Extreme State Aggregation beyond Markov Decision Processes

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Abstract

We consider a Reinforcement Learning setup where an agent interacts with an environment in observation-reward-action cycles without any (esp. MDP) assumptions on the environment. State aggregation and more generally feature reinforcement learning is concerned with mapping histories/raw-states to reduced/aggregated states. The idea behind both is that the resulting reduced process (approximately) forms a small stationary finite-state MDP, which can then be efficiently solved or learnt. We considerably generalize existing aggregation results by showing that even if the reduced process is not an MDP, the (q-)value functions and (optimal) policies of an associated MDP with same state-space size solve the original problem, as long as the solution can approximately be represented as a function of the reduced states. This implies an upper bound on the required state space size that holds uniformly for all RL problems. It may also explain why RL algorithms designed for MDPs sometimes perform well beyond MDPs.

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Keywords

state aggregation, reinforcement learning, non-MDP.

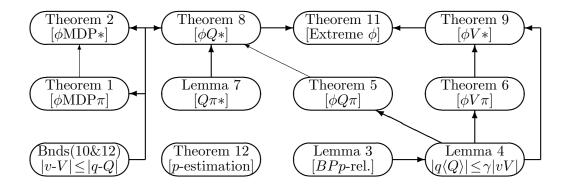
1 Introduction

In Reinforcement Learning (RL) [SB98], an agent Π takes actions in some environment P and observes its consequences and is rewarded for them. A well-understood and efficiently solvable [Put94] and efficiently learnable [SLL09, LH14b] case is where the environment is (modelled as) a finite-state stationary Markov Decision Process (MDP). Unfortunately most interesting real-world problems P are neither finite-state, nor stationary, nor Markov. One way of dealing with this mismatch is to somehow transform the real-world problem into a small MDP: Feature Reinforcement Learning (FRL) [Hut09c] and U-tree [McC96] deal with the case of arbitrary unknown environments, while state aggregation assumes the environment is a large known stationary MDP [GDG03, EDM03, FPP04]. The former maps histories into states (Section 2), the latter groups raw states into aggregated states.

Here we follow the FRL approach and terminology, since it is arguably most general: It subsumes the cases where the original process P is an MDP, a k-order MDP, a POMDP, and others (Section 3). Thinking in terms of histories also naturally stifles any temptation of a naive frequency estimate of P (no history ever repeats). Finally we find the history vs state terminologically somewhat neater than raw state vs aggregated state.

More importantly, we consider maps ϕ from histories to states for which the reduced process P_{ϕ} is not (even approximately) an MDP (Section 4). At first this seems to defeat the original purpose, namely of reducing P to a well-understood and efficiently solvable problem class, namely small MDPs. The main novel contribution of this paper is to show that there is still an associated finite-state stationary MDP p whose solution (approximately) solves the original problem P, as long as the solution can still be represented (Section 5). Indeed, we provide an upper bound on the required state space size that holds uniformly for all P (Section 6). While these are interesting theoretical insights, it is a-priori not clear whether they could by utilized to design (better) RL algorithms. We also show how to learn p from experience (Section 7), and sketch an overall learning algorithm and regret/PAC analysis based on our main theorems (Section 8). We briefly discuss how to relax one of the conditions in our main theorems by permuting actions (Section 9). We conclude with an outlook on future work and open problems (Section 10). A list of notation can be found in Appendix A.

The diagram below depicts the dependencies between our results:



2 Feature Markov Decision Processes (ΦMDP)

This section formally describes the setup of [Hut09c]. It consists of the agent-environment framework and maps ϕ from observation-reward-action histories to MDP states. This arrangement is called "Feature MDP" or short Φ MDP. We use upper-case letters P, Q, V, and Π for the Probability, (Q-)Value, and Policy of the original (agent-environment interactive) Process, and lower-case letters p, q, v, and π for the probability, (q-)value, and policy of the (reduced/aggregated) MDP.

Agent-environment setup [Hut09c]. We start with the standard agent-environment setup [RN10] in which an agent Π interacts with an environment P. The agent can choose from actions $a \in \mathcal{A}$ and the environment provides observations $o \in \mathcal{O}$ and real-valued rewards $r \in \mathcal{R} \subseteq [0;1]$ to the agent. This happens in cycles t = 1,2,3,...: At time t, after observing o_t and receiving reward r_t , the agent takes action a_t based on history

$$h_t := o_1 r_1 a_1 \dots o_{t-1} r_{t-1} a_{t-1} o_t r_t \in \mathcal{H}_t := (\mathcal{O} \times \mathcal{R} \times \mathcal{A})^{t-1} \times \mathcal{O} \times \mathcal{R}$$

Then the next cycle t+1 starts. The agent's objective is to maximize its long-term reward. To avoid integrals and densities, we assume spaces \mathcal{O} and \mathcal{R} are finite. They may be huge, so this is not really restrictive. Indeed, the Φ MDP framework has been specifically developed for huge observation spaces. Generalization to continuous \mathcal{O} and \mathcal{R} is routine [Hut09a]. Furthermore we assume that \mathcal{A} is finite and smallish, which is restrictive. Potential extensions to continuous \mathcal{A} are discussed in Section 10.

The agent and environment may be viewed as a pair of interlocking functions of the history $\mathcal{H} := (\mathcal{O} \times \mathcal{R} \times \mathcal{A})^* \times \mathcal{O} \times \mathcal{R} \cup \{\epsilon\}$, where ϵ is the empty history.

where \rightsquigarrow indicates that mappings \rightarrow are in general stochastic. We make no (stationarity or Markov or other) assumption on environment P. For most parts, environment P is assumed to be fixed, so dependencies on P will be suppressed. For

convenience and since optimal policies can be chosen to be deterministic (see Eq.(4)), we consider deterministic policies $a_t = \Pi(h_t)$ only.

