boldsymbol{w})\|_{D}^{2} \right] - \frac{\lambda}{N} KL \left( q_{\boldsymbol{\xi}}(\boldsymbol{w}) \mid\mid p(\boldsymbol{w}) \right)$$
(2)

Intuitively, the approximate posterior trades-off between placing probability mass over those weights  $\boldsymbol{w}$  that have low TD error (first term), and staying close to the prior distribution (second term). Assuming that we are able to compute the gradients of (2) w.r.t. the variational parameters  $\boldsymbol{\xi}$ , our objective can be easily optimized with any stochastic optimization algorithm.

We now highlight our general transfer procedure in Alg. 1, while deferring a description of practical implementations with specific choices for the distributions involved to the next two sections. Given a set of weights  $W_s$  from the source tasks, we start by estimating the prior distribution (line 1) and we initialize the variational parameters by minimizing the KL divergence w.r.t. such distribution<sup>2</sup> (line

<sup>&</sup>lt;sup>1</sup>In practice, this is easily achieved by truncation.

<sup>&</sup>lt;sup>2</sup>If the prior and approximate posterior were in the same family of distributions we could simply set  $\xi$  to the prior parameters, however this does not always hold in practice.

#### **Algorithm 1** Variational Transfer

**Require:** Target task  $\tau$ , source Q-function weights  $W_s$ , batch sizes  $M_D$  and  $M_W$ , prior weight  $\lambda$ 

```
1: Estimate prior p(w) from W_s
  2: Initialize variational parameters: \pmb{\xi} \leftarrow \operatorname{argmin}_{\pmb{\xi}} KL(q_{\pmb{\xi}}||p)
  3: Initialize replay buffer: D = \emptyset
                Sample initial state: s_0 \sim p_0^{(\tau)}
  5:
  6:
                while s_h is not terminal do
  7:
                      Sample weights: \boldsymbol{w} \sim q_{\boldsymbol{\xi}}(\boldsymbol{w})
                      Take action a_h = \operatorname{argmax}_a Q_{\boldsymbol{w}}(s_h, a)
  8:
                    Observe transition s_{h+1} \sim \mathcal{P}^{(\tau)}(\cdot|s_h, a_h)

Collect reward r_h = \mathcal{R}^{(\tau)}(s_h, a_h)

Add sample to the replay buffer: D \leftarrow D \cup \langle s_h, a_h, r_h, s_{h+1} \rangle

Sample batch D' = \langle s_i, a_i, r_i, s_i' \rangle_{i=1}^{M_D} from D and \mathcal{W} = \{ \boldsymbol{w}_1, \boldsymbol{w}_2, \dots, \boldsymbol{w}_{M_{\mathcal{W}}} \} from q_{\boldsymbol{\xi}}

Approximate objective: \mathcal{L}(\boldsymbol{\xi}) = \frac{1}{M_{\mathcal{W}}} \sum_{\boldsymbol{w} \in \mathcal{W}} \|B(\boldsymbol{w})\|_{D'}^2 - \frac{\lambda}{N} KL(q_{\boldsymbol{\xi}} \parallel p)
  9:
10:
11:
12:
13:
                      Compute the gradient \nabla_{\boldsymbol{\xi}} \mathcal{L}(\boldsymbol{\xi})
14:
                      Update \xi in the direction of \nabla_{\xi} \mathcal{L}(\xi) using any stochastic optimizer (e.g., ADAM)
15:
16:
                end while
17: until forever
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2). Then, at each time step of interaction, we re-sample the weights from the current approximate posterior and act greedily w.r.t. the corresponding *Q*-function (lines 7,8). This resembles the well-known Thompson sampling approach adopted in multi-armed bandits []and allows our algorithm to efficiently explore the target task. In some sense, at each time we guess what is the task we are trying to solve based on our current belief and we act as if such guess were actually true. After collecting and storing the new experience (lines 9-11), we draw a batch of samples from the replay buffer and a batch of weights from the posterior (line 12). We use these to approximate the negative ELBO, compute its gradient, and finally update the variational parameters (lines 13-15).

The main advantage of our approach is that it exploits knowledge from the source tasks to perform an efficient adaptive exploration. Intuitively, during the first steps of interaction, our algorithm has no idea about what is the current task. However, it can rely on the learned prior to take early informed decisions. As the learning process goes on, it will quickly figure out which task is being solved, thus moving all probability mass over the weights minimizing the TD error. From that point, sampling from the posterior is approximately equivalent to deterministically taking such weights, and no more exploration will be performed. Finally, notice the generality of the proposed approach: as far as the objective  $\mathcal{L}$  is differentiable in the variational parameters  $\boldsymbol{\xi}$ , and its gradients can be efficiently computed, any function approximator for the Q-functions and any family for the pior and posterior distributions can be adopted. For the latter, we describe two practical choices in the next two sections.

