# Planning to Be Surprised: Optimal Bayesian Exploration in Dynamic Environments

Yi Sun, Faustino Gomez, and Jürgen Schmidhuber

IDSIA

**Abstract.** To maximize its success, an AGI typically needs to explore its initially unknown world. Is there an optimal way of doing so? Here we derive an affirmative answer for a broad class of environments.

### 1 Introduction

An intelligent agent is sent to explore an unknown environment. Over the course of its mission, the agent makes observations, carries out actions, and incrementally builds up a model of the environment from this interaction. Since the way in which the agent selects actions may greatly affect the efficiency of the exploration, the following question naturally arises:

How should the agent choose the actions such that the knowledge about the environment accumulates as quickly as possible?

In this paper, this question is addressed under a classical framework, in which the agent improves its model of the environment through probabilistic inference, and learning progress is measured in terms of Shannon information gain. We show that the agent can, at least in principle, optimally choose actions based on previous experiences, such that the cumulative expected information gain is maximized. We then consider a special case, namely exploration in finite MDPs, where we demonstrate, both in theory and through experiment, that the optimal Bayesian exploration strategy can be effectively approximated by solving a sequence of dynamic programming problems.

The rest of the paper is organized as follows: Section 2 reviews the basic concepts and establishes the terminology; Section 3 elaborates the principle of optimal Bayesian exploration; Section 4 focuses on exploration in finite MDP; Section 5 presents a simple experiment; The related works are briefly reviewed in Section 6; Section 7 concludes the paper.

### 2 Preliminaries

Suppose that the agent interacts with the environment in discrete time cycles t = 1, 2, ... In each cycle, the agent performs an action a, then receives a sensory input o. A history h is either the empty string  $\emptyset$  or a string of the form  $a_1o_1 \cdots a_to_t$  for some t, and ha and hao refer to the strings resulting from appending a and ao to h, respectively.

#### 2.1 Learning from Sequential Interactions

To facilitate the subsequent discussion under a probabilistic framework, we make the following assumptions:

- Assumption I. The models of the environment under consideration are fully described by a random element  $\Theta$  which *depends solely on the environment*. Moreover, the agent's initial knowledge about  $\Theta$  is summarized by a prior density  $p(\theta)$ .
- Assumption II. The agent is equipped with a conditional predictor  $p(o|ha; \theta)$ , i.e. the agent is capable of refining its prediction in the light of information about  $\Theta$ .

Using  $p(\theta)$  and  $p(o|ha;\theta)$  as building blocks, it is straightforward to formulate learning in terms of probabilistic inference. From Assumption I, given the history h, the agent's knowledge about  $\Theta$  is fully summarized by  $p(\theta|h)$ . According to Bayes rule,  $p(\theta|hao) = \frac{p(\theta|ha)p(o|ha;\theta)}{p(o|ha)}$ , with  $p(o|ha) = \int p(o|ha, \theta) p(\theta|h) d\theta$ . The term  $p(\theta|ha)$  represents the agent's current knowledge about  $\Theta$  given history h and an additional action a. Since  $\Theta$  depends solely on the environment, and, importantly, knowing the action without subsequent observations cannot change the agent's state of knowledge about  $\Theta$ ,  $p(\theta|ha) = p(\theta|h)$ , hence the knowledge about  $\Theta$  can be updated using

$$p(\theta|hao) = p(\theta|h) \cdot \frac{p(o|ha;\theta)}{p(o|ha)}.$$
(1)

It is worth pointing out that  $p(o|ha;\theta)$  is chosen a priori. It is not required that they match the true dynamics of the environment, but the effectiveness of the learning certainly depends on the choices of  $p(o|ha;\theta)$ . For example, if  $\Theta \in \mathbb{R}$ , and  $p(o|ha;\theta)$  depends on  $\theta$  only through its sign, then no knowledge other than the sign of  $\Theta$  can be learned.

### 2.2 Information Gain as Learning Progress

Let h and h' be two histories such that h is a prefix of h'. The respective posterior of  $\Theta$  are  $p(\theta|h)$  and  $p(\theta|h')$ . Using h as a reference point, the amount of information gained when the history grows to h', can be measured using the KL divergence between  $p(\theta|h)$  and  $p(\theta|h')$ . This *information gain* from h to h' is defined as

$$g(h'||h) = KL\left(p\left(\theta|h'\right)||p\left(\theta|h\right)\right) = \int p\left(\theta|h'\right)\log\frac{p\left(\theta|h'\right)}{p\left(\theta|h\right)}d\theta.$$

As a special case, if  $h = \emptyset$ , then  $g(h') = g(h' || \emptyset)$  is the *cumulative information* gain with respect to the prior  $p(\theta)$ . We also write g(ao || h) for g(hao || h), which denotes the information gained from an additional action-observation pair.

From an information theoretic point of view, the KL divergence between two distributions p and q represents the additional number of bits required to encode

elements sampled from p, using optimal coding strategy designed for q. This can be interpreted as the degree of 'unexpectedness' or 'surprise' caused by observing samples from p when expecting samples from q.

The key property information gain for the treatment below is the following decomposition: Let h be a prefix of h' and h' be a prefix of h'', then

$$\begin{split} & \mathbb{E}_{h''|h'}g\left(h''\|h\right) \\ &= \mathbb{E}_{h''|h'}\int p\left(\theta|h''\right)\log\frac{p\left(\theta|h''\right)}{p\left(\theta|h\right)}d\theta \\ &= \mathbb{E}_{h''|h'}\int p\left(\theta|h''\right)\left[\log\frac{p\left(\theta|h''\right)}{p\left(\theta|h'\right)} + \log\frac{p\left(\theta|h'\right)}{p\left(\theta|h\right)}\right]d\theta \\ &= \mathbb{E}_{h''|h'}\int p\left(\theta|h''\right)\log\frac{p\left(\theta|h''\right)}{p\left(\theta|h'\right)}d\theta + \int \mathbb{E}_{h''|h'}p\left(\theta|h''\right)\log\frac{p\left(\theta|h'\right)}{p\left(\theta|h\right)}d\theta \\ &= \mathbb{E}_{h''|h'}g\left(h''\|h'\right) + \int \mathbb{E}_{h''|h'}p\left(\theta|h''\right)\log\frac{p\left(\theta|h'\right)}{p\left(\theta|h\right)}d\theta. \end{split}$$

From updating formula Eq.1,

$$\sum_{o} p(o|ha) p(\theta|hao) = \sum_{o} p(\theta|h) p(o|ha, \theta)$$
$$= p(\theta|h) \sum_{o} p(o|ha, \theta)$$
$$= p(\theta|h).$$

Using this relation recursively,

$$\mathbb{E}_{h''|h'} p\left(\theta|h''\right) = \sum_{a_1} \sum_{o_1} \cdots \sum_{a_t} \sum_{o_t} p\left(\theta|h'a_1 o_1 \cdots a_t o_t\right)$$
$$= \sum_{a_1} \sum_{o_1} \cdots \sum_{a_{t-1}} \sum_{o_{t-1}} p\left(\theta|h'a_1 o_1 \cdots a_{t-1} o_{t-1}\right)$$
$$= \cdots$$
$$= p\left(\theta|h'\right),$$

therefore

$$\mathbb{E}_{h''|h'}g(h''\|h) = g(h'\|h) + \mathbb{E}_{h''|h'}g(h''\|h').$$
(2)

That is, the information gain is additive in expectation.

Having defined the information gain from trajectories ending with observations, one may proceed to define the *expected information gain* of performing action a, before observing the outcome o. Formally, the *expected information gain* of performing a with respect to the current history h is given by

 $g(a||h) = \mathbb{E}_{o|ha}g(ao||h)$ . A simple derivation gives

$$\begin{split} g\left(a\|h\right) &= \sum_{o} p\left(o|ha\right) \int p\left(\theta|hao\right) \log \frac{p\left(\theta|hao\right)}{p\left(\theta|h\right)} d\theta \\ &= \sum_{o} \int p\left(o,\theta|ha\right) \log \frac{p\left(\theta|hao\right) p\left(o|ha\right)}{p\left(\theta|h\right) p\left(o|ha\right)} d\theta \\ &= \sum_{o} \int p\left(o,\theta|ha\right) \log \frac{p\left(o,\theta|ha\right)}{p\left(\theta|ha\right) p\left(o|ha\right)} d\theta \\ &= I\left(O;\Theta|ha\right), \end{split}$$

which means that g(a||h) is the mutual information between  $\Theta$  and the random variable O representing the unknown observation, conditioned on the history h and action a.<sup>1</sup>

# **3** Optimal Bayesian Exploration

In this section, the general principle of optimal Bayesian exploration in dynamic environments is presented. We first give results obtained by assuming a fixed limited life span for our agent, then discuss a condition required to extend this to infinite time horizons.

### 3.1 Results for Finite Time Horizon

Suppose that the agent has experienced history h, and is about to choose  $\tau$  more actions in the future. Let  $\pi$  be a policy mapping the set of histories to the set of actions, such that the agent performs a with probability  $\pi(a|h)$  given h. Define the *curiosity Q-value*  $q_{\pi}^{\tau}(h, a)$  as the expected information gained from the additional  $\tau$  actions, assuming that the agent performs a in the next step and follows policy  $\pi$  in the remaining  $\tau - 1$  steps. Formally, for  $\tau = 1$ ,

$$q_{\pi}^{1}(h,a) = \mathbb{E}_{o|ha}g\left(ao||h\right) = g\left(a||h\right),$$

and for  $\tau > 1$ ,

$$q_{\pi}^{\tau}(h,a) = \mathbb{E}_{o|ha} \mathbb{E}_{a_1|hao} \mathbb{E}_{o_1|haoa_1} \cdots \mathbb{E}_{o_{\tau-1}|h\cdots a_{\tau-1}} g(haoa_1o_1\cdots a_{\tau-1}o_{\tau-1}\|h) = \mathbb{E}_{o|ha} \mathbb{E}_{a_1o_1\cdots a_{\tau-1}o_{\tau-1}|hao} g(haoa_1o_1\cdots a_{\tau-1}o_{\tau-1}\|h).$$

<sup>&</sup>lt;sup>1</sup> Side note: To generalize the discussion, concepts from algorithmic information theory, such as compression distance, may also be used here. However, restricting the discussion under a probabilistic framework greatly simplifies the matter.

The curiosity Q-value can be defined recursively. Applying Eq. 2 for  $\tau = 2$ ,

$$q_{\pi}^{\tau}(h,a) = \mathbb{E}_{o|ha} \mathbb{E}_{a_1o_1|hao}g(haoa_1o_1||h)$$
  
=  $\mathbb{E}_{o|ha} \left[ g(ao||h) + \mathbb{E}_{a_1o_1|hao}g(a_1o_1||hao) \right]$   
=  $g(a||h) + \mathbb{E}_{o|ha} \mathbb{E}_{a'|hao} q_{\pi}^1(hao,a').$ 

And for  $\tau > 2$ ,

$$q_{\pi}^{\tau}(h,a) = \mathbb{E}_{o|ha} \mathbb{E}_{a_{1}o_{1}\cdots a_{\tau-1}o_{\tau-1}|hao}g(haoa_{1}o_{1}\cdots a_{\tau-1}o_{\tau-1}\|h) = \mathbb{E}_{o|ha} \left[g(ao\|h) + \mathbb{E}_{a_{1}o_{1}\cdots a_{\tau-1}o_{\tau-1}}g(haoa_{1}o_{1}\cdots a_{\tau-1}o_{\tau-1}\|hao)\right] = g(a\|h) + \mathbb{E}_{o|ha} \mathbb{E}_{a'|hao} q_{\pi}^{\tau-1}(hao,a').$$
(3)

Noting that Eq.3 bears great resemblance to the definition of state-action values (Q(s, a)) in reinforcement learning, one can similarly define the *curiosity value* of a particular history as  $v_{\pi}^{\tau}(h) = \mathbb{E}_{a|h} q_{\pi}^{\tau}(h, a)$ , analogous to state values (V(s)), which can also be iteratively defined as  $v_{\pi}^{1}(h) = \mathbb{E}_{a|h} g(a||h)$ , and

$$v_{\pi}^{\tau}(h) = \mathbb{E}_{a|h} \left[ g\left( a \| h \right) + \mathbb{E}_{o|ha} v_{\pi}^{\tau-1} \left( hao \right) \right].$$

The curiosity value  $v_{\pi}^{\tau}(h)$  is the expected information gain of performing the additional  $\tau$  steps, assuming that the agent follows policy  $\pi$ . The two notations can be combined to write

$$q_{\pi}^{\tau}(h,a) = g(a||h) + \mathbb{E}_{o|ha} v_{\pi}^{\tau-1}(hao).$$
(4)

This equation has an interesting interpretation: since the agent is operating in a dynamic environment, it has to take into account not only the immediate expected information gain of performing the current action, i.e., g(a||h), but also the expected curiosity value of the situation in which the agent ends up due to the action, i.e.,  $v_{\pi}^{\tau-1}$  (hao). As a consequence, the agent needs to choose actions that balance the two factors in order to improve its total expected information gain.