Value functions, optimal Policies, and history Bellman equations. We measure the performance of a policy Π in terms of the P-expected γ -discounted reward sum $(0 \le \gamma < 1)$, called (Q-)Value of Policy Π at history h_t (and action a_t)

$$V^{\Pi}(h_t) := \mathbb{E}^{\Pi}[R_t|h_t] \text{ and } Q^{\Pi}(h_t, a_t) := \mathbb{E}^{\Pi}[R_t|h_t a_t], \text{ where } R_t := \sum_{\tau=t+1}^{\infty} \gamma^{\tau-t} r_{\tau}$$

The optimal Policy and (Q-)Value functions are

$$V^{*}(h_{t}) := \max_{\Pi} V^{\Pi}(h_{t})$$

$$Q^{*}(h_{t}, a_{t}) := \max_{\Pi} Q^{\Pi}(h_{t}, a_{t})$$

$$\Pi^{*} :\in \arg\max_{\Pi} V^{\Pi}(\epsilon)$$

$$(1)$$

The maximum over all policies Π always exists [LH14a] but may not be unique, in which case argmax denotes the set of optimal policies and Π^* denotes a representative or the whole set of optimal policies. Despite being history-based we can write down (pseudo)recursive Bellman (optimality) equations for the (optimal) (Q-)Values [Hut05, Sec.4.2]:

$$Q^{\Pi}(h_t, a_t) = \sum_{o_{t+1}r_{t+1}} P(o_{t+1}r_{t+1}|h_t a_t) [r_{t+1} + \gamma V^{\Pi}(h_{t+1})]$$

$$V^{\Pi}(h_t) = Q^{\Pi}(h_t, \Pi(h_t))$$
(2)

$$Q^{*}(h_{t}, a_{t}) = \sum_{o_{t+1}r_{t+1}} P(o_{t+1}r_{t+1}|h_{t}a_{t})[r_{t+1} + \gamma V^{*}(h_{t+1})]$$

$$V^{*}(h_{t}) = \max_{a_{t} \in \mathcal{A}} Q^{*}(h_{t}, a_{t})$$
(3)

$$\Pi^*(h_t) \in \arg\max_{a_t \in \mathcal{A}} Q^*(h_t, a_t)$$
(4)

Unlike their classical state-space cousins (see below), they are *not* self-consistency equations: The r.h.s. refers to a longer history h_{t+1} which is always different from the history h_t on the l.h.s, which precludes any learning algorithm based on estimating the frequency of state/history visits. Still the recursions will be convenient for the mathematical development.

From histories to states (ϕ). The space of histories is huge and unwieldy and no history ever repeats. Standard ways of dealing with this are to define a similarity metric on histories [McC96] or to aggregate histories [Hut09c]. We pursue the latter via a feature map $\phi: \mathcal{H} \to \mathcal{S}$ which reduces histories $h_t \in \mathcal{H}$ to states $s_t := \phi(h_t) \in \mathcal{S}$. W.l.g. we assume that ϕ is surjective. We also assume that state space \mathcal{S} is finite; indeed we are interested in small \mathcal{S} . This corresponds and indeed is equivalent to a partitioning of histories $\{\phi^{-1}(s): s \in \mathcal{S}\}$. Classical state aggregation usually uses the

partitioning view [GDG03, Ort07], but the map notation is a bit more convenient here.

The state s_t is supposed to summarize all relevant information in history h_t , which lower bounds the size of S. We pass from the complete history $o_1r_1a_1...o_nr_n$ to a 'reduced' history $s_1r_1a_1...s_nr_n$. Traditionally, 'relevant' means that the future is predictable from s_t (and a_t) alone, or technically that the reduced history forms a Markov decision process. This is precisely the condition this paper intends to lift (later).

From histories to MDPs. The probability of the successor states and rewards can be obtained by marginalization

$$P_{\phi}(s_{t+1}r_{t+1}|h_t a_t) := \sum_{\tilde{o}_{t+1}:\phi(h_t a_t \tilde{o}_{t+1}r_{t+1}) = s_{t+1}} P(\tilde{o}_{t+1}r_{t+1}|h_t a_t)$$
 (5)

Note that rewards (and actions) of the reduced process P_{ϕ} are the same as rewards (and actions) of the original process. The reduced process P_{ϕ} is a Markov Decision Process, or Markov for short, if P_{ϕ} only depends on h_t through s_t , i.e. is the same for all histories mapped to the same state. Formally

$$P_{\phi} \in \text{MDP} \quad : \iff \quad \exists p : P_{\phi}(s_{t+1}r_{t+1}|\tilde{h}_{t}a_{t}) = p(s_{t+1}r_{t+1}|s_{t}a_{t}) \quad \forall \phi(\tilde{h}_{t}) = s_{t} \quad (6)$$

Here and elsewhere a quantifier such as $\forall \phi(\tilde{h}_t) = s_t$ shall mean: for all values of all involved variables consistent with the constraint $\phi(\tilde{h}_t) = s_t$. The MDP P_{ϕ} is assumed to be stationary, i.e. independent of t; another condition to be lifted later. Condition (6) is essentially the stochastic bisimulation condition generalized to histories and being somewhat more restrictive regarding rewards: It is a condition on the reward distribution, while [GDG03] constrains its expectation only. This could easily be rectified but is besides the point of this paper. The bisimulation metric [FPP04] is an approximate version of (6), which measures the deviation of P_{ϕ} from being an MDP.

Many problems P can be reduced (approximately) to stationary MDPs [Hut09c]: Full-information games such as chess with a static opponent are already Markov, classical physics is approximately 2nd-order Markov, (conditional) i.i.d. processes such as Bandits have counting sufficient statistics, and for a POMDP planning problem, the belief vector is Markov.

Markov decision processes (MDP). We have used and continue to use uppercase letters V, Q, Π for the general process P. We will use lower-case letters v, q, π for (stationary) MDPs p. We use s and a for the current state and action, and s' and r' for successor state and reward. Consider a stationary finite-state MDP $p: \mathcal{S} \times \mathcal{A} \leadsto \mathcal{S} \times \mathcal{R}$ and stationary deterministic policy $\pi: \mathcal{S} \to \mathcal{A}$. Only in Section 3 will this p be given by (6), but in general p will be different from (6). In any case, the p-expected γ -discounted reward sum, called (q-)value of (optimal) policy $\pi^{(*)}$ in MDP p, are given by the Bellman (optimality) equations

$$q^{\pi}(s,a) = \sum_{s'r'} p(s'r'|sa)[r'+\gamma v^{\pi}(s')] \text{ and } v^{\pi}(s) = q^{\pi}(s,\pi(s))$$
 (7)

$$q^*(s,a) = \sum_{s'r'}^{s'r'} p(s'r'|sa)[r'+\gamma v^*(s')] \quad \text{and} \quad v^*(s) = \max_a q^*(s,a)$$
 (8)

$$\pi^*(s) \in \arg\max_{a} q^*(s, a).$$
 Note: $v^{\pi}(s) \le v^*(s), \ q^{\pi}(s, a) \le q^*(s, a)$ (9)

Using p(s'r'|sa) = p(r'|sas')p(s'|sa) we could also rewrite (7) and (8) in terms of transition matrix p(s'|sa) and expected reward $\mathbb{E}[r'|sa]$ [SB98].

More notation. While our equations often assume or imply $s = s_t$, $a = a_t$, $s' = s_{t+1}$, $r' = r_{t+1}$, (and $h_{t+1} = h_t a o' r'$) for some t, technically s, a, s', r' are different variables from all variables in history $h_n = o_1 r_1 a_1 \dots o_t r_t a_t o_{t+1} r_{t+1} \dots a_n r_n$. Less prone to confusion are $o = o_t$, $o' = o_{t+1}$, $h = h_t$, h' = h a o' r'.