#### 3.2 Gaussian Variational Transfer

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We now restrict ourselves to a specific choice of the prior and posterior families that makes our 96 algorithm very efficient and easy to implement. We assume that optimal Q-functions according to our 97 task distribution (or better, their weights) follow a multivariate Gaussian law. That is, we model the 98 prior as  $p(w) = \mathcal{N}(\mu_p, \Sigma_p)$  and we learn its parameters from the set of source weights using, e.g., 99 maximum likelihood estimation (with small regularization to make sure the covariance is positive 100 definite). Then, our variational family is the set of all well-defined Gaussian distributions, i.e., the variational parameters are  $\Xi = \{(\mu, \Sigma) \mid \mu \in \mathbb{R}^K, \Sigma \in \mathbb{R}^{K \times K}, \Sigma \succ 0\}$ . To prevent the covariance 101 102 from going not positive definite, we consider its Cholesky decomposition  $\Sigma = LL^T$  and learn the lower-triangular Cholesky factor L instead. Under Gaussian distributions, all quantity of interest for using Alg. 1 can be computed very easily. The KL divergence between the prior and approximate posterior can be computed in closed-form as:

$$KL\left(q_{\boldsymbol{\xi}}(\boldsymbol{w}) \mid\mid p(\boldsymbol{w})\right) = \frac{1}{2} \left( \log \frac{|\boldsymbol{\Sigma}_p|}{|\boldsymbol{\Sigma}|} + \operatorname{Tr}\left(\boldsymbol{\Sigma}_p^{-1} \boldsymbol{\Sigma}\right) + (\boldsymbol{\mu} - \boldsymbol{\mu}_p)^T \boldsymbol{\Sigma}_p^{-1} (\boldsymbol{\mu} - \boldsymbol{\mu}_p) - K \right)$$
(3)

for  $\boldsymbol{\xi} = (\boldsymbol{\mu}, \boldsymbol{L})$  and  $\boldsymbol{\Sigma} = \boldsymbol{L}\boldsymbol{L}^T$ . Its gradients with respect to the variational parameters are []:

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$$\nabla_{\boldsymbol{\mu}} KL\left(q_{\boldsymbol{\xi}}(\boldsymbol{w}) \mid\mid p(\boldsymbol{w})\right) = \boldsymbol{\Sigma}_{p}^{-1}(\boldsymbol{\mu} - \boldsymbol{\mu}_{p})$$
(4)

$$\nabla_{\boldsymbol{L}} KL\left(q_{\boldsymbol{\xi}}(\boldsymbol{w}) \mid\mid p(\boldsymbol{w})\right) = \boldsymbol{\Sigma}_{p}^{-1} \boldsymbol{L} - (\boldsymbol{L}^{-1})^{T}$$
(5)

Finally, the gradients w.r.t. the expected likelihood term of the variational objective (2) can be computed using the reparameterization trick (e.g., []):

$$\nabla_{\boldsymbol{\mu}} \mathbb{E}_{\boldsymbol{w} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{L} \boldsymbol{L}^T)} \left[ ||B(\boldsymbol{w})||_D^2 \right] = \mathbb{E}_{\boldsymbol{v} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I})} \left[ \nabla_{\boldsymbol{w}} ||B(\boldsymbol{w})||_D^2 \right] \text{ for } \boldsymbol{w} = \boldsymbol{L} \boldsymbol{v} + \boldsymbol{\mu}$$
 (6)

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$$\nabla_{\boldsymbol{L}} \mathbb{E}_{\boldsymbol{w} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{L} \boldsymbol{L}^T)} \left[ ||B(\boldsymbol{w})||_D^2 \right] = \mathbb{E}_{\boldsymbol{v} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I})} \left[ \nabla_{\boldsymbol{w}} ||B(\boldsymbol{w})||_D^2 \cdot \boldsymbol{v}^T \right] \text{ for } \boldsymbol{w} = \boldsymbol{L} \boldsymbol{v} + \boldsymbol{\mu} \quad (7)$$

#### 3.3 Mixture of Gaussian Variational Transfer

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See the original paper for the proof.