Now we show that there is a optimal policy  $\pi_*$ , which leads to the maximum cumulative expected information gain given any history h. To obtain the optimal policy, one may work backwards in  $\tau$ , taking greedy actions with respect to the curiosity Q-values at each time step. Namely, for  $\tau = 1$ , let

$$q^{1}(h,a) = g(a||h), \pi^{1}_{*}(h) = \arg\max_{a} g(a||h), \text{ and } v^{1}(h) = \max_{a} g(a||h),$$

such that  $v^{1}(h) = q^{1}(h, \pi^{1}(h))$ , and for  $\tau > 1$ , let

$$q^{\tau}(h,a) = g(a||h) + \mathbb{E}_{o|ha} \left[ \max_{a'} q^{\tau-1} (a'|hao) \right] = g(a||h) + \mathbb{E}_{o|ha} v^{\tau-1} (hao),$$

with  $\pi_*^{\tau}(h) = \arg \max_a q^{\tau}(h, a)$  and  $v^{\tau}(h) = \max_a q^{\tau}(h, a)$ . We show that  $\pi_*^{\tau}(h)$  is indeed the optimal policy for any given  $\tau$  and h in the sense that

the curiosity value, when following  $\pi^{\tau}_{*}$ , is maximized. To see this, take any other strategy  $\pi$ , first notice that

$$v^{1}(h) = \max_{a} g(a \| h) \ge \mathbb{E}_{a|h} g(a \| h) = v_{\pi}^{1}(h).$$

Moreover, assuming  $v^{\tau}(h) \geq v_{\pi}^{\tau}(h)$ ,

$$v^{\tau+1}(h) = \max_{a} \left[ g\left(a\|h\right) + \mathbb{E}_{o|ha}v^{\tau}\left(hao\right) \right] \ge \max_{a} \left[ g\left(a\|h\right) + \mathbb{E}_{o|ha}v^{\tau}_{\pi}\left(hao\right) \right]$$
$$\ge \mathbb{E}_{a|h} \left[ g\left(a\|h\right) + \mathbb{E}_{o|ha}v^{\tau}_{\pi}\left(hao\right) \right] = v^{\tau+1}_{\pi}(h) \,.$$

Therefore  $v^{\tau}(h) \ge v_{\pi}^{\tau}(h)$  holds for arbitrary  $\tau$ , h, and  $\pi$ . The same can be shown for curiosity Q-values, namely,  $q^{\tau}(h, a) \ge q_{\pi}^{\tau}(h, a)$ , for all  $\tau$ , h, a, and  $\pi$ . It may be beneficial to write  $q^{\tau}$  in explicit forms, namely,

$$q^{\tau}(h,a) = \mathbb{E}_{o|ha} \max_{a_1} \mathbb{E}_{o_1|haoa_1} \cdots \max_{a_{\tau-1}} \mathbb{E}_{o_{\tau-1}|h\cdots a_{\tau-1}} g(haoa_1o_1 \cdots a_{\tau-1}o_{\tau-1}||h).$$

Now consider that the agent has a fixed life span T. It can be seen that at time t, the agent has to perform  $\pi_*^{T-t}(h_{t-1})$  to maximize the expected information gain in the remaining T-t steps. Here  $h_{t-1} = a_1 o_1 \cdots a_{t-1} o_{t-1}$  is the history at time t. However, from Eq.2,

$$\mathbb{E}_{h_T|h_{t-1}}g(h_T) = g(h_{t-1}) + \mathbb{E}_{h_T|h_{t-1}}g(h_T||h_{t-1}).$$

Note that at time t,  $g(h_{t-1})$  is a constant, thus maximizing the cumulative expected information gain in the remaining time steps is equivalent to maximizing the expected information gain of the whole trajectory with respect to the prior. The result is summarized in the following proposition:

**Proposition 1.** Let  $q_1(h, a) = \bar{g}(a||h), v_1(h) = \max_a q_1(h, a), and$ 

$$q_{\tau}(h,a) = \bar{g}(a||h) + \mathbb{E}_{o|ha}v_{\tau-1}(hao), v_{\tau}(h) = \max_{a} q_{\tau}(h,a),$$

then the policy  $\pi_{\tau}^{*}(h) = \arg \max_{a} q_{\tau}(h, a)$  is optimal in the sense that  $v_{\tau}(h) \geq v_{\tau}^{\pi}(h)$ ,  $q_{\tau}(h, a) \geq q_{\tau}^{\pi}(h, a)$  for any  $\pi, \tau$ , h and a. In particular, for an agent with fixed life span T, following  $\pi_{T-t}^{*}(h_{t-1})$  at time  $t = 1, \ldots, T$  is optimal in the sense that the expected cumulative information gain with respect to the prior is maximized.

### 3.2 Non-triviality of the Result

Intuitively, the interpretation of the recursive definition of the curiosity (Q) value is simple, and bears clear resemblance to their counterparts in reinforcement learning. It might be tempting to think that the result is nothing more than solving the finite horizon reinforcement learning problem using g(a||h) or g(ao||h) as the reward signals. However, this is not the case.

First, note that the decomposition Eq.2 is a direct consequence of the formulation of the KL divergence. The decomposition does not necessarily hold if g(h) is replaced with other types of measures of information gain.

Second, it is worth pointing out that g(ao||h) and g(a||h) behave differently from normal reward signals in the sense that they are *additive only in expectation*, while in the reinforcement learning setup, the reward signals are usually assumed to be additive, i.e., adding reward signals together is always meaningful. Consider a simple problem with only two actions. If g(ao||h) is a plain reward function, then g(ao||h) + g(a'o'||hao) should be meaningful, no matter if a and o is known or not. But this is not the case, since the sum does not have a valid information theoretic interpretation. On the other hand, the sum is meaningful *in expectation*. Namely, when o has *not* been observed, from Eq.2,

$$g(ao||h) + \mathbb{E}_{o'|haoa'}g(a'o'||hao) = \mathbb{E}_{o'|haoa'}g(aoa'o'||h),$$

the sum can be interpreted as the expectation of the information gained from h to haoa'o'. This result shows that g(a||h) or g(ao||h) can be treated as additive reward signals only when one is planning ahead.

To emphasize the difference further, note that all immediate information gains g(ao||h) are non-negative since they are essentially KL divergence. A natural assumption would be that the information gain g(h), which is the sum of all g(ao||h) in expectation, grows monotonically when the length of the history increases. However, this is not the case, see Figure 1 for example. Although g(ao||h) is always non-negative, some of the gain may pull  $\theta$  closer to its prior density  $p(\theta)$ , resulting in a decrease of KL divergence between  $p(\theta|h)$  and  $p(\theta)$ . This is never the case if one considers the normal reward signals in reinforcement learning, where the accumulated reward would never decrease if all rewards are non-negative.

### 3.3 The Algorithm

The definition of the optimal exploration policy is constructive, which means that it can be readily implemented, provided that the number of actions and possible observations is finite so that the expectation and maximization can be computed exactly.

The following two algorithms computes the maximum curiosity value  $v^{\tau}(h)$ and the maximum curiosity Q-value  $q^{\tau}(h, a)$ , respectively, assuming that the expected immediate gain g(a||h) can be computed.



**Fig. 1.** Illustration of the difference between the sum of one-step information gain and the cumulative information gain with respect to the prior. In this case, 1000 independent samples are generated from a distribution over finite sample space  $\{1, 2, 3\}$ , with p(x = 1) = 0.1, p(x = 2) = 0.5, and p(x = 3) = 0.4. The task of learning is to recover the mass function from the samples, assuming a Dirichlet prior  $Dir\left(\frac{50}{3}, \frac{50}{3}, \frac{50}{3}\right)$ . The KL divergence between two Dirichlet distributions are computed according to [6]. It is clear from the graph that the cumulative information gain fluctuates when the number of samples increases, while the sum of the one-step information gain increases monotonically. It also shows that the difference between the two quantities can be large.

$\fbox{CuriosityValue}(h,\tau)$
Input: history $h$ , look-ahead $\tau$
Output: curiosity value $v^{\tau}(h)$
$\boxed{1   v \leftarrow 0}$
2 <b>for</b> all possible a
3 $v \leftarrow \max(v, \texttt{CuriosityQValue}(h, a, \tau))$
4 end for
5 return $v$

CuriosityQValue(h, a,  au)
Input: history $h$ , action $a$ , look-ahead $\tau$
Output: curiosity Q-value $q^{\tau}(h, a)$
$1   q \leftarrow g \left( a \  h \right)$
$2 \mathbf{if} \ \tau \neq 0$
3 for all possible o
$4 \left   q \leftarrow q + p\left(o ha\right) \cdot \texttt{CuriosityValue}(hao, \tau - 1) \right $
5 end for
6 end if
7 return $q$

The complexity of both CuriosityValue and CuriosityQValue are  $O((n_o n_a)^{\tau})$ , where  $n_o$  and  $n_a$  are the number of possible observations and actions, respectively. Since the cost is exponential on  $\tau$ , planning with large number of look ahead steps is infeasible, and approximation heuristics must be used in practice.

### 3.4 Extending to Infinite Horizon

Having to restrict the maximum life span of the agent is rather inconvenient. It is tempting to define the curiosity Q-value in the infinite time horizon case as the limit of curiosity Q-values with increasing life spans,  $T \to \infty$ . However, this cannot be achieved without additional technical constraints. For example, consider simple coin tossing. Assuming a *Beta* (1, 1) over the probability of seeing heads, then the expected cumulative information gain for the next T flips is given by

$$v^T(h_1) = I(\Theta; X_1, \dots, X_T) \sim \log T.$$

With increasing T,  $v^T(h_1) \to \infty$ . A frequently used approach to simplifying the math is to introduce a discount factor  $\gamma$ , as used in reinforcement learning. Assume that the agent has a maximum  $\tau$  actions left, but before finishing the  $\tau$  actions it may be forced to leave the environment with probability  $1 - \gamma$  $(0 \le \gamma < 1)$  at each time step. In this case, the curiosity Q-value becomes  $q_{\pi}^{1,\gamma}(h, a) = g(a||h)$ , and

$$\begin{aligned} q_{\pi}^{\tau,\gamma}\left(h,a\right) &= \left(1-\gamma\right)g\left(a\|h\right) + \gamma\left[g\left(a\|h\right) + \mathbb{E}_{o|ha}\mathbb{E}_{a'|hao}q_{\pi}^{\tau-1,\gamma}\left(hao,a'\right)\right] \\ &= g\left(a\|h\right) + \gamma\mathbb{E}_{o|ha}\mathbb{E}_{a'|hao}q_{\pi}^{\tau-1,\gamma}\left(hao,a'\right). \end{aligned}$$

One may also interpret  $q_{\pi}^{\tau,\gamma}(h,a)$  as a linear combination of curiosity Q-values without the discount,

$$q_{\pi}^{\tau,\gamma}\left(h,a\right) = \left(1-\gamma\right)\sum_{t=1}^{\tau}\gamma^{t-1}q_{\pi}^{t}\left(h,a\right) + \gamma^{\tau}q_{\pi}^{\tau}\left(h,a\right),$$

Note that curiosity Q-values with larger look-ahead steps are weighed exponentially less.

The optimal policy in the discounted case is given by

$$q^{1,\gamma}(h,a) = g(a||h), v^{1,\gamma}(h) = \max_{a} q^{1,\gamma}(h,a),$$

and

$$q^{\tau,\gamma}(h,a) = g\left(a\|h\right) + \gamma \mathbb{E}_{o|ha} v^{\tau-1,\gamma}(hao), v^{\tau,\gamma}(h) = \max_{a} q^{\tau,\gamma}(h,a).$$

The optimal actions are given by  $\pi_*^{\tau,\gamma}(h) = \arg \max_a q^{\tau,\gamma}(h,a)$ . The proof that  $\pi_*^{\tau,\gamma}$  is optimal is similar to the one for no-discount case and thus is omitted here.

Adding the discount enables one to define the curiosity Q-value in infinite time horizon in a number of cases. However, it is still possible to construct scenarios where such discount fails. Consider a infinite list of bandits. For bandit n,

there are *n* possible outcomes with Dirichlet prior  $Dir\left(\frac{1}{n}, \ldots, \frac{1}{n}\right)$ . The expected information gain of pulling bandit *n* for the first time is then given by

$$\log n - \psi(2) + \log\left(1 + \frac{1}{n}\right) \sim \log n.$$

Assume at time t, only the first  $e^{e^{2t}}$  bandits are available, thus the curiosity Q-value in finite time horizon is always finite. However, since the largest expected information gain grows at speed  $e^{t^2}$ , for any given  $\gamma > 0$ ,  $q^{\tau,\gamma}$  goes to infinity with increasing  $\tau$ . This example gives the intuition that to make the curiosity Q-value meaningful, the 'total information content' of the environment (or its growing speed) must be bounded.

The following two Lemmas are useful for later discussion.