We call a function f(h), piecewise constant or ϕ -uniform iff $f(h) = f(\tilde{h})$ for all $\phi(h) = \phi(\tilde{h})$. Here and elsewhere $\forall \phi(h) = \phi(\tilde{h})$ is short for $\forall h, \tilde{h}: \phi(h) = \phi(\tilde{h})$. Similarly $\forall s = \phi(h)$ is short for $\forall s, h: s = \phi(h)$. Etc.

The Iverson bracket, $[\![R]\!] := 1$ if R = true and $[\![R]\!] := 0$ if R = false, denotes the indicator function. Throughout, $\varepsilon, \delta \ge 0$ denote approximation accuracy. Note that this includes the exact = 0 case.

We now show that if P reduces via ϕ to an MDP p, the solution of these equations yields (Q-)Values and optimal Policy of the original process P. This is not surprising and are just history-based versions of classical state-aggregation results [GDG03]. We state and prove them here, since notation and setup are somewhat different, and proof ideas and fragments will be reused later.

3 Exact Aggregation for $P_{\phi} \in MDP$

The following two theorems show that if ϕ reduces P to a stationary MDP via (5) and (6), then V and Q (and Π^*) essentially coincide with v and q (and π^*), where policy Π (Π^*) has to be assumed (will be shown) constant within each partition $\phi^{-1}(s)$. This allows to efficiently solve for (and learn in the case of unknown P) V and Q (and Π^*) in time polynomial in S by solving/learning (7) (or (8) and (9)) instead of (2) (or (3) and (4)).

Theorem 1 (ϕ MDP π) Let ϕ be a reduction such that $P_{\phi} \in MDP$ reduces to MDP p defined in (6), and let Π be some policy such that $\Pi(h) = \Pi(\tilde{h})$ for all $\phi(h) = \phi(\tilde{h})$. Then for all a and h it holds:

$$V^\Pi(h) = v^\pi(s) \quad and \quad Q^\Pi(h,a) = q^\pi(s,a), \quad where \quad \pi(s) := \Pi(h) \quad and \quad s = \phi(h)$$

Note that $\pi(s)$ is well-defined, since ϕ is surjective and $\Pi(h)$ is the same for all $h \in \phi^{-1}(s)$. The standard proof considers an m-horizon truncated MDP and induction

on m and $m \to \infty$. Besides the adaptation to histories, the proof below is a slight variation that avoids such truncation and limit. This style will be useful later. We explain all steps in detail here, since variations will be utilized later.

Proof. Let $\delta := \sup_{s=\phi(h),a} |q^{\pi}(s,a) - Q^{\Pi}(h,a)|$. Using $a' := \pi(s') = \Pi(h')$ for $s' = \phi(h')$ and (2) and (7) lets us bound the value difference

$$|v^{\pi}(s') - V^{\Pi}(h')| = |q^{\pi}(s', a') - Q^{\Pi}(h', a')| \le \delta \quad \forall s' = \phi(h')$$
 (10)

For any a and h, this implies

$$Q^{\Pi}(h,a) \stackrel{(a)}{=} \sum_{o'r'} P(o'r'|ha)[r' + \gamma V^{\Pi}(h')] \qquad [h' = hao'r']$$

$$\stackrel{(b)}{\leq} \sum_{s'r'} \sum_{o':\phi(h')=s'} P(o'r'|ha)[r' + \gamma(v^{\pi}(s') \pm \delta)] \qquad (11)$$

$$\stackrel{(c)}{=} \sum_{s'r'} P_{\phi}(s'r'|ha)[r' + \gamma v^{\pi}(s')] \pm \gamma \delta$$

$$\stackrel{(d)}{=} \sum_{s'r'} p(s'r'|sa)[r' + \gamma v^{\pi}(s')] \pm \gamma \delta \qquad [s := \phi(h)]$$

$$\stackrel{(e)}{=} q^{\pi}(s,a) \pm \gamma \delta$$

(a) is just (2). In (b) we sum over all o' by first summing over all o' such that $\phi(hao'r') = s'$ and then summing over all s'. We have also upper/lower bounded $V^{\Pi}(h')$ via (10). (c) is the definition (5) of P_{ϕ} and pulls out $\gamma\delta$ using that probability P_{ϕ} sums to 1. (d) is the definition (6) of p. (e) is simply (7). The chain (11a-e) holds for all $s = \phi(h)$ and a, hence

$$\delta = \sup_{s=\phi(h),a} |q^{\pi}(s,a) - Q^{\Pi}(h,a)| \leq \gamma \delta \quad \Rightarrow \quad \delta \leq 0$$

Hence
$$v^{\pi}(s) = V^{\Pi}(h)$$
 and $q^{\pi}(s,a) = Q^{\Pi}(h,a)$ for all $s = \phi(h)$ and a .

Theorem 2 (ϕ MDP*) Let ϕ be a reduction such that $P_{\phi} \in MDP$ reduces to MDP p defined in (6), Then for all a and h it holds:

$$\Pi^*(h) = \pi^*(s) \quad and \quad V^*(h) = v^*(s) \quad and \quad Q^*(h,a) = q^*(s,a), \quad where \quad s = \phi(h)$$

In case optimal policies/actions are not unique, $\Pi^*(h) = \pi^*(s)$ means that the set $\pi^*(s)$ of optimal actions in state $s = \phi(h)$ coincides with the set of optimal actions in history h. The core of the proof follows the same steps (11a-e) as for the previous theorem, but the rest is slightly different. Additionally we have to show that some Π^* is piecewise constant (in Theorem 1 we assumed Π was).

Proof. Let $\delta := \sup_{s=\phi(h),a} |q^*(s,a) - Q^*(h,a)|$. We can bound the value difference

$$|v^*(s) - V^*(h)| \stackrel{(a)}{=} |\max_{a} q^*(s, a) - \max_{a} Q^*(h, a)|$$

$$\stackrel{(b)}{\leq} \max_{a} |q^*(s, a) - Q^*(h, a)| \stackrel{(c)}{\leq} \delta \quad \forall s = \phi(h)$$

$$(12)$$

(a) follows from the definitions (3) and (8). (b) follows from the following general elementary frequently used bound

$$\left| \max_{x} f(x) - \max_{x} g(x) \right| \le \max_{x} \left| f(x) - g(x) \right| \tag{13}$$

(c) follows from the definition of δ .