Although the Gaussian assumption of the previous section is very appealing as it allows for a simple 113 and efficient way of computing the variational objective and its gradients, we believe that such 114 assumption almost never holds in practice. In fact, even for families of tasks in which the reward and 115 transition models follow a Gaussian law, the Q-values might be far from it. Depending on the family 116 of tasks under consideration and, since we are learning a distribution over weights, on the chosen 117 function approximator, the prior might have arbitrarily complex shapes. When the information loss 118 due to the Gaussian approximation becomes too severe, the algorithm is likely too fail at transferring 119 knowledge, thus reducing to almost random exploration. We now propose a variant to successfully 120 solve this problem, while keeping the algorithm simple and efficient enough to be applied in practice. 121 In order to capture arbitrarily complex distributions, we use a kernel estimator [for learning our prior.] 122 Assume we are given a set  $W_s$  of weights from the source tasks. Then, our estimated prior places a 123 single isotropic Gaussian over each weight:  $p(w) = \frac{1}{|W_s|} \sum_{w_s \in W_s} \mathcal{N}(w|w_s, \sigma_p^2 I)^3$ . This takes the form of a mixture of Gaussians with equally weighted components. Consistently with the prior, we 124 125 model our approximate posterior as a mixture of Gaussians. However, we allow a different number 126 of components (typically much less than the prior's) and we adopt full covariances instead of only 127 diagonals, so that our posterior has the potential to match complex distributions with less components. 128 Using C components, our posterior is  $q_{\boldsymbol{\xi}}(\boldsymbol{w}) = \frac{1}{C} \sum_{i=1}^{C} \mathcal{N}(\boldsymbol{w} | \boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i)$ , with variational parameters  $\boldsymbol{\xi} = (\boldsymbol{\mu}_1, \dots, \boldsymbol{\mu}_C, \boldsymbol{\Sigma}_1, \dots, \boldsymbol{\Sigma}_C)$ . Once again, we learn Cholesky factors instead of full covariances. 129 130

Although this new model has the potential to capture much more complex distributions, it poses a major complication: the KL divergence between two mixture of Gaussians is well-known to have no closed-form equation. To solve this issue, we can rely on an upper bound to such quantity, so that negative ELBO we are optimizing still represents an upper bound on the KL between the approximate and true posterior. However, this turns out to be non-trivial as well. In fact, it is very easy to bound the KL between two mixtures with the KLs between each couple of components. However, the loss of information is such that minimizing the upper bound via gradient methods converges to a local optimum in which all components tend to go to the same point, thus almost reducing to the single Gaussian case. To solve this issue, we adopt the variational upper bound proposed in [], which we found to be able to preserve the needed information. We report it here for the sake of completeness.

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Theorem 1. Let  $p=\sum_i c_i^{(p)} f_i^{(p)}$  and  $q=\sum_j c_j^{(q)} f_j^{(q)}$  be two mixture of Gaussian distributions, where  $f_i^{(p)}=\mathcal{N}(\boldsymbol{\mu}_i^{(p)},\boldsymbol{\Sigma}_i^{(p)})$  denotes the i-th component of  $p,c_i^{(p)}$  denotes its weight, and similarly for q. Introduce two vectors  $\chi^{(1)}$  and  $\chi^{(2)}$  such that  $c_i^{(p)}=\sum_j \chi_{j,i}^{(2)}$  and  $c_j^{(q)}=\sum_i \chi_{i,j}^{(1)}$ . Then:

$$KL(p||q) \le KL(\chi^{(2)}||\chi^{(1)}) + \sum_{i,j} \chi_{j,i}^{(2)} KL(f_i^{(p)}||f_j^{(q)})$$
(8)

Our new algorithm replaces the KL with the above-mentioned upper bound. Each time we require its value, we have to recompute the parameters  $\chi^{(1)}$  and  $\chi^{(2)}$  that tighten the bound. As shown in [], this can be achieved by a simple fixed-point procedure. Furthermore, both terms in the approximate negative ELBO are now linear combinations of functions of the variational parameters for different components, thus their gradients can be straightforwardly derived from the ones of the Gaussian case.