Lemma 1.  $q_{\pi}^{\tau+1,\gamma}(h,a) - q_{\pi}^{\tau,\gamma}(h,a) = \gamma^{\tau} \mathbb{E}_{oa_1\cdots o_{\tau-1}a_{\tau}|hag}(a_{\tau}||h\cdots o_{\tau-1}).$ 

*Proof.* Expand  $q_{\pi}^{\tau,\gamma}$  and  $q_{\pi}^{\tau+1,\gamma}$ ,

$$\begin{aligned} q_{\pi}^{\tau+1,\gamma} - q_{\pi}^{\tau,\gamma} &= (1-\gamma) \sum_{t=1}^{\tau+1} \gamma^{t-1} q_{\pi}^{t} + \gamma^{\tau+1} q_{\pi}^{\tau+1} \\ &- (1-\gamma) \sum_{t=1}^{\tau} \gamma^{t-1} q_{\pi}^{t} - \gamma^{\tau} q_{\pi}^{\tau} \\ &= \gamma^{\tau} \left( q_{\pi}^{\tau+1} - q_{\pi}^{\tau} \right). \end{aligned}$$

By definition,

$$\begin{aligned} q_{\pi}^{\tau+1} - q_{\pi}^{\tau} &= \mathbb{E}_{o|ha} \mathbb{E}_{a_{1}o_{1}\cdots a_{\tau}o_{\tau}|haog} \left(haoa_{1}o_{1}\cdots a_{\tau}o_{\tau} \| h\right) \\ &- \mathbb{E}_{o|ha} \mathbb{E}_{a_{1}o_{1}\cdots a_{\tau-1}o_{\tau-1}|haog} \left(haoa_{1}o_{1}\cdots a_{\tau-1}o_{\tau-1} \| h\right) \\ &= \mathbb{E}_{o|ha} \mathbb{E}_{a_{1}o_{1}\cdots a_{\tau-1}o_{\tau-1}|hao} \\ &\left[ \mathbb{E}_{a_{\tau}o_{\tau}|h\cdots o_{\tau-1}g} \left(haoa_{1}o_{1}\cdots a_{\tau}o_{\tau} \| h\right) - g \left(haoa_{1}o_{1}\cdots a_{\tau-1}o_{\tau-1} \| h\right) \right]. \end{aligned}$$

Using Eq.2,

$$\mathbb{E}_{a_{\tau}o_{\tau}|h\cdots o_{\tau-1}}g\left(haoa_{1}o_{1}\cdots a_{\tau}o_{\tau}\|h\right) - g\left(haoa_{1}o_{1}\cdots a_{\tau-1}o_{\tau-1}\|h\right)$$
$$= \mathbb{E}_{a_{\tau}|h\cdots a_{\tau}}, q\left(a_{\tau}\|h\cdots o_{\tau-1}\right),$$

thus

$$q_{\pi}^{\tau+1,\gamma} - q_{\pi}^{\tau,\gamma} = \gamma^{\tau} \mathbb{E}_{o|ha} \mathbb{E}_{a_1 o_1 \cdots a_{\tau-1} o_{\tau-1}|hao} \mathbb{E}_{a_\tau | h \cdots o_{\tau-1}} g\left(a_\tau \| h \cdots o_{\tau-1}\right)$$
$$= \gamma^{\tau} \mathbb{E}_{oa_1 \cdots o_{\tau-1} a_\tau | hag} \left(a_\tau \| h \cdots o_{\tau-1}\right).$$

**Lemma 2.**  $q^{\tau+1,\gamma}(h,a) - q^{\tau,\gamma}(h,a) \leq \gamma^{\tau} \mathbb{E}_{o|ha} \max_{a_1} \mathbb{E}_{o_1|haoa_1} \cdots \max_{a_{\tau}} g(a_{\tau} || h \cdots o_{\tau-1}).$ 

*Proof.* Expand  $q^{\tau,\gamma}$  and  $q^{\tau+1,\gamma}$ , and note that  $\max X - \max Y \leq \max |X - Y|$ , then

$$\begin{split} q^{\tau+1,\gamma}(h,a) &- q^{\tau,\gamma}(h,a) \\ &= \mathbb{E}_{o|ha} \max_{a_1} \mathbb{E}_{o_1|haoa_1} \cdots \max_{a_{\tau}} \left[ g\left( a \| h \right) + \gamma g\left( a_1 \| hao \right) + \dots + \gamma^{\tau} g\left( a_{\tau} \| h \cdots o_{\tau-1} \right) \right] \\ &- \mathbb{E}_{o|ha} \max_{a_1} \mathbb{E}_{o_1|haoa_1} \cdots \max_{a_{\tau-1}} \left[ g\left( a \| h \right) + \gamma g\left( a_1 \| hao \right) + \dots + \gamma^{\tau-1} g\left( a_{\tau-1} \| h \cdots o_{\tau-2} \right) \right] \\ &\leq \mathbb{E}_{o|ha} \max_{a_1} \left\{ \mathbb{E}_{o_1|haoa_1} \cdots \max_{a_{\tau}} \left[ g\left( a \| h \right) + \gamma g\left( a_1 \| hao \right) + \dots + \gamma^{\tau} g\left( a_{\tau} \| h \cdots o_{\tau-1} \right) \right] \\ &- \mathbb{E}_{o_1|haoa_1} \cdots \max_{a_{\tau-1}} \left[ g\left( a \| h \right) + \gamma g\left( a_1 \| hao \right) + \dots + \gamma^{\tau-1} g\left( a_{\tau-1} \| h \cdots o_{\tau-2} \right) \right] \right\} \\ &\leq \dots \\ &\leq \gamma^{\tau} \mathbb{E}_{o|ha} \max_{a_1} \mathbb{E}_{o_1|haoa_1} \cdots \max_{a_{\tau}} g\left( a_{\tau} \| h \cdots o_{\tau-1} \right). \end{split}$$

It can be seen that if  $\mathbb{E}_{oa_1\cdots o_{\tau-1}a_\tau|ha}g(a_\tau||h\cdots o_{\tau-1})$  is bounded, then both  $q_{\pi}^{\gamma,\tau}$  and  $q^{\gamma,\tau}$  are a Cauchy sequences with respect to  $\tau$ .

# 4 Exploration in Finite Markovian Environment with Dirichlet Priors

In this section we restrict the discussion to a simple case, where the possible actions and sensory inputs are finite, and the agent assumes that the environment is Markovian, namely, the current sensory input and action is sufficient for determining the (probabilities of the) next sensory inputs. Formally, let  $S = \{1, \dots, S\}$  and  $\mathcal{A} = \{1, \dots, A\}$  be the space of possible sensory inputs, to which we referred as 'states', and actions. The dynamics of the environment is fully determined by the transition probability p(s'|s, a).

The agent tries to learn the transition probabilities. Initially, it assumes for each  $\langle s, a \rangle$  a Dirichlet prior over the random variable  $\Theta_{s,a}$  corresponding to the distribution  $p(\cdot|s, a)$ . Through time, the agent observes the transitions when performing a at s, and updates its estimate of  $\Theta_{s,a}$  through probabilistic inference. Since the Dirichlet distribution is conjugate with multinomial distribution, the posterior is still a Dirichlet distribution over  $\Theta_{s,a}$ . Therefore, at any time, the agent's knowledge about the environment can be fully summarized by a three dimensional array  $\alpha(s, a, s')$ , such that  $Dir(\alpha_{s,a,1}, \cdots, \alpha_{s,a,S})$  is the current (prior or posterior) density of  $\Theta_{s,a}$ , and the definition of the optimal curiosity Q-value can be written  $as^2$ 

$$q_{\alpha}^{\gamma,\tau}(s,a) = g(\alpha_{s,a}) + \gamma \sum_{s'} p_{\alpha}(s'|s,a) \max_{a'} q_{\alpha \triangleleft \langle s,a,s' \rangle}^{\gamma,\tau-1}(s',a')$$
$$= g(\alpha_{s,a}) + \gamma \sum_{s'} \frac{\alpha_{s,a,s'}}{\alpha_{s,a}} \max_{a'} q_{\alpha \triangleleft \langle s,a,s' \rangle}^{\gamma,\tau-1}(s',a').$$

Here  $g(\alpha_{s,a})$  is the expected immediate information gain for  $\Theta_{s,a}$  given the current parameterization of the Dirichlet distribution. By definition,  $g(\alpha_{s,a})$  is also the mutual information between  $\Theta$  and an additional observation. According to [6], the precise form of g is given by

$$g([n_1, \cdots, n_S]) = \log n^* - \psi(n^* + 1) - \sum_{s=1}^S \frac{n_s}{n^*} [\log n_s - \psi(n_s + 1)],$$

where  $n^* = \sum_s n_s$ , and  $\psi(\cdot)$  is the standard digamma function. By marginalizing out  $\Theta_{s,a}$ , the predictive probability is given by  $p_{\alpha}(s'|s,a) = \frac{\alpha_{s,a,s'}}{\alpha_{s,a}}$ , and  $\triangleleft$  is the operator<sup>3</sup> such that  $\alpha \triangleleft \langle s, a, s' \rangle$  is the same as  $\alpha$ , except that the entry indexed by  $\langle s, a, s' \rangle$  is increased by 1. Similarly, for a given policy  $\pi$ , the curiosity Q-value can be written as

$$q_{\pi,\alpha}^{\gamma,\tau}\left(s,a\right) = g\left(\alpha_{s,a}\right) + \gamma \sum_{s'} \frac{\alpha_{s,a,s'}}{\alpha_{s,a}} \sum_{a'} \pi_{\alpha}\left(a'|s'\right) q_{\pi,\alpha \triangleleft \langle s,a,s' \rangle}^{\gamma,\tau-1}\left(s',a'\right).$$

### 4.1 Curiosity Q-value in Infinite Time Horizon

In this subsection we extend the definition of curiosity Q-value to infinite horizon. We show that a) the limit  $\lim_{\tau\to\infty} q_{\pi,\alpha}^{\gamma,\tau}$  exists, b) the limit  $\lim_{\tau\to\infty} q_{\alpha}^{\gamma,\tau}$  exists, and c) the limit is the solution of the infinite recursion.

**Proposition 2.**  $q_{\pi,\alpha}^{\gamma}(s,a) = \lim_{\tau \to \infty} q_{\pi,\alpha}^{\gamma,\tau}(s,a)$  exists for any  $\pi$ ,  $\alpha$ , s, a, and  $\gamma \in [0,1)$ . Moreover, the convergence is uniform with respect to  $\langle s,a \rangle$  in the sense that

$$0 \leq q_{\pi,\alpha}^{\gamma}\left(s,a\right) - q_{\pi,\alpha}^{\gamma,\tau}\left(s,a\right) \leq \frac{g_{\alpha}}{1-\gamma}\gamma^{\tau}, \, \forall s,a$$

where  $g_{\alpha} = \max_{s} \max_{a} g(\alpha_{s,a}).$ 

*Proof.* Rewrite the result in Lemma.1 in this context:

$$\begin{aligned} q_{\pi,\alpha}^{\gamma,\tau+1}\left(s,a\right) - q_{\pi,\alpha}^{\gamma,\tau}\left(s,a\right) &= \gamma^{\tau} \mathbb{E}_{oa_{1}\cdots o_{\tau-1}a_{\tau}|ha} g\left(a_{\tau} \| h \cdots o_{\tau-1}\right) \\ &= \gamma^{\tau} \mathbb{E}_{s_{1}a_{2}s_{2}\cdots s_{\tau}a_{\tau+1}|ha} g\left(\alpha_{s_{\tau}a_{\tau+1}}'\right), \end{aligned}$$

<sup>&</sup>lt;sup>2</sup> We use  $\alpha_{s,a}$  both for the vector  $[\alpha_{s,a,1}, \cdots, \alpha_{s,a,S}]$  and the number  $\sum_{s'} \alpha_{s,a,s'}$ . The meaning should be clear from the context.

<sup>&</sup>lt;sup>3</sup> Assume that the operator  $\triangleleft$  is right associative, so one can write  $\alpha \triangleleft \langle s_1, a_2, s_2 \rangle \triangleleft \langle s_2, a_3, s_3 \rangle \cdots$ , or simply  $\alpha \triangleleft \langle s_1 a_2 s_2 a_3 s_3 \cdots \rangle$ .

where

$$\alpha' = \alpha \triangleleft \langle s, a, s_1 \rangle \triangleleft \langle s_1, a_2, s_2 \rangle \triangleleft \cdots \triangleleft \langle s_{\tau-1}, a_{\tau}, s_{\tau} \rangle.$$

Because  $g(\alpha'_{s,a})$  depends only on the transitions when performing a at s, and all such transitions are exchangeable since they are assumed to be i.i.d. when  $\Theta_{s,a}$  is given, one can rewrite the expectation in the following form:

$$\mathbb{E}_{s_1 a_2 s_2 \cdots s_\tau a_{\tau+1} | hag} \left( \alpha'_{s_\tau a_{\tau+1}} \right) = \mathbb{E}_s \mathbb{E}_a \mathbb{E}_n \mathbb{E}_{x_1} \cdots \mathbb{E}_{x_n} g \left( \alpha'_{s,a} \right).$$

The first and second expectations are taken over the possible final state-action pairs  $\langle s_{\tau}, a_{\tau+1} \rangle$ , from which  $g\left(\alpha'_{s_{\tau}a_{\tau+1}}\right)$  is computed. Once  $\langle s, a \rangle$  is fixed, the third expectation is taken over the time n that  $\langle s, a \rangle$ -pair appears in the trajectory  $sas_1a_2\cdots s_{\tau}$ , i.e., the time that transitions starting from s with action aoccurs. The rest of the expectations are over the n destinations of the transitions, denoted as  $x_1, \cdots, x_n$ . By definition,  $Dir\left(\alpha'_{s,a}\right)$  is the posterior distribution after seeing  $x_1, \cdots, x_n$ , and  $g\left(\alpha'_{s,a}\right)$  is the expected information gain of seeing the outcome of the (n + 1)-th transition, which we denote  $x_{n+1}$ , thus

$$g\left(\alpha_{s,a}'\right) = I\left(\Theta_{s,a}; X_{n+1} | x_1, \cdots, x_n\right),$$

and

$$\mathbb{E}_{x_1}\cdots\mathbb{E}_{x_n}g\left(\alpha'_{s,a}\right)=I\left(\Theta_{s,a};X_{n+1}|X_1,\cdots,X_n\right).$$

Note that  $X_1, \dots, X_{n+1}$  are i.i.d. given  $\Theta_{s,a}$ , therefore

$$\begin{split} I\left(\Theta_{s,a}; X_{n+1} | X_1, \cdots, X_n\right) \\ &= I\left(\Theta_{s,a}; X_1, \cdots, X_{n+1}\right) - I\left(\Theta_{s,a}; X_1, \cdots, X_n\right) \\ &= H\left(X_1, \cdots, X_{n+1}\right) - \sum_{i=1}^{n+1} H\left(X_i | \Theta\right) - H\left(X_1, \cdots, X_n\right) + \sum_{i=1}^n H\left(X_i | \Theta\right) \\ &= H\left(X_{n+1} | X_1, \cdots, X_n\right) - H\left(X_{n+1} | \Theta\right) \\ &\leq H\left(X_{n+1}\right) - H\left(X_{n+1} | \Theta\right) \\ &= I\left(\Theta; X_{n+1}\right) \\ &= I\left(\Theta; X_1\right). \end{split}$$