One now can show that $Q^*(h,a) \leq q^*(s,a) \pm \gamma \delta$ for $s = \phi(h)$ by following exactly the same steps as (11a-e) just with Π and π replaced by * and using (12) instead of (10), and using the Bellman optimality equations (3) and (8) instead of the Bellman equations (2) and (7). Also as before, this implies $\delta \leq \gamma \delta$, hence $\delta \leq 0$, hence $v^*(s) = V^*(h)$ and $q^*(s,a) = Q^*(h,a)$ for all $s = \phi(h)$ and a. Finally, the latter implies $\pi^*(s) = \operatorname{argmax}_a q^*(s,a) = \operatorname{argmax}_a Q^*(h,a) = \Pi^*(h)$.

Approximate aggregation results if P_{ϕ} is approximately MDP can also be derived [EDM03]. The core results in the next section show that aggregation is possible far beyond P_{ϕ} being approximately MDP.

4 Approximate Aggregation for General P

This section prepares for the main technical contribution of the paper in the next section. The key quantity to relate original and reduced Bellman equations is a form of stochastic inverse of ϕ , whose choice and analysis will be deferred to Section 7.

Dispersion probability B. Let $B_{\phi}: \mathcal{S} \times \mathcal{A} \rightsquigarrow \mathcal{H}$ be a probability distribution on finite histories for each state-action pair such that $B_{\phi}(h|sa) = 0$ if $s \neq \phi(h)$. $B \equiv B_{\phi}$ may be viewed as a stochastic inverse of ϕ that assigns non-zero probability only to $h \in \phi^{-1}(s)$. The formal constraints we pose on B are

$$B(h|sa) \ge 0$$
 and $\sum_{h \in \mathcal{H}} B(h|sa) = \sum_{h:\phi(h)=s} B(h|sa) = 1 \quad \forall s, a$ (14)

This implicitly requires ϕ to be surjective, i.e. $\phi(\mathcal{H}) = \mathcal{S}$, which can always be made true by defining $\mathcal{S} := \mathcal{S}_{\phi} := \phi(\mathcal{H})$. Note that the sum is taken over histories of any/mixed length. In general, B is a somewhat weird distribution, since it assigns probabilities to past and future observations given the current state and action. The interpretation and choice of B does not need to concern us, except later when we want to learn p.

The MDP requirement (6) will be replaced by the following definition:

$$p(s'r'|sa) := \sum_{h \in \mathcal{H}} P_{\phi}(s'r'|ha)B(h|sa)$$

$$\equiv \sum_{t=1}^{\infty} \sum_{h_{t} \in \mathcal{H}_{t}} P_{\phi}(s_{t+1} = s', r_{t+1} = r'|h_{t}, a_{t} = a)B(h_{t}|sa)$$
(15)

That is, the finite-state stationary MDP p is built from feature map ϕ , dispersion probability B, and environment P: The p-probability of observing state-reward pair (s',r') from state-action pair (s,a) is defined as the B-average of P_{ϕ} over all histories h consistent with (s,a), where $P_{\phi}(s'r'|ha)$ is the P_{ϕ} -probability of observing (s',r'), obtained from P by ϕ -marginalization, given history h and action a. The r.h.s. of the first line is merely shorthand for the second line. Note that sas'r' are fixed and do not appear in h which ranges over histories \mathcal{H} of all lengths. It is easy to see that p is a probability distribution, and it is Markov by definition. If $P_{\phi} \in \text{MDP}$, then definition (15) coincides with p defined in (6). In general, the MDP p, depending on arbitrary B, is not the state distribution induced by P (and Π), which in general is non-Markov. Note that p is a stationary MDP for any B satisfying (14) and $any \phi$ and P. We need the following lemmas:

Some lemmas. The first lemma establishes the key relation between P and p via B used later to relate original history Bellman (optimality) equations (2–4) with reduced state Bellman (optimality) equations (7–9).

Lemma 3 (B-P-p relation) For any function $f: S \times R \to \mathbb{R}$ and p defined in (15) in terms of P via (5), and $s' := \phi(h')$ and h' := hao'r' it holds

$$\sum_{h \in \mathcal{H}} B(h|sa) \sum_{o'r'} P(o'r'|ha) f(s',r') = \sum_{s'r'} p(s'r'|sa) f(s',r')$$

$$\underset{depends \ on \ hao'r'}{\uparrow} p(s'r'|sa) f(s',r')$$

Proof.

$$\sum_{h \in \mathcal{H}} B(h|sa) \sum_{o'r'} P(o'r'|ha) f(s',r')$$

$$\stackrel{(a)}{=} \sum_{h \in \mathcal{H}} B(h|sa) \sum_{s'r'} \sum_{o':\phi(h')=s'} P(o'r'|ha) f(s',r')$$

$$\stackrel{(b)}{=} \sum_{h \in \mathcal{H}} B(h|sa) \sum_{s'r'} P_{\phi}(s'r'|ha) f(s',r')$$

$$\stackrel{(c)}{=} \sum_{r'} p(s'r'|sa) f(s',r')$$

In (a) we sum over all o' by first summing over all o' such that $\phi(hao'r') = s'$ and then summing over all s'. In (b) we used the definition (5) of P_{ϕ} . In (c) we used the definition (15) of p.

Inequalities (10) and (12) trivially bound v-V differences in terms of q-Q differences: $|v-V| \le \max_a |q-Q|$. The following lemma shows that a reverse holds in expectation, i.e. $|q-\langle Q\rangle_B| \le \gamma |v-V|$. The expectation can (only) be dropped if Q is constant for $h \in \phi^{-1}(s)$. Formally define

$$\langle f(h,a)\rangle_B := \sum_{\tilde{h}\in\mathcal{H}} B(\tilde{h}|sa)f(\tilde{h},a), \text{ where } s := \phi(h)$$
 (16)

That is, $\langle f(h,a)\rangle_B$ takes a *B*-average over all \tilde{h} that ϕ maps to the same state as h. For convenience we will sometimes drop the tilde over h when using (16), which we can do if we declare $s := \phi(h)$ to refer to the 'global' h in $\langle f(h,a)\rangle_B$ and not to the 'local' variable in the $h \in \mathcal{H}$ sum.

Lemma 4 $(|q - \langle Q \rangle| \leq \gamma |v - V|)$ For any P, ϕ , B, Π , π , define p via (15) and (5).

(i) If $|v^{\pi}(s) - V^{\Pi}(h)| \le \delta \ \forall s = \phi(h)$ then $|q^{\pi}(s,a) - \langle Q^{\Pi}(h,a) \rangle_B| \le \gamma \delta \ \forall s = \phi(h) \ \forall a.$

(ii) If $|v^*(s) - V^*(h)| \le \delta \ \forall s = \phi(h)$ then $|q^*(s,a) - \langle Q^*(h,a) \rangle_B| \le \gamma \delta \ \forall s = \phi(h) \ \forall a$.