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<sup>&</sup>lt;sup>3</sup>Notice that this is slightly different than the typical kernel estimator (e.g., [])

#### 3.4 Optimizing the TD error

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From Sections 3.2 and 3.3, we know that differentiating the negative ELBO  $\mathcal{L}$  w.r.t.  $\boldsymbol{\xi}$  requires differentiating  $\|B(\boldsymbol{w})\|_D^2$  w.r.t.  $\boldsymbol{w}$ . Unfortunately, the TD error is well-known to be non-differentiable due to the presence of the max operator. This rarely represents a problem since typical value-based algorithms are actually semi-gradient methods, i.e., they do not differentiate the targets (see, e.g., Chapter 11 of []). However, our transfer settings are rather different than common RL. In fact, our algorithm is likely to always start from Q-functions that are very close to the optimum, and the only thing that needs to be done is to adapt the weights in a direction of lower error (i.e., higher likelihood) so as to quickly converge to the solution of the task that is being solved. Unfortunately, this property cannot be guaranteed for most semi-gradient algorithms. Even worse, many online RL algorithms combined with complex function approximators (e.g., DQNs) are well-known to be unstable, especially when approaching the optimum, and require a lot of tuning and tricks to work well. This is obviously an undesirable property in our case, as we only aim at adapting already good solutions. Thus, we consider using a residual gradient algorithm (after []). In order to differentiate the targets, we replace the optimal Bellman operator with the mellow Bellman operator introduced in [], which adopts a softened version of max called *mellowmax*:

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$$\min_{a} Q_{\boldsymbol{w}}(s, a) = \frac{1}{\kappa} \log \frac{1}{|\mathcal{A}|} \sum_{a} e^{\kappa Q_{\boldsymbol{w}}(s, a)} \tag{9}$$

where  $\kappa$  is a hyperparameter and  $|\mathcal{A}|$  is the number of actions. The mellow Bellman operator, which 166 we denote as T, has several appealing properties that make it suitable for our settings: (i) it converges 167 to the maximum as  $\kappa \to \infty$ , (ii) it has a unique fixed point, and (iii) it is differentiable. Denoting 168 by  $\widetilde{B}(w) = \widetilde{T}Q_w - Q_w$  the Bellman residual w.r.t. the mellow Bellman operator  $\widetilde{T}$ , we have 169 that the corresponding TD error,  $\left\|\widetilde{B}(\boldsymbol{w})\right\|_{D}^{2}$ , is now differentiable with respect to  $\boldsymbol{w}$ . Although 170 residual algorithms have the sought guaranteed convergence, they are typically much slower than 171 their semi-gradient counterpart. This problem was addressed in [], where the authors proposed a 172 simple remedy consisting in projecting the gradient in a direction that sill guarantees convergence but 173 is also closer to the one of the semi-gradient, thus achieving higher learning speed. This can be easily 174 done by including a parameter  $\psi \in [0,1]$  in the TD error gradient such that: 175

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$$\nabla_{\boldsymbol{w}} \left\| \widetilde{B}(\boldsymbol{w}) \right\|_{D}^{2} = \frac{2}{N} \sum_{i=1}^{N} b_{i}(\boldsymbol{w}) \left( \gamma \psi \nabla_{\boldsymbol{w}} \min_{a'} Q_{\boldsymbol{w}}(s'_{i}, a') - \nabla_{\boldsymbol{w}} Q_{\boldsymbol{w}}(s_{i}, a_{i}) \right)$$
(10)

where  $b_i(\boldsymbol{w}) = r_i + \gamma \, \text{mm}_{a'} \, Q_{\boldsymbol{w}}(s_i', a') - Q_{\boldsymbol{w}}(s_i, a_i)$ . Notice that  $\psi$  trades-off between the semi-gradient ( $\psi = 0$ ) and the full residual gradient ( $\psi = 1$ ). A good criterion for choosing such parameter is to start with values close to zero (to have faster learning) and move to higher values when approaching the optimum (to guarantee converge). Since in our case we are likely to start from this latter point, we consider only higher values (e.g., above 0.5).

### 4 Theoretical Analysis

In this section, we theoretically analyze our variational transfer algorithm...

A first important question that we need to answer is whether replacing max with mellow-max in the Bellman operator constitutes a strong approximation or not. It has been proved [] that the mellow Bellman operator is a contraction under the  $L_{\infty}$ -norm and, thus, has a unique fixed-point. However, how such fixed-point differs from the one of the optimal Bellman operator remains an open question. Since mellow-max monotonically converges to max as  $\kappa \to \infty$ , it would be desirable if the corresponding operator also monotonically converged to the optimal one. We confirm that this property actually holds in the following theorem.

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Theorem 2. Let V be the fixed-point of the optimal Bellman operator T, and Q the corresponding action-value function. Define the action-gap function g(s) as the difference between the value of the best action and the second best action at each state s. Let  $\widetilde{V}$  be the fixed-point of the mellow Bellman operator  $\widetilde{T}$  with parameter  $\kappa > 0$  and denote by  $\beta > 0$  the inverse temperature of the induced Boltzmann distribution (as in []). Let  $\nu$  be a probability measure over the state-space. Then,

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195 for any  $p \geq 1$ :

$$\left\|V - \widetilde{V}\right\|_{\nu,p}^{p} \le \frac{2R_{max}}{(1-\gamma)^{2}} \left\|1 - \frac{1}{1+|\mathcal{A}|e^{-\beta g}}\right\|_{\nu,p}^{p}$$
 (11)

- 196 5 Related Works
- 197 **6 Experiments**
- 198 6.1 Gridworld
- 199 6.2 Classic Control
- 200 6.3 Maze Navigation
- 7 Conclusion
- 202 References
- [1] Martin L. Puterman. Markov Decision Processes: Discrete Stochastic Dynamic Programming. John Wiley
   & Sons, Inc., New York, NY, USA, 1994.