This means that  $I(\Theta_{s,a}; X_{n+1}|X_1, \dots, X_n)$  is upper bounded by  $I(\Theta; X_1)$ , which is the expected information gain of seeing the outcome of the transition for the first time. By definition  $I(\Theta; X_1) = g(\alpha_{s,a})$ , and it follows that

$$\mathbb{E}_{n}\mathbb{E}_{x_{1}}\cdots\mathbb{E}_{x_{n}}g\left(\alpha_{s,a}'\right)\leq g\left(\alpha_{s,a}\right).$$

Therefore,

$$q_{\pi,\alpha}^{\gamma,\tau+1}(s,a) - q_{\pi,\alpha}^{\gamma,\tau}(s,a) = \gamma^{\tau} \mathbb{E}_{s_1 a_2 s_2 \cdots s_\tau a_{\tau+1} | hag} \left( \alpha'_{s_\tau a_{\tau+1}} \right)$$
$$= \gamma^{\tau} \mathbb{E}_s \mathbb{E}_a \mathbb{E}_n \mathbb{E}_{x_1} \cdots \mathbb{E}_{x_n} g \left( \alpha'_{s,a} \right)$$
$$\leq \gamma^{\tau} \mathbb{E}_s \mathbb{E}_a g \left( \alpha_{s,a} \right)$$
$$\leq \gamma^{\tau} \max_s \max_a g \left( \alpha_{s,a} \right)$$
$$\leq \gamma^{\tau} g_{\alpha}.$$

Since  $g_{\alpha}$  depends on  $\alpha$  only, for any T

$$q_{\pi,\alpha}^{\gamma,\tau+T}\left(s,a\right) - q_{\pi,\alpha}^{\gamma,\tau}\left(s,a\right) \le \frac{g_{\alpha}}{1-\gamma}\gamma^{\tau}.$$

This means that  $q_{\pi,\alpha}^{\gamma,\tau}(s,a)$  is a Cauchy sequence with respect to  $\tau$ , thus  $\lim_{\tau\to\infty} q_{\pi,\alpha}^{\gamma,\tau}(s,a)$  exists. Also note that the convergence is uniform since  $g_{\alpha}$  does not depend on  $\langle s, a \rangle$ .

**Proposition 3.**  $q_{\alpha}^{\gamma}(s,a) = \lim_{\tau \to \infty} q_{\alpha}^{\gamma,\tau}(s,a)$  exists for any  $\alpha$ , s, a, and  $\gamma \in [0,1)$ . Also the convergence is uniform in the sense that

$$0 \le q^{\gamma}(s,a) - q_{\alpha}^{\gamma,\tau}(s,a) \le \frac{g_{\alpha}}{1-\gamma}\gamma^{\tau}.$$

Proof. Rewrite the result in Lemma.2,

$$q_{\alpha}^{\gamma,\tau+1}(s,a) - q_{\alpha}^{\gamma,\tau}(s,a) \leq \gamma^{\tau} \mathbb{E}_{s_{1}|sa} \max_{a_{2}} \mathbb{E}_{s_{2}|s_{1}a_{2},\alpha \triangleleft \langle s,a,s_{1} \rangle} \\ \cdots \mathbb{E}_{s_{\tau}|s_{\tau-1}a_{\tau},\alpha \triangleleft \langle sas_{1}\cdots s_{\tau-1} \rangle} \max_{a_{\tau+1}} g\left(\alpha'_{s_{\tau},\alpha_{\tau+1}}\right).$$

Since the max operator is only over actions, the proof in the previous proposition still holds, so

$$q_{\alpha}^{\gamma,\tau+1}\left(s,a\right) - q_{\alpha}^{\gamma,\tau}\left(s,a\right) \le \gamma^{\tau}g_{\alpha},$$

and the result follows.

The next proposition shows that  $q_{\alpha}^{\gamma}$  is the solution to the infinite recursion.

**Proposition 4.**  $q_{\alpha}^{\gamma}$  is the solution to the recursion

$$q_{\alpha}^{\gamma}\left(s,a\right) = g\left(\alpha_{s,a}\right) + \gamma \sum_{s'} \frac{\alpha_{s,a,s'}}{\alpha_{s,a}} \max_{a'} q_{\alpha \triangleleft \left\langle s,a,s'\right\rangle}^{\gamma}\left(s',a'\right),$$

and for any other policy  $\pi$ ,  $q_{\alpha}^{\gamma}(s, a) \geq q_{\pi,\alpha}^{\gamma}(s, a)$ .

*Proof.* To see that  $q_{\alpha}^{\gamma}$  is the solution, taking any  $\varepsilon > 0$ , one can find a  $\tau$  such that  $\left|q_{\alpha}^{\gamma,\tau+1}-q_{\alpha}^{\gamma}\right| < \frac{\varepsilon}{2}$ , and  $\left|q_{\alpha \triangleleft \langle s,a,s' \rangle}^{\gamma,\tau}-q_{\alpha \triangleleft \langle s,a,s' \rangle}^{\gamma}\right| < \frac{\varepsilon}{2}$  for any  $\langle s,a,s' \rangle$ , thanks to the fact that there are only finite number of  $\langle s,a,s' \rangle$  triples, and the convergence from  $q_{\alpha}^{\gamma,\tau+1}(s,a)$  to  $q_{\alpha}^{\gamma}(s,a)$  is uniform. It follows that

$$\left| g\left(\alpha_{s,a}\right) + \gamma \sum_{s'} \frac{\alpha_{s,a,s'}}{\alpha_{s,a}} \max_{a'} q_{\alpha \triangleleft \langle s,a,s' \rangle}^{\gamma}\left(s',a'\right) - q_{\alpha}^{\gamma}\left(s,a\right) \right| \\ \leq \left| q_{\alpha}^{\gamma,\tau+1} - q_{\alpha}^{\gamma} \right| + \gamma \left| q_{\alpha \triangleleft \langle s,a,s' \rangle}^{\gamma,\tau} - q_{\alpha \triangleleft \langle s,a,s' \rangle}^{\gamma} \right| \\ \leq \varepsilon$$

Since  $\varepsilon$  is chosen arbitrary,  $q_{\alpha}^{\gamma}(s, a)$  must be the solution of the infinite recursion.

The fact that  $q_{\alpha}^{\gamma}(s,a) \geq q_{\pi,\alpha}^{\gamma}(s,a)$  follows from the fact that  $q_{\alpha}^{\gamma,\tau}$  and  $q_{\pi,\alpha}^{\gamma,\tau}$  are monotonically increasing on  $\tau$  (by Lemma.1), and  $q_{\alpha}^{\gamma,\tau} \geq q_{\pi,\alpha}^{\gamma,\tau}$  for any given  $\tau$  and  $\pi$ .

The propositions above guarantees the existence and optimality of  $q_{\alpha}^{\gamma}$ , and the following discussions would focus on  $q_{\alpha}^{\gamma}$ . We drop the super-script  $\gamma$  in the rest of this section.

### 4.2 Approximation through Dynamic Programming

The optimal curiosity Q-value is given by the infinite recursion

$$q_{\alpha}(s,a) = g\left(\alpha_{s,a}\right) + \gamma \sum_{s'} \frac{\alpha_{s,a,s'}}{\alpha_{s,a}} \max_{a'} q_{\alpha \triangleleft \langle s,a,s' \rangle}\left(s',a'\right).$$
(5)

It is impossible to solve this equation directly. A natural idea is to approximate this infinite recursion by solving at each time step the following Bellman equation,

$$\tilde{q}_{\alpha}\left(s,a\right) = g\left(\alpha_{s,a}\right) + \gamma \sum_{s'} \frac{\alpha_{s,a,s'}}{\alpha_{s,a}} \max_{a'} \tilde{q}_{\alpha}\left(s',a'\right).$$
(6)

The Bellman equation can be solved by dynamic programming in time polynomial on S and A. The algorithm is given below.

CuriosityExploreDP $(\alpha, \gamma, s, T)$ Input: prior  $\alpha$ , discount factor  $\gamma$ , initial state s, number of steps T. Output: posterior stored in  $\alpha$ 

```
\begin{array}{c} 1 \ G \leftarrow [g(\alpha_{s,a})]_{\langle s,a \rangle \in \mathcal{S} \times \mathcal{A}} \\ 2 \ P \leftarrow \left[\frac{\alpha_{s,a,s'}}{\alpha_{s,a}}\right]_{\langle s,a,s' \rangle \in \mathcal{S} \times \mathcal{A} \times \mathcal{S}} \\ 3 \ \text{for } t \ \text{in 1 to } T \\ 4 \ \pi \leftarrow \text{PolicyIteration}(G, P, \gamma) \\ 5 \ a \leftarrow \pi_s \\ 6 \ s' \leftarrow \text{NextState}(a) \\ 7 \ \alpha_{s,a,s'} \leftarrow \alpha_{s,a,s'} + 1 \\ 8 \ G_{s,a} \leftarrow g(\alpha_{s,a}) \\ 9 \ \text{for } s' \ \text{in 1 to } S \\ 10 \ P_{s,a,s'} \leftarrow \frac{\alpha_{s,a,s'}}{\alpha_{s,a}} \\ 11 \ \text{end for} \\ 12 \ s \leftarrow s' \\ 13 \ \text{end for} \end{array}
```

A surprising fact is that when  $\alpha$  is large,  $\tilde{q}_{\alpha}$  is in fact a very good approximation of  $q_{\alpha}$ , which is the central result in this section. We start by investigating the properties of the gain  $g\left(\alpha_{s,a}^{t}\right)$ .

### 4.3 Properties of Expected Information Gain in Dirichlet Case

The expected information gain of a Dirichlet distribution  $Dir(n_1, \dots, n_S)$  is given by

$$g(n) = \log(n) - \psi(n+1) - \sum_{s} \frac{n_s}{n} \left[ \log(n_s) - \psi(n_s+1) \right].$$

Define

$$f(x) = x [\psi(x+1) - \log x] = 1 - x [\log x - \psi(x)].$$

then

$$g(n) = \frac{1}{n} \left[ \sum_{s} f(n_{s}) - f(n) \right].$$

The following important properties has been proved by Alzer in [1].

**Theorem 1.** f has the following properties<sup>4</sup>:

a)  $\lim_{x \to 0} f(x) = 0$ ,  $\lim_{x \to \infty} f(x) = \frac{1}{2}$ 

<sup>&</sup>lt;sup>4</sup> Alzer's original paper considers the function  $x (\log x - \psi(x)) = 1 - f(x)$ . Here the statements are modified accordingly.

b) f is strictly completely monotonic, in the sense that

$$(-1)^{n+1} \frac{d^n f(x)}{dx^n} > 0.$$

In particular, Theorem.1 shows that f is strictly monotonically increasing, and also strictly concave. The following Lemma summarizes the properties about f used in this paper.

**Lemma 3.** Define  $\delta_m(x) = f(x+m) - f(x)$  for m > 0. Then

a) f is sub-additive, i.e., f(x) + f(y) > f(x+y) for x, y > 0b)  $\delta_m(x)$  is monotonically decreasing on  $(0, \infty)$ . c)  $0 < x\delta_m(x) < \frac{1-e^{-1}}{2}m$  for  $x \in (0, \infty)$ .

*Proof.* a) Note that g(n) is mutual information, and the unknown observation depends on the parameters of the distribution, therefore g(n) > 0, and

$$0 < g([x, y]) = \frac{1}{x + y} [f(x) + f(y) - f(x + y)].$$

b) Note that

$$\delta_m(x) = \int_0^m f'(x+s) \, ds,$$

and the result follows from f''(x) < 0.

c) Clearly,  $x\delta_m(x) > 0$  because f is strictly increasing. From Intermediate Value Theorem, there some  $\delta \in (0, m)$ , such that

$$\begin{aligned} x\delta_m\left(x\right) &= x\left[f\left(x+m\right) - f\left(x\right)\right] \\ &= mxf'\left(x+\delta\right) \\ &= mxf'\left(x\right) + mx\left[f'\left(x+\delta\right) - f'\left(x\right)\right] \\ &< mxf'\left(x\right). \end{aligned}$$

The inequality is because f is strictly concave. From [1],

$$f(x) = 1 - x \int_0^\infty \phi(t) e^{-tx} dt,$$

where

$$\phi(t) = \frac{1}{1 - e^{-t}} - \frac{1}{t}$$

is strictly increasing, with  $\lim_{t\to 0}\phi\left(t\right)=\frac{1}{2}$  and  $\lim_{t\to\infty}\phi\left(t\right)=1.$  Therefore,

$$\begin{aligned} xf'(x) &= x \int_0^\infty \phi(t) \, e^{-tx} \, (xt-1) \, dt \\ &= x^2 \int_0^{\frac{1}{x}} \phi(t) \, e^{-tx} \left(t - \frac{1}{x}\right) dt + x^2 \int_{\frac{1}{x}}^\infty \phi(t) \, e^{-tx} \left(t - \frac{1}{x}\right) dt \\ &< x^2 \phi(0) \int_0^{\frac{1}{x}} e^{-tx} \left(t - \frac{1}{x}\right) dt + x^2 \phi(\infty) \int_{\frac{1}{x}}^\infty e^{-tx} \left(t - \frac{1}{x}\right) dt \\ &= \frac{x^2}{2} \int_0^\infty e^{-tx} \left(t - \frac{1}{x}\right) dt + \frac{x^2}{2} \int_{\frac{1}{x}}^\infty e^{-tx} t dt - \frac{x}{2} \int_{\frac{1}{x}}^\infty e^{-tx} dt \\ &< \frac{x^2}{2} \int_0^\infty e^{-tx} \left(t - \frac{1}{x}\right) dt + \frac{x^2}{2} \int_0^\infty e^{-tx} t dt - \frac{x}{2} \int_{\frac{1}{x}}^\infty e^{-tx} dt. \end{aligned}$$

Note that

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$$\int_{0}^{\infty} e^{-tx} t dt = \frac{1}{x^2}, \ \int_{0}^{\infty} e^{-tx} dt = \frac{1}{x},$$

and

$$x\int_{\frac{1}{x}}^{\infty}e^{-tx}dt = e^{-1},$$

it follows that

$$xf'(x) < \frac{1-e^{-1}}{2}.$$

The properties of f guarantee that g(n) decreases at the rate of  $\frac{1}{n}$ . The result is formulated in the following Lemma.