Proof. (i) Let $s := \phi(h)$ and h' := hao'r' and $s' := \phi(h')$. Then

$$\langle Q^{\Pi}(h,a)\rangle_{B} \stackrel{\text{(16)}}{\equiv} \sum_{h\in\mathcal{H}} B(h|sa)Q^{\Pi}(h,a)$$

$$\stackrel{\text{(2)}}{\equiv} \sum_{h\in\mathcal{H}} B(h|sa) \sum_{o'r'} P(o'r'|ha)[r' + \gamma V^{\Pi}(h')]$$

$$\stackrel{\text{(a)}}{\leq} \sum_{h\in\mathcal{H}} B(h|sa) \sum_{o'r'} P(o'r'|ha)[r' + \gamma (v^{\pi}(s') \pm \delta)]$$

$$\stackrel{\text{Lem.3}}{\equiv} \sum_{s'r'} p(s'r'|sa)[r' + \gamma v^{\pi}(s')] \pm \gamma \delta$$

$$\stackrel{\text{(7)}}{\equiv} q^{\pi}(s,a) \pm \gamma \delta$$

In (a) we used the assumption (i) of the Lemma. The derived upper and lower bounds imply $|q^{\pi}(s,a) - \langle Q^{\Pi}(h,a) \rangle_B| \leq \gamma \delta$ (for all $s = \phi(h)$ and a).

(ii) follows the same steps except with Π and π replaced by Π^* and π^* , and using (3) and (8) instead of (2) and (7) to justify the steps. Note that in general $\Pi^* \neq \pi^*$!

5 Approximate Aggregation Results

This section contains the main technical contribution of the paper. We show that histories (or raw states) can be aggregated and modeled by an MDP even if the true

aggregated process is actually not an MDP. A necessary condition for successful aggregation is of course that the quantities of interest, namely (Q-)Value functions and Policies can be represented as functions of the aggregated states. The results in this section roughly show that these necessary conditions, which are significantly weaker than the MDP requirements, are also sufficient. All but one result also hold for approximate aggregation, i.e. approximate conditions lead to approximate reductions. We also lift the stationarity assumption.

- Theorem 5 shows how (approximately) ϕ -uniform Q^{Π} and Π can be obtained from the reduced Bellman equations (7).
- Theorem 6 weakens the assumptions and conclusions to (approximately) ϕ uniform V^{Π} and Π .
- Theorem 8 shows that for (approximately) ϕ -uniform Q^* , the optimal policy is (approximately) ϕ -uniform, and (an approximation of it) can be obtained via the reduced Bellman optimality equations (8).
- Theorem 9 shows that for (approximately) ϕ -uniform V^* and Π^* we can obtain similar but somewhat weaker results. The proof of the latter involves extra complications not present in the other three proofs. Indeed, the arguably most desirable bound (28) does not hold.

Note that all theorems crucially differ in their conditions and conclusions.

Theorem 5 $(\phi Q\pi)$ For any P, ϕ , and B, define p via (15) and (5). Let Π be some policy such that $|Q^{\Pi}(h,a)-Q^{\Pi}(\tilde{h},a)| \leq \varepsilon_q$ and either $\Pi(h)=\Pi(\tilde{h})$ with $\varepsilon_v:=0$ or $|V^{\Pi}(h)-V^{\Pi}(\tilde{h})| \leq \varepsilon_v$, for all $\phi(h)=\phi(\tilde{h})$ and all a. Then for all a and h it holds:

$$|Q^{\Pi}(h,a) - q^{\pi}(s,a)| \le \frac{\varepsilon}{1-\gamma} \quad and \quad |V^{\Pi}(h) - v^{\pi}(s)| \le \frac{\varepsilon}{1-\gamma},$$

$$where \quad \pi(s) := \Pi(h) \quad and \quad s = \phi(h) \quad and \quad \varepsilon := \varepsilon_v + \varepsilon_q$$

For the either-condition, $\pi(s)$ is uniquely defined, since $\Pi(h)$ is the same for all $h \in \phi^{-1}(s)$. For the or-condition, $\pi(s)$ is not unique, but any choice of $h \in \phi^{-1}(s)$ will do. Ignoring a factor 2 in the bounds, the or-condition is weaker than the either-condition; it allows to aggregate histories on which Π differs, as long as their (Q-)Values are close.

Proof. Let
$$\delta := \sup_{s=\phi(h),a} |q^{\pi}(s,a) - Q^{\Pi}(h,a)| \tag{17}$$

We first show

$$|v^{\pi}(s) - V^{\Pi}(h)| \le \delta + \varepsilon_v \quad \forall s = \phi(h)$$
 (18)

Under the *either*-condition this follows immediately from (10). For the *or*-condition, let $\pi(s) := \Pi(\tilde{h})$ for some $\tilde{h} \in \phi^{-1}(s)$. Then

$$|v^{\pi}(s) - V^{\Pi}(h)| \stackrel{(a)}{\leq} |v^{\pi}(s) - V^{\Pi}(\tilde{h})| + \varepsilon_v \stackrel{(b)}{=} |q^{\pi}(s, \tilde{a}) - Q^{\Pi}(\tilde{h}, \tilde{a})| + \varepsilon_v \stackrel{(c)}{\leq} \delta + \varepsilon_v$$

where (a) follows from the assumption by a triangle inequality, (b) from (2) and (7) and $\tilde{a} := \pi(s) \equiv \Pi(\tilde{h})$, and (c) from the definition of δ .

Now in both cases, (18) implies

$$|q^{\pi}(s, a) - \langle Q^{\Pi}(h, a) \rangle_B| \le \gamma(\delta + \varepsilon_v) \quad \forall s = \phi(h), a \tag{19}$$

by Lemma 4i. By assumption on Q^{Π} and B, for $s = \phi(h)$ we have

Together with (19) this implies $|q^{\pi}(s,a) - Q^{\Pi}(h,a)| \leq \gamma(\delta + \varepsilon_v) + \varepsilon_q$, hence $\delta \leq \gamma(\delta + \varepsilon_v) + \varepsilon_q$, hence $\delta \leq \frac{\varepsilon_q + \gamma \varepsilon_v}{1 - \gamma}$. Inserting this δ into (17) and (18) establishes the bounds in the theorem.