### 205 A Proofs

Theorem 2. Let V be the fixed-point of the optimal Bellman operator T, and Q the corresponding action-value function. Define the action-gap function g(s) as the difference between the value of the best action and the second best action at each state s. Let  $\widetilde{V}$  be the fixed-point of the mellow Bellman operator  $\widetilde{T}$  with parameter  $\kappa > 0$  and denote by  $\beta > 0$  the inverse temperature of the induced Boltzmann distribution (as in []). Let  $\nu$  be a probability measure over the state-space. Then, Cite MM for any  $p \geq 1$ :

$$\left\| V - \widetilde{V} \right\|_{\nu,p}^{p} \le \frac{2R_{max}}{(1 - \gamma)^{2}} \left\| 1 - \frac{1}{1 + |\mathcal{A}| e^{-\beta g}} \right\|_{\nu,p}^{p} \tag{11}$$

212 *Proof.* We begin by noticing that:

$$\begin{split} \left\| V - \widetilde{V} \right\|_{\nu,p}^{p} &= \left\| TV - \widetilde{T}\widetilde{V} \right\|_{\nu,p}^{p} \\ &= \left\| TV - \widetilde{T}V + \widetilde{T}V - \widetilde{T}\widetilde{V} \right\|_{\nu,p}^{p} \\ &\leq \left\| TV - \widetilde{T}V \right\|_{\nu,p}^{p} + \left\| \widetilde{T}V - \widetilde{T}\widetilde{V} \right\|_{\nu,p}^{p} \\ &\leq \left\| TV - \widetilde{T}V \right\|_{\nu,p}^{p} + \gamma \left\| V - \widetilde{V} \right\|_{\nu,p}^{p} \end{split}$$

where the first inequality follows from Minkowsky's inequality and the second one from the contraction property of the mellow Bellman operator. This implies that:

$$\left\|V - \widetilde{V}\right\|_{\nu,p}^{p} \le \frac{1}{1 - \gamma} \left\|TV - \widetilde{T}V\right\|_{\nu,p}^{p} \tag{12}$$

Let us bound the norm on the right-hand side separately. In order to do that, we will bound the function  $\left|TV(s) - \widetilde{T}V(s)\right|$  point-wisely for any state s. By applying the definition of the optimal and mellow Bellman operators, we obtain:

$$\begin{aligned} \left| TV(s) - \widetilde{T}V(s) \right| &= \left| \max_{a} \{ R(s, a) + \gamma \mathbb{E} \left[ V(s') \right] \} - \min_{a} \{ R(s, a) + \gamma \mathbb{E} \left[ V(s') \right] \} \right| \\ &= \left| \max_{a} Q(s, a) - \min_{a} Q(s, a) \right| \end{aligned}$$

Recall that applying the mellow-max is equivalent to computing an expectation under a Boltzmann distribution with inverse temperature  $\beta$  induced by  $\kappa$  []. Thus, we can write:

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$$\left| \max_{a} Q(s, a) - \min_{a} Q(s, a) \right| = \left| \sum_{a} \pi^{*}(a|s)Q(s, a) - \sum_{a} \pi_{\beta}(a|s)Q(s, a) \right|$$

$$= \left| \sum_{a} Q(s, a) \left( \pi^{*}(a|s) - \pi_{\beta}(a|s) \right) \right|$$

$$\leq \sum_{a} |Q(s, a)| \left| \pi^{*}(a|s) - \pi_{\beta}(a|s) \right|$$

$$\leq \frac{R_{max}}{1 - \gamma} \sum_{a} |\pi^{*}(a|s) - \pi_{\beta}(a|s)$$

$$(13)$$

where  $\pi^*$  is the optimal (deterministic) policy w.r.t. Q and  $\pi_{\beta}$  is the Boltzmann distribution induced by Q with inverse temperature  $\beta$ :

$$\pi_{\beta}(a|s) = \frac{e^{\beta Q(s,a)}}{\sum_{a'} e^{\beta Q(s,a')}}$$

Denote by  $a_1(s)$  the optimal action for state s under Q. We can then write:

$$\sum_{a} |\pi^{*}(a|s) - \pi_{\beta}(a|s)| = |\pi^{*}(a_{1}(s)|s) - \pi_{\beta}(a_{1}(s)|s)| + \sum_{a \neq a_{1}(s)} |\pi^{*}(a|s) - \pi_{\beta}(a|s)|$$