**Lemma 4.** Let  $Dir(n_1^0, \dots, n_S^0)$  and  $Dir(n_1^t, \dots, n_S^t)$  be the prior and the posterior distribution, such that  $n^t = n^0 + t$ . Let  $s^* = \arg \max_s n_s^0$ . Then

$$\frac{\sum_{s \neq s^*} f\left(n_s^0\right) - f\left(\sum_{s \neq s^*} n_s^0\right)}{2n} < g\left(n^t\right) < \frac{S-1}{2n}.$$

*Proof.* The upper bound is because  $0 < f(x) < \frac{1}{2}$  and f is increasing, thus

$$\sum_{s} f\left(n_{s}^{t}\right) - f\left(n^{t}\right) = f\left(n_{1}^{t}\right) - f\left(n^{t}\right) + \sum_{s \neq 1} f\left(n_{s}^{t}\right)$$
$$< \frac{S-1}{2}.$$

The lower bound follows from the fact that f(x+m) - f(x) is decreasing. We show that the trajectory minimizing  $g(n^t)$  is the one such that all t observations equal to  $s^*$ . To see this, let  $m_s$  be the number of times observing  $s \neq s^*$ , then

$$f(n_s^0 + m_s) + f(n_{s^*}^0 + m_{s^*}) = f(n_s^0) + f(n_{s^*}^0 + m_{s^*} + m_s) + f(n_s^0 + m_s) - f(n_s^0) - (f(n_{s^*}^0 + m_{s^*} + m_s) - f(n_{s^*}^0 + m_{s^*})).$$

Note that  $n_{s^*}^0 + m_{s^*} \ge n_s^0$ , so

$$f(n_s^0 + m_s) + f(n_{s^*}^0 + m_{s^*}) \ge f(n_s^0) + f(n_{s^*}^0 + m_{s^*} + m_s).$$

Now assume the observations are all  $s^*$ , from sub-additivity,

$$\begin{split} \sum_{s} f\left(n_{s}^{t}\right) - f\left(n^{t}\right) \\ &= \sum_{s \neq s^{*}} f\left(n_{s}^{0}\right) + f\left(n_{s^{*}}^{0} + t\right) - f\left(n^{0} + t\right) \\ &= \sum_{s \neq s^{*}} f\left(n_{s}^{0}\right) - f\left(\sum_{s \neq s^{*}} n_{s}^{0}\right) + \left[f\left(\sum_{s \neq s^{*}} n_{s}^{0}\right) + f\left(n_{s^{*}}^{0} + t\right) - f\left(n^{0} + t\right)\right] \\ &> \sum_{s \neq s^{*}} f\left(n_{s}^{0}\right) - f\left(\sum_{s \neq s^{*}} n_{s}^{0}\right). \end{split}$$

A little remark: The bounds hold irrespective of the data generating process, namely, it holds for *any* sequences of observations, *including sequences with zero probabilities*.

The following Lemma bound the variation of the expected information gain, when one single observation is added.

**Lemma 5.** Let  $n = [n_1, \dots, n_S]$  and  $n' = [n_1, \dots, n_{s-1}, n_s + 1, n_{s+1}, \dots, n_S]$ , then

$$\frac{n_s}{n} \left| g\left(n'\right) - g\left(n\right) \right| \le \frac{S}{2n^2}, \, \forall n_s > 0.$$

*Proof.* Without loss of generality let s = 1. Note that

$$\begin{split} &\frac{n_1}{n} \left[ g\left(n'\right) - g\left(n\right) \right] \\ &= \frac{n_1}{n} \left\{ \frac{1}{n+1} \left[ \sum_{s \neq 1} f\left(n_s\right) + f\left(n_1 + 1\right) - f\left(n+1\right) \right] - \frac{1}{n} \left[ \sum_s f\left(n_s\right) - f\left(n\right) \right] \right\} \\ &= \frac{n_1}{n} \left\{ \frac{\sum_s f\left(n_s\right)}{n+1} - \frac{f\left(n+1\right)}{n+1} + \frac{f\left(n_1 + 1\right) - f\left(n_1\right)}{n+1} + \frac{f\left(n\right)}{n} - \frac{\sum_s f\left(n_s\right)}{n} \right\} \\ &= \frac{n_1}{n} \left\{ -\frac{f\left(n+1\right)}{n+1} - \frac{\sum_s f\left(n_s\right)}{n\left(n+1\right)} + \frac{f\left(n_1 + 1\right) - f\left(n_1\right)}{n+1} + \frac{f\left(n\right)}{n} \right\} \\ &= \frac{n_1}{n} \left\{ -\frac{f\left(n+1\right)}{n+1} - \frac{ng\left(n\right) + f\left(n\right)}{n\left(n+1\right)} + \frac{f\left(n_1 + 1\right) - f\left(n_1\right)}{n+1} + \frac{f\left(n\right)}{n} \right\} \\ &= \frac{n_1}{n\left(n+1\right)} \left\{ -\delta_1\left(n\right) + \delta_1\left(n_1\right) - g\left(n\right) \right\} \\ &= \frac{1}{n\left(n+1\right)} \left\{ n_1\delta_1\left(n_1\right) - \frac{n_1}{n} \cdot n\delta_1\left(n\right) - \frac{n_1}{n} \left[ \sum_s f\left(n_s\right) - f\left(n\right) \right] \right\} \end{split}$$

From the previous Lemma,

$$0 < x\delta_1(x) < \frac{1}{2}, \ 0 < f(x) < \frac{1}{2},$$

 $\mathbf{SO}$ 

$$-\frac{S}{2n^{2}} < -\frac{n_{1}}{n}\frac{S}{2n^{2}} < \frac{n_{1}}{n}\left[g\left(n'\right) - g\left(n\right)\right] < \frac{1}{2n^{2}},$$

thus

$$\frac{n_{1}}{n}\left|g\left(n'\right)-g\left(n\right)\right|<\frac{S}{2n^{2}}.$$

# 4.4 Bounding the Difference Between $q_{\alpha}$ and $\tilde{q}_{\alpha}$

In this subsection we present the result bounding the difference between  $q_{\alpha}$  and  $\tilde{q}_{\alpha}$ , without making any assumptions to the environment. Let  $c_{\alpha} = \min_{s} \min_{a} \alpha_{s,a}$ , the main conclusion of this subsection is that

$$\left|q_{\alpha}\left(s,a\right)-\tilde{q}_{\alpha}\left(s,a\right)\right|\sim\frac{1}{c_{\alpha}^{2}}.$$

Lemma 6.  $q_{\alpha}(s,a) \leq \frac{S-1}{2(1-\gamma)c_{\alpha}}$ .

*Proof.* From Lemma.4, write  $K_0 = \frac{S-1}{2}$ , then

$$g\left(\alpha_{s,a}\right) < \frac{K_0}{\alpha_{s,a}} < \frac{K_0}{c_{\alpha}}, \forall s, a$$

By definition,

$$q_{\alpha}^{\gamma,2}(s,a) = g(\alpha_{s,a}) + \gamma \sum_{s'} \frac{\alpha_{s,a,s'}}{\alpha_{s,a}} \max_{a'} q_{\alpha \triangleleft \langle s,a,s' \rangle}^{\gamma,1}(s',a')$$
$$< K_0 \left(\frac{1}{c_{\alpha}} + \gamma \frac{1}{c_{\alpha \triangleleft \langle s,a,s' \rangle}}\right)$$
$$\leq \frac{K_0}{c_{\alpha}} (1+\gamma),$$

since  $c_{\alpha \triangleleft \langle s, a, s' \rangle} \ge c_{\alpha}$ . Repeat the process, it follows that for any  $\tau$ ,

$$q_{\alpha}^{\gamma,\tau}\left(s,a\right) \leq \frac{K_{0}}{c_{\alpha}}\left(1+\gamma+\dots+\gamma^{\tau-1}\right) < \frac{K_{0}}{\left(1-\gamma\right)c_{\alpha}} = \frac{S-1}{2\left(1-\gamma\right)c_{\alpha}},$$

thus

$$q_{\alpha}^{\gamma}(s,a) = \lim_{\tau \to \infty} q_{\alpha}^{\gamma,\tau}(s,a) \le \frac{K_{0}}{(1-\gamma)c_{\alpha}}$$

**Lemma 7.** Let  $n = [n_1, \dots, n_S]$ , and  $n' = [n_1 + 1, n_2, \dots, n_S]$ . Let  $x_1, \dots, x_S$  be S non-negative numbers. Define  $p_s = \frac{n_s}{n}$ ,  $p'_1 = \frac{n_{1+1}}{n+1}$  and  $p'_s = \frac{n_s}{n+1}$  for  $s = 2, \dots, S$ . Then

$$p_1\left|\sum_s \left(p'_s - p_s\right)x_s\right| \le \frac{1}{n}\sum_s p_s x_s.$$

*Proof.* Simple derivation gives

$$p_1 \left| \sum_{s} \left( p'_s - p_s \right) x_s \right| = \left( \sum_{s} p_s x_s \right) \cdot p_1 \left| \frac{\sum_{s} \left( p'_s - p_s \right) x_s}{\sum_{s} p_s x_s} \right|$$
$$\leq \left( \sum_{s} p_s x_s \right) \max_{s} \frac{p_1 \cdot |p'_s - p_s|}{p_s}.$$

If s = 1,

$$\frac{p_1 \cdot |p_1' - p_1|}{p_1} = \frac{n_1}{n} \cdot \frac{\frac{n_1 + 1}{n+1} - \frac{n_1}{n}}{\frac{n_1}{n}} = \frac{n - n_1}{n(n+1)} \le \frac{1}{n}$$

If  $s \neq 1$ ,

$$\frac{p_1 \cdot |p'_s - p_s|}{p_s} = \frac{n_1}{n} \cdot \frac{\frac{n_s}{n} - \frac{n_s}{n+1}}{\frac{n_s}{n}} = \frac{n_1}{n(n+1)} \le \frac{1}{n}.$$

Therefore,

$$\max_{s} \frac{p_1 \cdot |p_s' - p_s|}{p_s} \le \frac{1}{n}$$

and

$$p_1 \left| \sum_s \left( p'_s - p_s \right) x_s \right| \le \frac{1}{n} \sum_s p_s x_s$$

**Lemma 8.** For any  $\alpha$ ,  $s^{\dagger}$ ,  $a^{\dagger}$ , there is some constant K depending on S and  $\gamma$  only, such that

$$\sum_{s} \frac{\alpha_{s^{\dagger},a^{\dagger},s}}{\alpha_{s^{\dagger},a^{\dagger}}} \max_{a} \left| q_{\alpha \triangleleft \langle s^{\dagger},a^{\dagger},s \rangle} \left(s,a\right) - q_{\alpha}\left(s,a\right) \right| \leq \frac{K}{c_{\alpha}^{2}}.$$

*Proof.* First change the notations. Let  $s_0 = s^{\dagger}$ ,  $a_0 = a^{\dagger}$ . Also let  $\alpha^1 = \alpha$ ,  $\beta^1 = \alpha \triangleleft \langle s^{\dagger}, a^{\dagger}, s \rangle$ . The result to prove becomes

$$\sum_{s_1} \frac{\alpha_{s_0 a_0 s_1}^1}{\alpha_{s_0 a_0}^1} \max_{a_1} \left| q_{\beta^1} \left( s_1, a_1 \right) - q_{\alpha^1} \left( s_1, a_1 \right) \right| \le \frac{K}{c_{\alpha}^2}.$$

Consider the finite time horizon approximations of  $q_{\beta^1}$  and  $q_{\alpha^1}$ , namely  $q_{\beta^1}^{\gamma,\tau}$ and  $q_{\alpha^1}^{\gamma,\tau}$ . With a little abuse of notation, we drop the superscript  $\gamma$  in this proof. Note that this shall not be confused with the finite time horizon curiosity Q-values without discount.