Theorem 6 $(\phi V\pi)$ For any P, ϕ , and B, define p via (15) and (5). Let Π be some policy such that $\Pi(h) = \Pi(\tilde{h})$ and $|V^{\Pi}(h) - V^{\Pi}(\tilde{h})| \le \varepsilon$ for all $\phi(h) = \phi(\tilde{h})$. Then for all a and h it holds:

$$|V^{\Pi}(h) - v^{\pi}(s)| \le \frac{\varepsilon}{1 - \gamma} \quad and \quad |q^{\pi}(s, a) - \langle Q^{\Pi}(h, a) \rangle_{B}| \le \frac{\varepsilon \gamma}{1 - \gamma}$$

$$where \quad \pi(s) := \Pi(h) \quad and \quad s = \phi(h)$$

Proof. Let $\delta := \sup_{s=\phi(h),a} |v^{\pi}(s) - V^{\Pi}(h)|$, fix some $s = \phi(h)$, and let $a^{\pi} := \Pi(h)$. Now

$$\langle Q^{\Pi}(h, a^{\pi}) \rangle_{B} \equiv \sum_{\tilde{h} \in \mathcal{H}: \phi(\tilde{h}) = s} B(\tilde{h} | s a^{\pi}) Q^{\Pi}(\tilde{h}, a^{\pi}) \stackrel{(a)}{=} \sum_{\tilde{h} \in \mathcal{H}: \phi(\tilde{h}) = s} B(\tilde{h} | s a^{\pi}) V^{\Pi}(\tilde{h})$$

$$\leq \sum_{\tilde{h} \in \mathcal{H}: \phi(\tilde{h}) = s} B(\tilde{h} | s a^{\pi}) [V^{\Pi}(h) \pm \varepsilon] = V^{\Pi}(h) \pm \varepsilon$$
(20)

where (a) follows from $a^{\pi} = \Pi(h) = \Pi(\tilde{h})$ and $Q^{\Pi}(\tilde{h},\Pi(\tilde{h})) = V^{\Pi}(\tilde{h})$. By Lemma 4i we have

$$|q^{\pi}(s,a) - \langle Q^{\Pi}(h,a)\rangle_B| \le \gamma \delta \quad \forall s = \phi(h), a$$
 (21)

We also have $q^{\pi}(s,a^{\pi}) = q^{\pi}(s,\pi(s)) = v^{\pi}(s)$ from (7). Together with (20) and (21) for $a = a^{\pi}$ this yields

$$|v^{\pi}(s) - V^{\Pi}(h)| \leq |v^{\pi}(s) - \langle Q^{\Pi}(h, a^{\pi}) \rangle_{B}| + |\langle Q^{\Pi}(h, a^{\pi}) \rangle_{B} - V^{\Pi}(h)| \leq \gamma \delta + \varepsilon$$

hence $\delta \leq \gamma \delta + \varepsilon$ by the definition of δ , hence $\delta \leq \frac{\varepsilon}{1-\gamma}$. Note that while $|q^{\pi}(s,a^{\pi}) - Q^{\Pi}(h,a^{\pi})| \leq \frac{\varepsilon}{1-\gamma}$, in general $|q^{\pi}(s,a) - Q^{\Pi}(h,a)| \not\leq \frac{\varepsilon}{1-\gamma}$ for $a \neq a^{\pi}$.

Example. Consider a process P which itself is an MDP in the observations with transition matrix T and reward function R, i.e. $P(o'r'|ha) = T^a_{oo'}R^{ar'}_{oo'}$, where o is the last observation in h. The example below has the special form $P(o'r'|ha) = T_{oo'} \cdot [r' = R(o)]$ with

$$T = \begin{pmatrix} \cdot & 1/2 & 1/2 & \cdot \\ 1/2 & \cdot & \cdot & 1/2 \\ \cdot & 1 & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot \end{pmatrix}, \quad R = \begin{pmatrix} \frac{\gamma/2}{1+\gamma} \\ \frac{1+\gamma/2}{1+\gamma} \\ 0 \\ 1 \end{pmatrix}, \quad r' = \frac{\gamma/2}{1+\gamma} \begin{pmatrix} 00 & 1/2 & 01 \end{pmatrix} r' = \frac{1+\gamma/2}{1+\gamma} \\ 1/2 & 1 & 1/2 \\ r' = 0 & 10 & 11 \end{pmatrix} r' = 1$$

It is an action-independent Markov process T with deterministic reward function R. The observation space is $\mathcal{O} = \{00,01,10,11\}$. For instance, $T_{00,01} = \frac{1}{2}$ and $R(00) = \frac{\gamma/2}{1+\gamma}$. Consider the reduction

$$s_t := \phi(h_t) := \begin{cases} 0 & \text{if } o_t = 00 \text{ or } 10 \\ 1 & \text{if } o_t = 01 \text{ or } 11 \end{cases} \in \mathcal{S} := \{0, 1\}$$

The reduced process P_{ϕ} is not (even approximately) Markov:

$$P_{\phi}(s'=0|o=00) = T_{00,00} + T_{00,10} = 0 + \frac{1}{2} = \frac{1}{2}$$

 $P_{\phi}(s'=0|o=10) = T_{10,00} + T_{10,10} = 0 + 0 = 0$

That is, P violates the bisimulation condition [GDG03], and raw states 00 and 10 have a large bisimulation distance [FPP04, Ort07]. On the other hand, the (Q-)Value function $V(o_t) := V^{\pi}(h_t) = Q^{\pi}(h_t, a_t) \forall a_t$ can easily be verified to be

$$V(00) = V(10) = \frac{\gamma}{1 - \gamma^2}$$
 and $V(01) = V(11) = \frac{1}{1 - \gamma^2}$

That is, V and Q are ϕ -uniform. The conditions of Theorems 5 and 6 are satisfied exactly ($\varepsilon = 0$), and hence the four raw states \mathcal{O} can be aggregated into two states \mathcal{S} despite $P_{\phi} \notin \text{MDP}$ (the policy is irrelevant and can be chosen constant). \diamondsuit

We now turn from the fixed policy case to similar theorems for optimal policies. For this we need the following lemma, which shows that if replacing the first action after h of the optimal policy Π^* by the action provided by Π thereafter following Π^* is at most ε -suboptimal, then always using Π is at most $\frac{\varepsilon}{1-\gamma}$ -suboptimal.

Lemma 7 ($Q\pi*$) If $Q^*(h,\Pi(h)) \ge V^*(h) - \varepsilon$ for all h for some policy Π , then for all h and a

$$0 \leq Q^*(h,a) - Q^{\Pi}(h,a) \leq \frac{\varepsilon \gamma}{1-\gamma} \quad and \quad 0 \leq V^*(h) - V^{\Pi}(h) \leq \frac{\varepsilon}{1-\gamma}$$

Proof. Let $\delta := \sup_{h,a} [Q^*(h,a) - Q^{\Pi}(h,a)]$. This implies

$$0 \stackrel{(a)}{\leq} V^*(h) - V^{\Pi}(h) \stackrel{(b)}{\leq} \varepsilon + Q^*(h, \Pi(h)) - Q^{\Pi}(h, \Pi(h)) \stackrel{(c)}{\leq} \varepsilon + \delta \qquad (22)$$

(a) follows from (1); (b) by assumption; and (c) by definition of δ for $a = \Pi(h)$. Now for any a and h, this implies

$$Q^{\Pi}(h,a) \overset{(1)}{\leq} Q^{*}(h,a) \overset{(3)}{=} \sum_{o'r'} P(o'r'|ha)[r'+\gamma V^{*}(h')] \qquad [h'=hao'r']$$

$$\overset{(22)}{\leq} \sum_{f} P(o'r'|ha)[r'+\gamma (V^{\Pi}(h')+\varepsilon+\delta)] \overset{(2)}{=} Q^{\Pi}(h,a)+\gamma(\varepsilon+\delta)$$

Hence $\delta \leq \gamma(\varepsilon + \delta)$, hence $\delta \leq \frac{\varepsilon \gamma}{1 - \gamma}$.