$$= |1 - \pi_{\beta}(a_{1}(s)|s)| + \sum_{a \neq a_{1}(s)} |\pi_{\beta}(a|s)|$$

$$= 2|1 - \pi_{\beta}(a_{1}(s)|s)| \tag{14}$$

Finally, let us bound this last term:

$$|1 - \pi_{\beta}(a_{1}(s)|s)| = \left|1 - \frac{e^{\beta Q(s,a_{1}(s))}}{\sum_{a'} e^{\beta Q(s,a')}}\right|$$

$$= \left|1 - \frac{e^{\beta(Q(s,a_{1}(s)) - Q(s,a_{2}(s)))}}{\sum_{a'} e^{\beta(Q(s,a') - Q(s,a_{2}(s)))}}\right|$$

$$= \left|1 - \frac{e^{\beta g(s)}}{\sum_{a'} e^{\beta(Q(s,a') - Q(s,a_{2}(s)))}}\right|$$

$$= \left|1 - \frac{e^{\beta g(s)}}{e^{\beta g(s)} + \sum_{a' \neq a_{1}(s)} e^{\beta(Q(s,a') - Q(s,a_{2}(s)))}}\right|$$

$$\leq \left|1 - \frac{e^{\beta g(s)}}{e^{\beta g(s)} + |\mathcal{A}|}\right|$$

$$= \left|1 - \frac{1}{1 + |\mathcal{A}| e^{-\beta g(s)}}\right|$$
(15)

224 Combining Eq. (13), (14), and (15), we obtain:

$$\left| \max_{a} Q(s, a) - \min_{a} Q(s, a) \right| \le \frac{2R_{max}}{1 - \gamma} \left| 1 - \frac{1}{1 + |\mathcal{A}| e^{-\beta g(s)}} \right|$$

- Taking the norm and plugging this into Eq. (12) concludes the proof.
- Lemma 1. Let p and  $\nu$  denote probability measures over Q-functions and state-action pairs, respectively. Assume  $Q^*$  is the unique fixed-point of the optimal Bellman operator T. Then, for any  $\delta > 0$ ,
- with probability at least  $1 \delta$  over the choice of a Q-function Q, the following holds:

$$\|Q - Q^*\|_{\nu}^2 \le \frac{\mathbb{E}_p\left[\|B(Q)\|_{\nu}^2\right]}{(1 - \gamma)\delta}$$
 (16)

229 *Proof.* First notice that:

$$\begin{split} \|Q - Q^*\| &= \|Q + TQ - TQ - TQ^*\| \\ &\leq \|Q - TQ\| + \|TQ - TQ^*\| \\ &\leq \|Q - TQ\| + \gamma \|Q - Q^*\| \\ &= \|B(Q)\| + \gamma \|Q - Q^*\| \end{split}$$

230 which implies that:

$$||Q - Q^*|| \le \frac{1}{1 - \gamma} ||B(Q)||$$

Then we can write:

$$P\left(\|Q - Q^*\| > \epsilon\right) \le P\left(\|B(Q)\| > \epsilon(1 - \gamma)\right) \le \frac{\mathbb{E}_p\left[\|B(Q)\|_{\nu}^2\right]}{(1 - \gamma)\epsilon}$$

Settings the right-hand side equal to  $\delta$  and solving for  $\epsilon$  concludes the proof.

Corollary 1. Let p and  $\nu$  denote probability measures over Q-functions and state-action pairs, respectively. Assume  $\widetilde{Q}$  is the unique fixed-point of the mellow Bellman operator  $\widetilde{T}$ . Then, for any  $\delta > 0$ , with probability at least  $1 - \delta$  over the choice of a Q-function Q, the following holds:

$$\left\| Q - \widetilde{Q} \right\|_{\nu}^{2} \leq \frac{\mathbb{E}_{p} \left[ \left\| \widetilde{B}(Q) \right\|_{\nu}^{2} \right]}{(1 - \gamma)\delta} \tag{17}$$

Lemma 2. Assume Q-functions belong to a parametric space of functions bounded by  $\frac{R_{max}}{1-\gamma}$ . Let p and q be arbitrary distributions over the parameter space W, and  $\nu$  be a probability measure over  $S \times A$ . Consider a dataset D of N samples and define  $v(w) \triangleq \mathbb{E}_{\nu} [Var_{\mathcal{P}}[b(w)]]$ . Then, for any  $\delta > 0$ , with probability at least  $1 - \delta$ , the following two inequalities hold simultaneously:

$$\mathbb{E}_{q}\left[\left\|B(\boldsymbol{w})\right\|_{\nu}^{2}\right] \leq \mathbb{E}_{q}\left[\left\|B(\boldsymbol{w})\right\|_{D}^{2}\right] - \mathbb{E}_{q}\left[v(\boldsymbol{w})\right] + \frac{\lambda}{N}KL(q||p) + 4\frac{R_{max}^{2}}{(1-\gamma)^{2}}\sqrt{\frac{\log\frac{2}{\delta}}{2N}}$$