For  $\tau = 2$ , consider the following inequality:

$$\begin{split} &\frac{\alpha_{s_{0}a_{0}s_{1}}^{1}}{\alpha_{s_{0}a_{0}}^{1}} \max_{a_{1}} \left| q_{\beta^{1}}^{2}\left(s_{1},a_{1}\right) - q_{\alpha^{1}}^{2}\left(s_{1},a_{1}\right) \right| \\ &\leq \frac{\alpha_{s_{0}a_{0}s_{1}}^{1}}{\alpha_{s_{0}a_{0}}^{1}} \max_{a_{1}} \left| g\left(\beta_{s_{1},a_{1}}^{1}\right) - g\left(\alpha_{s_{1},a_{1}}^{1}\right) \right| \\ &+ \gamma \frac{\alpha_{s_{0}a_{0}s_{1}}^{1}}{\alpha_{s_{0}a_{0}}^{1}} \max_{a_{1}} \left| \sum_{s_{2}} \left( \frac{\beta_{s_{1}a_{1}s_{2}}^{1}}{\beta_{s_{1}a_{1}}^{1}} - \frac{\alpha_{s_{1}a_{1}s_{2}}^{1}}{\alpha_{s_{1}a_{1}}^{1}} \right) \max_{a_{2}} q_{\beta^{2}}^{1}\left(s_{2},a_{2}\right) \right| \\ &+ \gamma \frac{\alpha_{s_{0}a_{0}s_{1}}^{1}}{\alpha_{s_{0}a_{0}}^{1}} \max_{a_{1}} \sum_{s_{2}} \frac{\alpha_{s_{1}a_{1}s_{2}}^{1}}{\alpha_{s_{1}a_{1}}^{1}} \max_{a_{2}} \left| q_{\beta^{2}}^{1}\left(s_{2},a_{2}\right) - q_{\alpha^{2}}^{1}\left(s_{2},a_{2}\right) \right|. \end{split}$$

Here  $\beta^2 = \beta^1 \triangleleft \langle s_1 a_1 s_2 \rangle$ ,  $\alpha^2 = \alpha^1 \triangleleft \langle s_1 a_1 s_2 \rangle$ . Note that the error between  $q_{\beta^1}^2$ and  $q_{\alpha^1}^2$  has been decomposed into three terms. The first term captures the difference between the immediate information gain, the second term captures the error between transition probabilities, and the third term is of the same form as the left side of the inequality, except  $\tau$  is decreased by 1. To simplify the notation, let  $\mathbb{F}^t$  be the operator

$$\mathbb{F}^{t}\left[\cdots\right] = \sum_{s_{t}} \frac{\alpha_{s_{t-1}a_{t-1}s_{t}}^{t-1}}{\alpha_{s_{t-1}a_{t-1}}^{t-1}} \max_{a_{t}}\left[\cdots\right].$$

For fixed  $\tau$ , let

$$\delta_{t} = \left| g\left(\beta_{s_{t},a_{t}}^{t}\right) - g\left(\alpha_{s_{t},a_{t}}^{t}\right) \right| \\ + \gamma \left| \sum_{s_{t+1}} \left( \frac{\beta_{s_{t}a_{t}s_{t+1}}^{t}}{\beta_{s_{t}a_{t}}^{t}} - \frac{\alpha_{s_{t}a_{t}s_{t+1}}^{t}}{\alpha_{s_{t}a_{t}}^{t}} \right) \max_{a_{t+1}} q_{\beta^{t+1}}^{\tau-t} \left( s_{t+1}, a_{t+1} \right) \right|,$$

and

$$\phi_t = q_{\beta^t}^{\tau+1-t} \left( s_t, a_t \right) - q_{\alpha^t}^{\tau+1-t} \left( s_t, a_t \right)$$

One can write

$$\mathbb{F}^1 \phi_1 \le \mathbb{F}^1 \delta_1 + \gamma \mathbb{F}^1 \mathbb{F}^2 \phi_2.$$

Repeat this process for general  $\tau$ , it follows that

$$\begin{split} \mathbb{F}^{1}\phi_{1} &\leq \mathbb{F}^{1}\delta_{1} + \gamma \mathbb{F}^{1}\mathbb{F}^{2}\phi_{2} \\ &\leq \mathbb{F}^{1}\delta_{1} + \gamma \mathbb{F}^{1}\left[\mathbb{F}^{2}\delta_{2} + \gamma \mathbb{F}^{2}\mathbb{F}^{3}\phi_{3}\right] \\ &= \mathbb{F}^{1}\delta_{1} + \gamma \mathbb{F}^{1}\mathbb{F}^{2}\delta_{2} + \gamma^{2}\mathbb{F}^{1}\mathbb{F}^{2}\mathbb{F}^{3}\phi_{3} \\ &= \cdots \\ &= \mathbb{F}^{1}\delta_{1} + \gamma \mathbb{F}^{1}\mathbb{F}^{2}\delta_{2} + \cdots + \gamma^{t-1}\mathbb{F}^{1}\cdots\mathbb{F}^{t}\delta_{t} + \cdots + \gamma^{\tau-2}\mathbb{F}^{1}\cdots\mathbb{F}^{\tau-1}\delta_{\tau-1} \\ &+ \gamma^{\tau-1}\mathbb{F}^{1}\cdots\mathbb{F}^{\tau}\phi_{\tau}. \end{split}$$

Now look at a particular term in the inequality above, for example,

$$\mathbb{F}^{1} \cdots \mathbb{F}^{t} \delta_{t} = \sum_{s_{1}} \frac{\alpha_{s_{0}a_{0}s_{1}}^{1}}{\alpha_{s_{0}a_{0}}^{1}} \max_{a_{1}} \cdots \sum_{s_{t}} \frac{\alpha_{s_{t-1}a_{t-1}s_{t}}^{t-1}}{\alpha_{s_{t-1}a_{t-1}}^{t-1}} \max_{a_{t}} \delta_{t}.$$

Note that if  $\langle s_t, a_t \rangle \neq \langle s^{\dagger}, a^{\dagger} \rangle$  then  $\delta_t = 0$ , since  $\beta^t$  and  $\alpha^t$  differ only in the entry indexed by  $\langle s^{\dagger}, a^{\dagger}, s_1 \rangle$ . The following discussion assumes that  $\langle s_t, a_t \rangle = \langle s^{\dagger}, a^{\dagger} \rangle$ . From Lemma.5, let  $K_1 = \frac{S}{2}$ , then

$$\left|g\left(\beta_{s_{t},a_{t}}^{t}\right) - g\left(\alpha_{s_{t},a_{t}}^{t}\right)\right| \leq \frac{K_{1}}{\alpha_{s_{t},a_{t}}^{t}\alpha_{s_{t},a_{t},s_{1}}^{t}}$$

From Lemma.6 and 7, there is some  $K_2$  depends only on S and  $\gamma$ , such that

$$\left| \sum_{s_{t+1}} \left( \frac{\beta_{s_{t}a_{t}s_{t+1}}^{t}}{\beta_{s_{t}a_{t}}^{t}} - \frac{\alpha_{s_{t}a_{t}s_{t+1}}^{t}}{\alpha_{s_{t}a_{t}}^{t}} \right) \max_{a_{t+1}} q_{\beta^{t+1}}^{\tau-t} \left( s_{t+1}, a_{t+1} \right) \right|$$
  
$$\leq \frac{1}{\alpha_{s_{0},a_{0},s_{1}}^{t}} \sum_{s_{t+1}} \frac{\alpha_{s_{t}a_{t}s_{t+1}}^{t}}{\alpha_{s_{t}a_{t}}^{t}} \max_{a_{t+1}} q_{\beta^{t+1}}^{\tau-t} \left( s_{t+1}, a_{t+1} \right)$$
  
$$\leq \frac{K_{2}}{\alpha_{s_{0},a_{0},s_{1}}^{t} c_{\alpha^{t}}},$$

where  $c_{\alpha^t} = \min_s \min_a \alpha_{s,a}^t$ . In combination, there is some  $K_0$  such that

$$\delta_t \le \frac{K_0}{c_{\alpha^t} \alpha_{s^\dagger, a^\dagger, s_1}^t}$$

The next step is tricky: Assume that the policy is given, say, it is already the policy maximize  $\mathbb{F}^1 \cdots \mathbb{F}^t \delta_t$ , so that each *a* is a deterministic function of the prior  $\alpha^1$  and the previous history. Consider a trajectory  $s_0 a_0 s_1 a_1 \cdots s_t a_t$ , the predictive probability of seeing such a trajectory is given by

$$p(s_1a_1\cdots s_ta_t|s_0a_0) = \frac{\alpha_{s_0a_0s_1}^1}{\alpha_{s_0a_0}^1}\frac{\alpha_{s_1a_1s_2}^2}{\alpha_{s_1a_1}^2}\cdots\frac{\alpha_{s_{t-1}a_{t-1}s_t}^{t-1}}{\alpha_{s_{t-1}a_{t-1}}^{t-1}}.$$

Again, if  $\langle s_t, a_t \rangle \neq \langle s^{\dagger}, a^{\dagger} \rangle$ , then  $p(s_1a_1 \cdots s_ta_t | s_0a_0) \delta_t = 0$ . Otherwise,

$$p\left(s_{1}a_{1}\cdots s_{t}a_{t}|s_{0}a_{0}\right)\delta_{t} = \frac{\alpha_{s_{1}a_{1}s_{2}}^{2}}{\alpha_{s_{1}a_{1}}^{2}}\cdots\frac{\alpha_{s_{t-1}a_{t-1}s_{t}}^{t-1}}{\alpha_{s_{t-1}a_{t-1}}^{t-1}}\cdot\left(\frac{\alpha_{s_{0}a_{0}s_{1}}^{1}}{\alpha_{s_{0}a_{0}}^{1}}\delta_{t}\right)$$

$$\leq \frac{\alpha_{s_{1}a_{1}s_{2}}^{2}}{\alpha_{s_{1}a_{1}}^{2}}\cdots\frac{\alpha_{s_{t-1}a_{t-1}s_{t}}^{t-1}}{\alpha_{s_{t-1}a_{t-1}}^{t-1}}\cdot\frac{K_{0}}{c_{\alpha^{t}}\alpha_{s_{0}a_{0}}^{1}}\cdot\frac{\alpha_{s_{0}a_{0}s_{1}}^{1}}{\alpha_{s_{0}a_{0},s_{1}}^{t}}$$

$$\leq \frac{\alpha_{s_{1}a_{1}s_{2}}^{2}}{\alpha_{s_{1}a_{1}}^{2}}\cdots\frac{\alpha_{s_{t-1}a_{t-1}s_{t}}^{t-1}}{\alpha_{s_{t-1}a_{t-1}}^{t-1}}\cdot\frac{K_{0}}{c_{\alpha^{t}}\alpha_{s_{0}a_{0}}^{1}}$$

$$\leq \frac{\alpha_{s_{1}a_{1}s_{2}}^{2}}{\alpha_{s_{1}a_{1}}^{2}}\cdots\frac{\alpha_{s_{t-1}a_{t-1}s_{t}}^{t-1}}{\alpha_{s_{t-1}a_{t-1}s_{t}}^{t-1}}\cdot\frac{K_{0}}{c_{\alpha^{1}}^{2}}.$$

Note that

$$\frac{\alpha_{s_1a_1s_2}^2}{\alpha_{s_1a_1}^2} \cdots \frac{\alpha_{s_{t-1}a_{t-1}s_t}^{t-1}}{\alpha_{s_{t-1}a_{t-1}}^{t-1}} = p\left(s_2a_2\cdots s_ta_t|s_1a_1\right)$$

is the probability of seeing the trajectory  $s_2a_2\cdots s_ta_t$ , when the agent assumes prior  $\alpha^1 \triangleleft \langle s_0, a_0, s_1 \rangle = \alpha^2$ , and follows the same policy starting from  $\langle s_1, a_1 \rangle$ . Clearly,

$$\sum_{s_2} \cdots \sum_{s_t} p\left(s_2 a_2 \cdots s_t a_t | s_1 a_1\right) = 1,$$

which leads to

$$\mathbb{F}^{1} \cdots \mathbb{F}^{t} \delta_{t} = \sum_{s_{1}} \sum_{s_{2}} \cdots \sum_{s_{t}} p\left(s_{1}a_{1} \cdots s_{t}a_{t} | s_{0}a_{0}\right) \delta_{t}$$
$$\leq \sum_{s_{1}} \frac{K_{0}}{c_{\alpha^{1}}^{2}} \sum_{s_{2}} \cdots \sum_{s_{t}} p\left(s_{2}a_{2} \cdots s_{t}a_{t} | s_{1}a_{1}\right)$$
$$\leq \frac{SK_{0}}{c_{\alpha^{1}}^{2}}.$$

Putting the equation back, and note that  $c_{\alpha^1}^2=c_\alpha^2$  is a constant on  $\alpha,$  one has

$$\mathbb{F}^{1}\phi_{1} \leq \mathbb{F}^{1}\delta_{1} + \gamma \mathbb{F}^{1}\mathbb{F}^{2}\delta_{2} + \dots + \gamma^{t-1}\mathbb{F}^{1}\cdots\mathbb{F}^{t}\delta_{t} + \dots + \gamma^{\tau-2}\mathbb{F}^{1}\cdots\mathbb{F}^{\tau-1}\delta_{\tau-1}$$

$$+ \gamma^{\tau-1}\mathbb{F}^{1}\cdots\mathbb{F}^{\tau}\phi_{\tau}$$

$$\leq \frac{SK_{0}}{c_{\alpha}^{2}}\left(1 + \gamma + \dots + \gamma^{\tau-2}\right) + \gamma^{\tau-1}\mathbb{F}^{1}\cdots\mathbb{F}^{\tau}\phi_{\tau}$$

$$\leq \frac{SK_{0}}{1 - \gamma}\frac{1}{c_{\alpha}} + \gamma^{\tau-1}\mathbb{F}^{1}\cdots\mathbb{F}^{\tau}\phi_{\tau}.$$

From Lemma.6, since the curiosity Q-values are bounded, there is some  $K_3$  such that

$$\begin{split} \phi_{\tau} &= \left| q_{\beta^{t}}^{1} \left( s_{t}, a_{t} \right) - q_{\alpha^{t}}^{1} \left( s_{t}, a_{t} \right) \right| \\ &\leq \left| q_{\beta^{t}}^{1} \left( s_{t}, a_{t} \right) \right| + \left| q_{\alpha^{t}}^{1} \left( s_{t}, a_{t} \right) \right| \\ &\leq \left| q_{\beta^{t}} \left( s_{t}, a_{t} \right) \right| + \left| q_{\alpha^{t}} \left( s_{t}, a_{t} \right) \right| \\ &\leq \frac{K_{3}}{c_{\alpha}}, \end{split}$$

thus

$$\mathbb{F}^1 \phi_1 \le \frac{SK_0}{1-\gamma} \frac{1}{c_\alpha} + \gamma^{\tau-1} \frac{K_3}{c_\alpha}.$$

Let  $\tau \to \infty$ , one has

$$\sum_{s_1} \frac{\alpha_{s_0 a_0 s_1}^1}{\alpha_{s_0 a_0}^1} \max_{a_1} \left| q_{\beta^1} \left( s_1, a_1 \right) - q_{\alpha^1} \left( s_1, a_1 \right) \right| \le \frac{K}{c_{\alpha}^2},$$

where  $K = \frac{SK_0}{1-\gamma}$  is a constant depending on S and  $\gamma$  only.