Theorem 8 $(\phi Q*)$ For any P, ϕ , and B, define p via (15) and (5). Assume $|Q^*(h,a)-Q^*(\tilde{h},a)| \leq \varepsilon$ for all $\phi(h)=\phi(\tilde{h})$ and all a. Then for all a and h and $s=\phi(h)$ it holds:

(i)
$$|Q^*(h,a) - q^*(s,a)| \le \frac{\varepsilon}{1-\gamma}$$
 and $|V^*(h) - v^*(s)| \le \frac{\varepsilon}{1-\gamma}$,

(ii)
$$0 \leq Q^*(h,a) - Q^{\tilde{\Pi}}(h,a) \leq \frac{2\varepsilon\gamma}{(1-\gamma)^2}$$
 and $0 \leq V^*(h) - V^{\tilde{\Pi}}(h) \leq \frac{2\varepsilon}{(1-\gamma)^2}$, where $\tilde{\Pi}(h) := \pi^*(s)$

(iii) If
$$\varepsilon = 0$$
 then $\Pi^*(h) = \pi^*(s)$

Proof. (i) The proof follows the same steps as the proof of Theorem 5, replacing all Π and π by * and using (12) instead of (10) and Lemma 4ii instead of Lemma 4i to justify the steps.

- (iii) If $\varepsilon = 0$, then $Q^*(h,a) = q^*(s,a)$ by (i) implies $\Pi^*(h) = \pi^*(s)$, where it is worthwhile to carefully check that the latter has actually not been used inadvertently in proving the former. Cf. the next theorem and proof.
 - (ii) For $s = \phi(h)$ and $\tilde{a} := \Pi(h) = \pi^*(s)$,

$$V^*(h) - \frac{\varepsilon}{1 - \gamma} \stackrel{(i)}{\leq} v^*(s) \stackrel{(8)}{=} q^*(s, \tilde{a}) \stackrel{(i)}{\leq} Q^*(h, \tilde{a}) + \frac{\varepsilon}{1 - \gamma}$$

which implies $Q^*(h,\tilde{\Pi}(h)) \ge V^*(h) - \frac{2\varepsilon}{1-\gamma}$. The claim now follows from Lemma 7.

Theorem 9 $(\phi V*)$ For any P, ϕ , and B, define p via (15) and (5). Assume $\Pi^*(h) = \Pi^*(\tilde{h})$ and $|V^*(h) - V^*(\tilde{h})| \le \varepsilon$ for all $\phi(h) = \phi(\tilde{h})$. Then for all a and h and $s = \phi(h)$ it holds:

$$(i) \quad |V^*(h) - v^*(s)| \le \frac{3\varepsilon}{(1 - \gamma)^2} \quad and \quad |q^*(s, a) - \langle Q^*(h, a) \rangle_B| \le \frac{3\varepsilon\gamma}{(1 - \gamma)^2},$$

(iii) If
$$\varepsilon = 0$$
 then $\Pi^*(h) = \pi^*(s)$

The proof (27) actually implies the stronger upper bound $V^*(h) - v^*(s) \le \frac{\varepsilon}{1-\gamma}$ and similarly for Q^* , but we do not know whether the upper bound can be improved.

Proof. While proofs start to get routine, here is a warning that care is in order when recycling similar proofs. Theorem 6 relies on the assumption that $\pi(s) = \Pi(h)$ for $s = \phi(h)$, while we were lucky that the proof of Theorem 8 worked for $\pi^*(s) \neq \Pi^*(h)$. Here we have to work a bit harder.

Let us define $a^0 := \pi^0(s) := \Pi^*(h)$ for $s = \phi(h)$. The Bellman equation for policy π^0 is

$$q^{\pi^0}(s,a) = \sum_{s'r'} p(s'r'|sa)[r' + \gamma v^{\pi^0}(s')] \quad \text{and} \quad v^{\pi^0}(s) = q^{\pi^0}(s,\pi^0(s))$$
 (23)

At this stage π^0 may well be different from π^* , since π^* satisfies (8), not (23), but we will now show that for $\varepsilon = 0$ it actually does. First note that

$$q^{\pi^0}(s, a^0) = v^{\pi^0}(s) \leq V^{\Pi^*}(h) \pm \frac{\varepsilon}{1 - \gamma} = V^*(h) \pm \frac{\varepsilon}{1 - \gamma}$$
 (24)

where the bounds follow from Theorem 6 applied to $\Pi := \Pi^*$ (with $\pi = \pi^0$). For general a we only get an upper bound:

$$q^{\pi^{0}}(s,a) - \frac{\varepsilon\gamma}{1-\gamma} \stackrel{Thm.6}{\leq} \langle Q^{\Pi^{*}}(h,a) \rangle_{B} \stackrel{(16)}{=} \sum_{\tilde{h} \in \mathcal{H}} B(\tilde{h}|sa)Q^{*}(\tilde{h},a) \qquad (25)$$

$$\stackrel{(4)}{\leq} \sum_{\tilde{h} \in \mathcal{H}} B(\tilde{h}|sa)Q^{*}(\tilde{h},\Pi^{*}(\tilde{h})) \stackrel{(14)}{=} \sum_{\tilde{h}:\phi(\tilde{h})=s} B(\tilde{h}|sa)V^{*}(\tilde{h})$$

$$\stackrel{(a)}{\leq} \sum_{\tilde{h}:\phi(\tilde{h})=s} B(\tilde{h}|sa)[V^{*}(h)+\varepsilon] \stackrel{(14)}{=} V^{*}(h)+\varepsilon$$

(a) uses the theorem's assumption on $V^*(h)$. Together, (24) and (25) imply

$$v^{\pi^0}(s) \stackrel{(23)}{=} q^{\pi^0}(s, a^0) \le \max_a q^{\pi^0}(s, a) \stackrel{(25)}{\le} V^*(h) + \frac{\varepsilon}{1 - \gamma} \stackrel{(24)}{\le} v^{\pi^0}(s) + \frac{2\varepsilon}{1 - \gamma}$$
 (26)