(18)

 $\mathbb{E}_{q}\left[\|B(\boldsymbol{w})\|_{D}^{2}\right] \leq \mathbb{E}_{q}\left[\|B(\boldsymbol{w})\|_{\nu}^{2}\right] + \mathbb{E}_{q}\left[v(\boldsymbol{w})\right] + \frac{\lambda}{N}KL(q||p) + 4\frac{R_{max}^{2}}{(1-\gamma)^{2}}\sqrt{\frac{\log\frac{2}{\delta}}{2N}}$ (19)

241 *Proof.* From Hoeffding's inequality we have:

240

$$P\left(\left|\mathbb{E}_{\nu,\mathcal{P}}\left[\left\|B(\boldsymbol{w})\right\|_{D}^{2}\right]-\left\|B(\boldsymbol{w})\right\|_{D}^{2}\right|>\epsilon\right)\leq 2exp\left(-\frac{2N\epsilon^{2}}{\left(2\frac{R_{max}}{1-\gamma}\right)^{4}}\right)$$

which implies that, for any  $\delta > 0$ , with probability at least  $1 - \delta$ :

$$\left| \mathbb{E}_{\nu,\mathcal{P}} \left[ \|B(\boldsymbol{w})\|_D^2 \right] - \|B(\boldsymbol{w})\|_D^2 \right| \le 4 \frac{R_{max}^2}{(1-\gamma)^2} \sqrt{\frac{\log \frac{2}{\delta}}{2N}}$$

243 Under independence assumptions, the expected TD error can be re-written as:

$$\mathbb{E}_{\nu,\mathcal{P}}\left[\left\|B(\boldsymbol{w})\right\|_{D}^{2}\right] = \mathbb{E}_{\nu,\mathcal{P}}\left[\frac{1}{N}\sum_{i=1}^{N}(r_{i} + \gamma \min_{a'}Q_{\boldsymbol{w}}(s'_{i}, a') - Q_{\boldsymbol{w}}(s_{i}, a_{i}))^{2}\right]$$

$$= \mathbb{E}_{\nu,\mathcal{P}}\left[\left(R(s, a) + \gamma \max_{a'}Q_{\boldsymbol{w}}(s', a') - Q_{\boldsymbol{w}}(s, a)\right)^{2}\right]$$

$$= \mathbb{E}_{\nu}\left[\mathbb{E}_{\mathcal{P}}\left[b(\boldsymbol{w})^{2}\right]\right]$$

$$= \mathbb{E}_{\nu}\left[Var_{\mathcal{P}}\left[b(\boldsymbol{w})\right] + \mathbb{E}_{\mathcal{P}}\left[b(\boldsymbol{w})\right]^{2}\right]$$

$$= v(\boldsymbol{w}) + \|B(\boldsymbol{w})\|_{\nu}^{2}$$

where  $v(\boldsymbol{w}) \triangleq \mathbb{E}_{\nu} \left[ Var_{\mathcal{P}} \left[ b(\boldsymbol{w}) \right] \right]$ . Thus:

$$\left| \|B(\boldsymbol{w})\|_{\nu}^{2} + v(\boldsymbol{w}) - \|B(\boldsymbol{w})\|_{D}^{2} \right| \leq 4 \frac{R_{max}^{2}}{(1 - \gamma)^{2}} \sqrt{\frac{\log \frac{2}{\delta}}{2N}}$$
 (20)

From the change of measure inequality [], we have that, for any measurable function f(w) and any two probability measures p and q:

Find a reference for this

$$\log \mathbb{E}_p \left[ e^{f(\boldsymbol{w})} \right] \ge \mathbb{E}_q \left[ f(\boldsymbol{w}) \right] - KL(q||p)$$

Thus, multiplying both sides of (20) by  $\lambda^{-1}N$  and applying the change of measure inequality with  $f(\boldsymbol{w}) = \lambda^{-1}N \left| \|B(\boldsymbol{w})\|_{\nu}^2 + v(\boldsymbol{w}) - \|B(\boldsymbol{w})\|_D^2 \right|$ , we obtain:

$$\mathbb{E}_{q}\left[f(\boldsymbol{w})\right] - KL(q||p) \le \log \mathbb{E}_{p}\left[e^{f(\boldsymbol{w})}\right] \le 4\frac{R_{max}^{2}\lambda^{-1}N}{(1-\gamma)^{2}}\sqrt{\frac{\log \frac{2}{\delta}}{2N}}$$

where the second inequality holds since the right-hand side of (20) does not depend on w. Finally, we can explicitly write:

$$\mathbb{E}_{q}\left[\left|\left\|B(\boldsymbol{w})\right\|_{\nu}^{2}+v(\boldsymbol{w})-\left\|B(\boldsymbol{w})\right\|_{D}^{2}\right|\right]\leq\frac{\lambda}{N}KL(q||p)+4\frac{R_{max}^{2}}{(1-\gamma)^{2}}\sqrt{\frac{\log\frac{2}{\delta}}{2N}}$$

251 from which the lemma follows straightforwardly.