The central result in this subsection is given by the following Proposition.

**Proposition 5.** There is some K > 0 depending on S and  $\gamma$  only, such that

$$\left|q_{\alpha}\left(s,a\right)-\tilde{q}_{\alpha}\left(s,a\right)\right|\leq rac{K}{c_{\alpha}^{2}}$$

 $\it Proof.$  Write Eq.5 into the following form

$$q_{\alpha}(s,a) = g(\alpha_{s,a}) + \gamma \sum_{s'} \frac{\alpha_{s,a,s'}}{\alpha_{s,a}} \max_{a'} q_{\alpha}(s',a') + \gamma \sum_{s'} \frac{\alpha_{s,a,s'}}{\alpha_{s,a}} \left[ \max_{a'} q_{\alpha \triangleleft \langle s,a,s' \rangle} \left(s',a'\right) - \max_{a'} q_{\alpha}\left(s',a'\right) \right].$$

The last term is bounded by

$$\delta = \sum_{s'} \frac{\alpha_{s,a,s'}}{\alpha_{s,a}} \left| \max_{a'} q_{\alpha \triangleleft \langle s, a, s' \rangle} \left( s', a' \right) - \max_{a'} q_{\alpha} \left( s', a' \right) \right|$$
  
$$\leq \sum_{s'} \frac{\alpha_{s,a,s'}}{\alpha_{s,a}} \max_{a'} \left| q_{\alpha \triangleleft \langle s, a, s' \rangle} \left( s', a' \right) - q_{\alpha} \left( s', a' \right) \right|.$$

Apply Lemma.7, it follows that there is some constant  $K_0$  depending on S and  $\gamma$  only, such that

$$\sum_{s'} \frac{\alpha_{s,a,s'}}{\alpha_{s,a}} \max_{a'} \left| q_{\alpha \triangleleft \langle s,a,s' \rangle} \left( s',a' \right) - q_{\alpha} \left( s',a' \right) \right| \le \frac{K_0}{c_{\alpha}^2}$$

Therefore  $\delta \leq \frac{K_0}{c_{\alpha}^2}$ . Now compare  $q_{\alpha}$  and  $\tilde{q}_{\alpha}$ :

$$\begin{split} \max_{s} \max_{a} &|q_{\alpha}\left(s,a\right) - \tilde{q}_{\alpha}\left(s,a\right)| \\ &= \max_{s} \max_{a} \left| \gamma \sum_{s'} \frac{\alpha_{s,a,s'}}{\alpha_{s,a}} \left( \max_{a'} q_{\alpha}\left(s',a'\right) - \max_{s'} \tilde{q}_{\alpha}\left(s',a'\right) \right) + \gamma \delta \right| \\ &\leq \gamma \max_{s} \max_{a} \left| q_{\alpha}\left(s,a\right) - \tilde{q}_{\alpha}\left(s,a\right) \right| + \frac{\gamma K_{0}}{c_{\alpha}^{2}}. \end{split}$$

Therefore

$$\max_{s} \max_{a} \left| q_{\alpha}\left(s,a\right) - \tilde{q}_{\alpha}\left(s,a\right) \right| \leq \frac{\gamma K_{0}}{1 - \gamma} \cdot \frac{1}{c_{\alpha}^{2}}.$$

Letting  $K = \frac{\gamma K_0}{1-\gamma}$  completes the proof.

### 4.5 Quality of the Approximation in Connected Markovian Environment

Proposition.5 guarantees that the difference between  $q_{\alpha}$  and  $\tilde{q}_{\alpha}$  decreases at the rate of  $c_{\alpha}^{-2}$ . However, this alone is not enough to guarantee that  $\tilde{q}_{\alpha}$  converges to  $q_{\alpha}$  when the agent operates in the environment. For example, consider the environment consists of two connected components. In this case,  $c_{\alpha}$  is upper bounded since that in one of the connected component  $\alpha_{s,a}$  never increases. Here we make the following assumption:

**Assumption III** The environment is finite Markovian with dynamics p(s'|s, a), and the Markov chain with transition kernel

$$p(s'|s) = \frac{1}{A} \sum_{a \in \mathcal{A}} p(s'|s, a)$$

is irreducible.

The first half of the assumption ensures that  $\frac{\alpha_{s,a,s'}}{\alpha_{s,a}}$  converges to p(s'|s,a) when  $\alpha_{s,a}$  goes to infinity by Law of Large Numbers. The second half of the assumption implies that it is always possible to navigate from one state to another with positive probability of success. Therefore, if some  $g(\alpha_{s,a})$  is large, the information is guaranteed to propagate to all the states. Under this assumption, we prove in this section that when  $t \to \infty$ ,

$$\left|\frac{q_{\alpha}\left(s,a\right)}{\tilde{q}_{\alpha}\left(s,a\right)}-1\right|\to0,$$

namely, the curiosity Q-value and the DP approximation are getting arbitrarily closer along time.

The proof is unwrapped in three steps.

**Lemma 9.** Assume IV), and the agent chooses the action greedily with respect to  $\tilde{q}_{\alpha^t}$ , where  $\alpha^t$  is the posterior after t time steps. Then for any s, a,

$$\lim_{t \to \infty} \alpha_{s,a}^t = \infty, \ a.s.$$

*Proof.* Note that  $\alpha_{s,a,s'}^t$  is non-decreasing, and can only increase by one if increasing. Therefore,  $\lim_{t\to\infty} \alpha_{s,a}^t < \infty$  implies that there is some  $T_{s,a}$  and  $c_{s,a}$  such that for all t > T,  $\alpha_{s,a}^t = c_{s,a}$ .

such that for all t > T,  $\alpha_{s,a}^t = c_{s,a}$ . The complement of  $\lim_{t\to\infty} \alpha_{s,a}^t = \infty$  for all  $\langle s, a \rangle$  is that  $\exists \Lambda \subset \mathcal{S} \times \mathcal{A}, \Lambda \neq \emptyset$ , and  $\exists T_{s,a}, c_{s,a}$  for all  $\langle s, a \rangle \in \Lambda$ , such that  $\alpha_{s,a}^t = c_{s,a}$  for all  $t > T_{s,a}$ . Since there are only finitely many  $\langle s, a \rangle$ , this can be simplified to  $\exists \Lambda \neq \emptyset, \exists T, \exists c_{s,a}$ , such that  $\alpha_{s,a}^t = c_{s,a}$  for all t > T and  $\langle s, a \rangle \in \Lambda$ . Fix  $\Lambda \neq \emptyset$ , T and  $c_{s,a}$ , we show that the event  $\alpha_{s,a}^t = c_{s,a}$  for t > T and  $\langle s, a \rangle \in \Lambda$  is a null event. Let  $\overline{\Lambda} = S \times A \setminus \Lambda$ , by definition,  $\alpha_{s,a}^t \to \infty$  for all  $\langle s, a \rangle \in \overline{\Lambda}$ . Clearly,  $\overline{\Lambda}$  is not empty. Define

$$\mathcal{S}_I = \{s \in \mathcal{S} : \exists a, a'' \text{ such that } \langle s, a \rangle \in \Lambda, \langle s, a'' \rangle \notin \Lambda \}.$$

Namely,  $S_I$  is the 'boundary' between  $\Lambda$  and  $\overline{\Lambda}$ .

The first step is to show  $S_I \neq \emptyset$  if  $\Lambda \neq \emptyset$ , or more precisely, the event  $S_I = \emptyset$ and  $\Lambda \neq \emptyset$  is null. Assume  $S_I = \emptyset$  and  $\Lambda \neq \emptyset$ , then  $\Lambda$  must satisfy that if  $\langle s, a \rangle \in \Lambda$  for some a, then  $\langle s, a \rangle \in \Lambda$  for all a. Let  $S_\Lambda \subset S$  be the set of s such that  $\langle s, a \rangle \in \Lambda$ . Clearly, once reaching  $s \in S_\Lambda$ , any action chosen would cause  $\Lambda$ be visited, which can only happen for finitely many times. This implies that for any  $s \in S_\Lambda$ , any state action pair  $\langle s', a' \rangle$  such that p(s|s', a') > 0 can only be visited finite number of times *almost surely*, because the probability of sampling from  $p(\cdot|s', a')$  for infinitely many times but only getting finite number of s is zero. From Assumption IV), for any  $S_\Lambda \neq S$ , there is always some  $\langle s', a' \rangle$  such that  $s' \notin S_\Lambda$  and p(s|s', a') > 0, so  $\langle s', a' \rangle$  can only be visited finitely many times, by definition  $\langle s', a' \rangle \in \Lambda$ , which contradicts with the fact that  $s' \notin S_\Lambda$ .

Next we show that at least for one  $s \in S_I$ , following the optimal strategy leads to some  $\langle s, a \rangle \in \Lambda$  being visited. For t > T, Define

$$\hat{q}\left(s,a\right) = r\left(s,a\right) + \gamma \sum_{s'} \hat{p}\left(s'|s,a\right) \max_{a'} \hat{q}\left(s',a'\right),$$

with

$$\hat{p}\left(s'|s,a\right) = \begin{cases} p\left(s'|s,a\right), \text{ if } \langle s,a \rangle \notin \Lambda \\ \frac{\alpha_{s,a,s'}^t}{\alpha_{s,a}^t}, \text{ if } \langle s,a \rangle \in \Lambda \end{cases}$$

and

$$r(s,a) = \begin{cases} 0, \text{ if } \langle s,a \rangle \notin \Lambda\\ g\left(\alpha_{s,a}^t\right), \text{ if } \langle s,a \rangle \in \Lambda \end{cases}$$

Clearly,  $\hat{p}$  and r do not depend on t, and  $\hat{q}$  is the unique optimal solution. Now let  $\langle s^{\dagger}, a^{\dagger} \rangle \in \Lambda$  be the pair such that  $s \in S_I$ , and

$$\hat{q}\left(s^{\dagger},a^{\dagger}\right) = \max_{\langle s,a\rangle\in\Lambda,s\in\mathcal{S}_{I}}\hat{q}\left(s,a\right).$$

It can be seen that for any a' such that  $\langle s^{\dagger}, a' \rangle \notin \Lambda$ ,  $\hat{q}(s^{\dagger}, a') \leq \gamma \hat{q}(s^{\dagger}, a^{\dagger})$ . The reason is the following: Performing a' leads to zero immediate reward since  $\langle s^{\dagger}, a' \rangle \notin \Lambda$ . Let s'' be the result of the transition, then either  $s'' \in S_I$ , so  $\max_{a''} \hat{q}(s'', a'') \leq \hat{q}(s^{\dagger}, a^{\dagger})$ , or s'' is some other state such that  $\langle s'', a'' \rangle \notin \Lambda$  for all a''. (Note that s'' cannot be a state such that  $\langle s'', a'' \rangle \in \Lambda$  for all a''.) In the latter case, since s'' is only connected to states in  $\Lambda$  through  $S_I$ , it must be that

$$\max_{a''} \hat{q}\left(s'', a''\right) \le \gamma \hat{q}\left(s^{\dagger}, a^{\dagger}\right),$$

since at least one more step must be made to reach  $S_I$  first. Taking into account the discount, it follows that

$$\hat{q}\left(s^{\dagger},a^{\dagger}\right) - \hat{q}\left(s^{\dagger},a'\right) \ge (1-\gamma)\,\hat{q}\left(s^{\dagger},a^{\dagger}\right).$$

Replace  $\hat{q}$  with  $\tilde{q}_{\alpha^t}$  leads to

$$\tilde{q}_{\alpha^{t}}\left(s^{\dagger},a^{\dagger}\right) - \tilde{q}_{\alpha^{t}}\left(s^{\dagger},a'\right) \geq (1-\gamma)\,\hat{q}\left(s^{\dagger},a^{\dagger}\right) \\ + \tilde{q}_{\alpha^{t}}\left(s^{\dagger},a^{\dagger}\right) - \hat{q}\left(s^{\dagger},a^{\dagger}\right) + \tilde{q}_{\alpha^{t}}\left(s^{\dagger},a'\right) - \hat{q}\left(s^{\dagger},a'\right)$$

From the initial assumption, when t > T,  $\langle s^{\dagger}, a^{\dagger} \rangle$  is never visited, also, the action is chosen greedily with respect to  $\tilde{q}_{\alpha^t}$ . This implies that at least for one a' such that  $\langle s^{\dagger}, a' \rangle \notin \Lambda$ ,

$$\tilde{q}_{\alpha^t}\left(s^{\dagger}, a^{\dagger}\right) - \tilde{q}_{\alpha^t}\left(s^{\dagger}, a'\right) \le 0$$

or

$$\begin{split} & 0 \ge (1-\gamma)\,\hat{q}\left(s^{\dagger},a^{\dagger}\right) + \tilde{q}_{\alpha^{t}}\left(s^{\dagger},a^{\dagger}\right) - \hat{q}\left(s^{\dagger},a^{\dagger}\right) + \tilde{q}_{\alpha^{t}}\left(s^{\dagger},a^{\prime}\right) - \hat{q}\left(s^{\dagger},a^{\prime}\right) \\ & \ge (1-\gamma)\,\hat{q}\left(s^{\dagger},a^{\dagger}\right) - 2\max_{s}\max_{a}\left|\tilde{q}_{\alpha^{t}}\left(s,a\right) - \hat{q}\left(s,a\right)\right|, \end{split}$$

which leads to

$$\max_{s} \max_{a} \left| \tilde{q}_{\alpha^{t}}\left(s,a\right) - \hat{q}\left(s,a\right) \right| \geq \frac{1-\gamma}{2} \hat{q}\left(s^{\dagger},a^{\dagger}\right).$$