Lemma 3. Let p be a prior distribution over the parameter space  $\mathcal{W}$ , and  $\nu$  be a probability measure over  $\mathcal{S} \times \mathcal{A}$ . Assume  $\widehat{\xi}$  is the minimizer of  $ELBO(\xi) = \mathbb{E}_{q_{\xi}} \left[ \|B(\boldsymbol{w})\|_{D}^{2} \right] + \frac{\lambda}{N} KL(q_{\xi}||p)$  for a dataset D of N samples. Define  $v(\boldsymbol{w}) \triangleq \mathbb{E}_{\nu} \left[ Var_{\mathcal{P}} \left[ b(\boldsymbol{w}) \right] \right]$ . Then, for any  $\delta > 0$ , with probability at least  $1 - \delta$ :

$$\mathbb{E}_{q_{\widehat{\xi}}}\left[\left\|B(\boldsymbol{w})\right\|_{\nu}^{2}\right] \leq \inf_{\xi \in \Xi} \left\{ \mathbb{E}_{q_{\xi}}\left[\left\|B(\boldsymbol{w})\right\|_{\nu}^{2}\right] + \mathbb{E}_{q_{\xi}}\left[v(\boldsymbol{w})\right] + 2\frac{\lambda}{N}KL(q_{\xi}||p)\right\} + 2\frac{R_{max}^{2}}{(1-\gamma)^{2}}\sqrt{\frac{\log\frac{2}{\delta}}{N}}$$

256 *Proof.* Let us use Lemma 2 for the specific choice  $q = q_{\widehat{\epsilon}}$ . From Eq. (18), we have:

$$\begin{split} \mathbb{E}_{q_{\widehat{\xi}}}\left[\left\|B(\boldsymbol{w})\right\|_{\nu}^{2}\right] &\leq \mathbb{E}_{q_{\widehat{\xi}}}\left[\left\|B(\boldsymbol{w})\right\|_{D}^{2}\right] - \mathbb{E}_{q_{\widehat{\xi}}}\left[v(\boldsymbol{w})\right] + \frac{\lambda}{N}KL(q_{\widehat{\xi}}||p) + 4\frac{R_{max}^{2}}{(1-\gamma)^{2}}\sqrt{\frac{\log\frac{2}{\delta}}{2N}} \\ &\leq \mathbb{E}_{q_{\widehat{\xi}}}\left[\left\|B(\boldsymbol{w})\right\|_{D}^{2}\right] + \frac{\lambda}{N}KL(q_{\widehat{\xi}}||p) + 4\frac{R_{max}^{2}}{(1-\gamma)^{2}}\sqrt{\frac{\log\frac{2}{\delta}}{2N}} \\ &= \inf_{\xi \in \Xi}\left\{\mathbb{E}_{q_{\xi}}\left[\left\|B(\boldsymbol{w})\right\|_{D}^{2}\right] + \frac{\lambda}{N}KL(q_{\xi}||p)\right\} + 4\frac{R_{max}^{2}}{(1-\gamma)^{2}}\sqrt{\frac{\log\frac{2}{\delta}}{2N}} \end{split}$$

where the second inequality holds since  $v(\boldsymbol{w}) > 0$ , while the equality holds from the definition of  $\widehat{\xi}$ .

We can now use Eq. (19) to bound  $\mathbb{E}_{q_{\xi}} \left[ \|B(\boldsymbol{w})\|_{D}^{2} \right]$ , thus obtaining:

$$\mathbb{E}_{q_{\widehat{\xi}}}\left[\left\|B(\boldsymbol{w})\right\|_{\nu}^{2}\right] \leq \inf_{\xi \in \Xi} \left\{\mathbb{E}_{q_{\xi}}\left[\left\|B(\boldsymbol{w})\right\|_{\nu}^{2}\right] + \mathbb{E}_{q_{\xi}}\left[v(\boldsymbol{w})\right] + 2\frac{\lambda}{N}KL(q_{\xi}||p)\right\} + 2\frac{R_{max}^{2}}{(1-\gamma)^{2}}\sqrt{\frac{\log\frac{2}{\delta}}{N}}$$

259 This concludes the proof.