Note that

$$\begin{aligned} \left| \tilde{q}_{\alpha^{t}}\left(s,a\right) - \hat{q}\left(s,a\right) \right| &\leq \left| g\left(\alpha_{s,a}^{t}\right) - r\left(s,a\right) \right| \\ &+ \gamma \sum_{s'} \left| \frac{\alpha_{s,a,s'}^{t}}{\alpha_{s,a}^{t}} - \hat{p}\left(s'|s,a\right) \right| \max_{a'} \tilde{q}_{\alpha^{t}}\left(s',a'\right) \\ &+ \gamma \sum_{s'} \hat{p}\left(s'|s,a\right) \max_{a'} \left| \tilde{q}_{\alpha^{t}}\left(s',a'\right) - \hat{q}\left(s,a\right) \right|, \end{aligned}$$

 $\mathbf{SO}$ 

$$\begin{split} & \max_{s} \max_{a} \left| \tilde{q}_{\alpha^{t}}\left(s,a\right) - \hat{q}\left(s,a\right) \right| \\ & \leq \frac{1}{1-\gamma} \left| g\left(\alpha_{s,a}^{t}\right) - r\left(s,a\right) \right| \\ & + \frac{\gamma}{1-\gamma} \max_{s} \max_{a} \sum_{s'} \left| \frac{\alpha_{s,a,s'}^{t}}{\alpha_{s,a}^{t}} - \hat{p}\left(s'|s,a\right) \right| \max_{a'} \tilde{q}_{\alpha^{t}}\left(s',a'\right). \end{split}$$

From Lemma.4,

$$\left|g\left(\alpha_{s,a}^{t}\right)-r\left(s,a\right)\right|=\max_{\left\langle s,a\right\rangle \notin A}g\left(\alpha_{s,a}^{t}\right)<\frac{S-1}{2\alpha_{s,a}^{t}}\rightarrow0.$$

Therefore, there is some T' such that  $\left|g\left(\alpha_{s,a}^{t}\right) - r\left(s,a\right)\right| < \frac{1-\gamma}{4}\hat{q}\left(s^{\dagger},a^{\dagger}\right)$  for all  $\langle s,a \rangle \notin \Lambda$ . Also note that

$$\tilde{q}_{\alpha^{t}}\left(s',a'\right) \leq \frac{S-1}{2\left(1-\gamma\right)c_{\alpha}}$$

where  $c_{\alpha} = \min_{\langle s,a \rangle \in \Lambda} c_{s,a}$ . Let  $K = \frac{\gamma(S-1)}{2(1-\gamma)^2 c_{\alpha}}$ , then

$$\begin{split} K \max_{s} \max_{a} \sum_{s'} \left| \frac{\alpha_{s,a,s'}^{t}}{\alpha_{s,a}^{t}} - \hat{p}\left(s'|s,a\right) \right| &+ \frac{1-\gamma}{4} \hat{q}\left(s^{\dagger},a^{\dagger}\right) \\ \geq \frac{\gamma}{1-\gamma} \max_{s} \max_{a} \sum_{s'} \left| \frac{\alpha_{s,a,s'}^{t}}{\alpha_{s,a}^{t}} - \hat{p}\left(s'|s,a\right) \right| \max_{a'} \tilde{q}_{\alpha^{t}}\left(s',a'\right) \\ &+ \frac{1}{1-\gamma} \left| g\left(\alpha_{s,a}^{t}\right) - r\left(s,a\right) \right| \\ \geq \max_{s} \max_{a} \left| \tilde{q}_{\alpha^{t}}\left(s,a\right) - \hat{q}\left(s,a\right) \right| \\ \geq \frac{1-\gamma}{2} \hat{q}\left(s^{\dagger},a^{\dagger}\right), \end{split}$$

thus

$$\begin{split} \max_{\langle s,a \rangle \notin \Lambda} \sum_{s'} \left| \frac{\alpha_{s,a,s'}^t}{\alpha_{s,a}^t} - p\left(s'|s,a\right) \right| &= \max_s \max_a \sum_{s'} \left| \frac{\alpha_{s,a,s'}^t}{\alpha_{s,a}^t} - \hat{p}\left(s'|s,a\right) \right| \\ &\geq \frac{1 - \gamma}{4K} \hat{q}\left(s^{\dagger},a^{\dagger}\right), \end{split}$$

for all t > T'. This implies that when  $t \to \infty$ , the empirical ratio  $\frac{\alpha_{s,a,s'}^t}{\alpha_{s,a}^t}$  does not converge to p(s'|s,a), which is a null event because it contradicts the Strong Law of Large Numbers. This in turn implies that for fixed  $\Lambda$ , T and  $c_{s,a}$ , the event  $\exists \Lambda \neq \emptyset$ ,  $\exists T$ ,  $\exists c_{s,a}$ , such that  $\alpha_{s,a}^t = c_{s,a}$  for all t > T and  $\langle s, a \rangle \in \Lambda$  is null.

As the last step, notice that there are only countably many such events, and since the union of countably many null events is still null, one can conclude that  $\lim_{t\to\infty} \alpha_{s,a}^t = \infty$  for all  $\langle s, a \rangle$  holds almost surely.

The next step is to show that all  $\tilde{q}_{\alpha^t}(s, a)$  decreases at the rate lower bounded by  $c_{\alpha}^{-1}$ . Let  $q_{s,a}$  be the Q-value of performing a at state s, assuming the reward is 1 at all states. Namely,  $q_{s,a}$  is the solution of the following Bellman equation

$$q_{s,a} = 1 + \gamma \sum_{s'} p(s'|s,a) \sum_{a'} q_{s',a'}$$

Clearly,  $q_{s,a} > 0$  from Assumption IV). Define  $q = \min_{s,a} q_{s,a}$ . Also, let

$$u_{s,a} = \frac{\sum_{s' \neq s^*} f\left(\alpha_{s,a,s'}^0\right) - f\left(\sum_{s' \neq s^*} \alpha_{s,a,s'}^0\right)}{2},$$

where  $\alpha^0$  is the initial  $\alpha$  representing the agent's prior, and  $s^* = \arg \max_{s'} \alpha^0_{s,a,s'}$  as defined in Lemma.4. Define  $u = \min_{s,a} u_{s,a}$ .

**Lemma 10.** Assume IV), and let  $c_{\alpha^t} = \min_s \min_a \alpha_{s,a}^t$ , then

$$\lim \inf_{t \to \infty} c_{\alpha^t} \tilde{q}_{\alpha^t} (s, a) \ge uq, \ a.s.$$

*Proof.* Let  $\hat{q}_{\alpha^t}$  be the solution to the following Bellman equation:

$$\hat{q}_{\alpha^{t}}\left(s,a\right) = g\left(\alpha_{s,a}^{t}\right) + \gamma \sum_{s'} p\left(s'|s,a\right) \max_{a'} \hat{q}_{\alpha^{t}}\left(s',a'\right).$$

Clearly, for any  $\langle s, a \rangle$ ,

$$g\left(\alpha_{s,a}^{t}\right) \geq \frac{u_{s,a}}{\alpha_{s,a}^{t}} \geq \frac{u}{c_{\alpha^{t}}}.$$

and because  $\hat{q}_{\alpha^t}$  is optimal,

$$\hat{q}_{\alpha^{t}}(s,a) \geq \frac{u}{c_{\alpha^{t}}}q_{s,a} \geq \frac{uq}{c_{\alpha^{t}}}, \forall s, a,$$

or  $c_{\alpha^t} \hat{q}_{\alpha^t}(s, a) \ge uq$ .

Fix an  $\varepsilon > 0$ , we show that

$$\lim \inf_{t \to \infty} c_{\alpha^{t}} \tilde{q}_{\alpha^{t}} \left( s, a \right) \le uq \left( 1 - \varepsilon \right), \, \forall s, a$$

is a null event. Assuming  $\liminf_{t\to\infty} c_{\alpha^t} \tilde{q}_{\alpha^t} \leq uq (1-\varepsilon)$ , and following similar procedure as in the proof of Lemma.9, let  $K = \frac{\gamma(S-1)}{2(1-\gamma)^2}$ , then

$$\max_{s} \max_{a} \sum_{s'} \left| \frac{\alpha_{s,a,s'}^{t}}{\alpha_{s,a}^{t}} - \hat{p}\left(s'|s,a\right) \right| \ge \frac{c_{\alpha}}{K} \max_{s} \max_{a} \left| \tilde{q}_{\alpha^{t}}\left(s,a\right) - \hat{q}\left(s,a\right) \right| \\\ge \frac{uq\varepsilon}{K}$$

holds for infinitely many t, which contradicts again with the Law of Large Numbers.

Let  $\varepsilon_n = \frac{1}{n}$ , then the union of the countably many events

$$\lim \inf_{t \to \infty} c_{\alpha^{t}} \tilde{q}_{\alpha^{t}} \left( s, a \right) \le uq \left( 1 - \varepsilon_{n} \right), \, \forall s, a$$

is again a null event, therefore

$$\lim \inf_{t \to \infty} c_{\alpha^t} \tilde{q}_{\alpha^t} (s, a) \ge uq, \text{ a.s.}$$

Combining Lemma.9 and 10 produces the following proposition.

**Proposition 6.** Assume IV), and that the agent acts greedily with respect to  $\tilde{q}_{\alpha}$ , then

$$\lim_{t \to \infty} \left| \frac{q_{\alpha^t}}{\tilde{q}_{\alpha^t}} - 1 \right| = 0, \ a.s.$$

and there is some K depending only on the dynamics and  $\gamma$ , such that

$$\lim \sup_{t \to \infty} c_{\alpha} \left| \frac{q_{\alpha^t}}{\tilde{q}_{\alpha^t}} - 1 \right| \le K.$$

*Proof.* Note that

$$\left|\frac{q_{\alpha}}{\tilde{q}_{\alpha}} - 1\right| \le \frac{K}{c_{\alpha}} \cdot \frac{1}{c_{\alpha}\tilde{q}_{\alpha}}$$

where K is given in Proposition.5. Use Lemma.9, 10, the result follows trivially.

# 5 Experiment

The idea presented in the previous section is illustrated through a simple experiment. The environment is an MDP consisting of two groups of densely connected states (cliques) linked by a long corridor. The agent has two actions allowing it to move along the corridor deterministically, whereas the transition probabilities inside each clique are randomly generated. The agent assumes Dirichlet priors over all transition probabilities, and the goal is to learn the transition model of the MDP. In the experiment, each clique consists of 5 states, (states 1 to 5 and states 56 to 60), and the corridor is of length 50 (states 6 to 55). The prior over each transition probability is  $Dir\left(\frac{1}{60}, \ldots, \frac{1}{60}\right)$ . We compare four different algorithms: i) random exploration, where the agent

We compare four different algorithms: i) random exploration, where the agent selects each of the two actions with equal probability at each time step; ii) Qlearning with the immediate information gain g(ao||h) as the reward; iii) greedy exploration, where the agent chooses at each time step the action maximizing g(a||h); and iv) a dynamic-programming (DP) approximation of the optimal Bayesian exploration, where at each time step the agent follows a policy which is computed using policy iteration, assuming that the dynamics of the MDP is given by the current posterior, and the reward is the expected information gain g(a||h).

Fig.2 shows the typical behavior of the four algorithms. The upper four plots show how the agent moves in the MDP starting from one clique. Both greedy exploration and DP approximation move back and forth between the two cliques. Random exploration has difficulty moving between the two cliques due to the random walk behavior in the corridor. Q-learning exploration, however, gets stuck in the initial clique. The reason for is that since the jump on the corridor is deterministic, the information gain decreases to virtually zero after only several attempts, therefore the Q-value of jumping into the corridor becomes much lower than the Q-value of jumping inside the clique. The bottom plot shows how the cumulative information gain grows over time, and how the DP approximation clearly outperforms the other algorithms, particularly in the early phase of exploration.

## 6 Related Work

The idea of actively selecting queries to accelerate learning process has a long history [2,3,8], and received a lot of attention in recent decades, primarily in the context of active learning [9] and artificial curiosity [7]. In particular, measuring learning progress using KL divergence dates back to the 50's [5,3]. In 1995 this was combined with reinforcement learning, with the goal of optimizing future expected information gain [11]. Others renamed this Bayesian surprise [4].

Our work differs from most previous work in two main points: First, like in [11], we consider the problem of exploring a dynamic environment, where actions change the environmental state, while most work on active learning and Bayesian experiment design focuses on queries that do not affect the environment [9]. Second, our result is theoretically sound and directly derived from first principles, in contrast to the more heuristic application [11] of traditional reinforcement learning to the problem of maximizing expected information gain. We formulated the concept of curiosity (Q) value, and highlighted the necessity of balancing immediate information gain and long-term expected information gain (see Eq.4). In particular, we pointed out a previously neglected subtlety of using KL divergence as learning progress.

Conceptually, however, our work is closely connected to artificial curiosity and intrinsically motivated reinforcement learning [7,10,8] for agents that actively explore the environment without external reward signal. In fact, the very definition of the curiosity (Q) value permits a firm connection between pure exploration and reinforcement learning.

### 7 Conclusion

We have presented the principle of optimal Bayesian exploration in dynamic environments, centered around the concept of the curiosity (Q) value. Our work provides a theoretically sound foundation for designing more effective exploration strategies. Based on this result, we establish the optimality of the DP approximation of the optimal Bayesian exploration in the MDP case.

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Fig. 2. The exploration process of a typical run of 4000 steps. The upper four plots shows the position of the agent between state 1 (the lowest) and 60 (the highest). The states at the top and the bottom correspond to the two cliques, and the states in the middle correspond to the corridor. The lowest plot is the cumulative information gain with respect to the prior.