We first prove (ii) of the theorem, then (i):

(iii) For $\varepsilon = 0$, the previous equation implies $v^{\pi^0}(s) = \max_a q^{\pi^0}(s,a)$, hence (23) can be rewritten as

$$q^{\pi^0}(s, a) = \sum_{s'r'} p(s'r'|sa)[r' + \gamma v^{\pi^0}(s')]$$
 and $v^{\pi^0}(s) = \max_a q^{\pi^0}(s, a)$

This shows that (q^{π^0}, v^{π^0}) satisfies the same Bellman optimality equation as (q^*, v^*) does. Since it has a unique solution, we must have $q^{\pi^0} \equiv q^*$ and $v^{\pi^0} \equiv v^*$ and $\pi^* \equiv \pi^0$, which for $s = \phi(h)$ implies $\Pi^*(h) = \pi^*(s)$ by definition of π^0 . It also implies $V^*(h) = v^*(s)$ by (24), and $q^*(s,a) = \langle Q^*(h,a) \rangle_B$ by Lemma 4ii, i.e. the $\varepsilon = 0$ version of (i).

(i) We now continue with the general $\varepsilon > 0$ case. For all s and a we have

$$0 \overset{(9)}{\leq} q^*(s,a) - q^{\pi^0}(s,a) \overset{(7)}{\underset{(8)}{=}} \sum_{s'r'} p(s'r'|sa) \gamma(v^*(s') - v^{\pi^0}(s')) \overset{(a)}{\leq} \gamma \max_{s'} \{v^*(s') - v^{\pi^0}(s')\}$$

$$0 \overset{(9)}{\leq} v^*(s) - v^{\pi^0}(s) \overset{(26)}{\underset{(8)}{\leq}} \max_a q^*(s,a) - \max_a q^{\pi^0}(s,a) + \frac{2\varepsilon}{1-\gamma} \overset{(13)}{\leq} \max_a \{q^*(s,a) - q^{\pi^0}(s,a)\} + \frac{2\varepsilon}{1-\gamma} \overset{(13)}{\leq} \underset{(13)}{\leq} \underset{(13$$

In (a) we have upper bounded the p-expectation by the maximum. Together this gives

$$\max_{s} \{v^{*}(s) - v^{\pi^{0}}(s)\} \leq \gamma \max_{s} \{v^{*}(s) - v^{\pi^{0}}(s)\} + \frac{2\varepsilon}{1 - \gamma}$$

$$\Rightarrow \max_{s} \{v^{*}(s) - v^{\pi^{0}}(s)\} \leq \frac{2\varepsilon}{(1 - \gamma)^{2}}$$
Hence for $s = \phi(h)$: $V^{*}(h) - \frac{\varepsilon}{1 - \gamma} \stackrel{(24)}{\leq} v^{\pi^{0}}(s) \stackrel{(9)}{\leq} v^{*}(s) \stackrel{(9)}{\leq} v^{\pi^{0}}(s) + \frac{2\varepsilon}{(1 - \gamma)^{2}}$ (27)
$$\stackrel{(24)}{\leq} V^{*}(h) + \frac{\varepsilon}{1 - \gamma} + \frac{2\varepsilon}{(1 - \gamma)^{2}} \leq V^{*}(h) + \frac{3\varepsilon}{(1 - \gamma)^{2}}$$

Together with Lemma 4ii this implies (i).

We are primarily interested in the optimal policy $\Pi^*(h)$; to correctly represent the value $V^*(h)$ is only of indirect interest. If Π^* is ϕ -uniform, it can be represented as $\Pi^*(h) = \pi^0(s)$ for some π^0 , but if the ϕ -uniformity condition on V^* in Theorem 9 is dropped, the conclusion $\Pi^*(h) = \pi^*(s)$ can fail as the following example shows.

Counter Example. Let P be the MDP $P(o'r'|ha) := T^a_{oo'} \cdot \llbracket r' = R^a_o \rrbracket$ with two raw states $o \in \{0,1\}$ and two actions $a \in \{\alpha,\beta\}$ formally defined on the left and depicted on the right:

$$T^{\alpha} := \begin{pmatrix} 1 & 0 \\ 1 & 0 \end{pmatrix}, \qquad R^{\alpha} := \begin{pmatrix} 1/6 \\ 1 \end{pmatrix},$$

$$T^{\beta} := \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix}, \qquad R^{\beta} := \begin{pmatrix} 0 \\ 1/2 \end{pmatrix},$$

$$\alpha, r' = \frac{1}{2}, p = \frac{1}{2}$$

$$\alpha, r' = \frac{1}{2}, p = \frac{1}{2}$$

The value of policy π in vector notation is $V^{\pi} = R^{\pi} + \gamma T^{\pi} V^{\pi}$, where $V_{o_t}^{\pi} := V^{\pi}(h_t)$. The 4 stationary policies are denoted by $\pi = a^0 a^1$, where a^o is the action taken in raw state o. For $\gamma = 0$, their values are

Policy $\pi = \alpha \alpha$ has the highest value, therefore $\Pi^*(h) \equiv \alpha$. Let us now aggregate raw states $o \in \{0,1\}$ to a 1-state MDP. The most natural and useful choice of dispersion

probability B is described in Section 7. For the stationary raw MDP and constant behavior policy of this example, (35) reduces to $p(s'r'|sa) = P_{\phi B}(s'r'|sa)$. One can show that for this B, the value of the 1-state MDP is $v = \frac{1}{1-\gamma}\rho^{\top}R = \rho^{\top}R$ for $\gamma = 0$, where ρ is the stationary distribution $\rho^{\top} = \rho^{\top}T$ of T, in particular $\rho^{\alpha} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ for T^{α} and $\rho^{\beta} = \begin{pmatrix} 1/2 \\ 1/2 \end{pmatrix}$ for T^{β} . Since there is only 1 aggregated state, there are only 2 stationary policies, one for each action. This leads to $v^{\alpha} = \frac{1}{6} < \frac{1}{4} = v^{\beta}$, hence $\pi^*(s) \equiv \beta \neq \alpha \equiv \Pi^*(h) \ \forall s,h$. That is, despite Π^* being constant, $\pi^* \neq \Pi^*$, which shows that the condition on V^* in Theorem 9 cannot be dropped. Note that $V^* = V^{\alpha\alpha} = \binom{1/6}{1}$ is far from constant. By continuity, the policy reversal also holds for $\gamma > 0$. Indeed, this example works for all $0 \leq \gamma < 1$.

Missing Bound (ii) in Theorem 9. The absence of an analogue of Theorem 8ii from Theorem 9 of the form

(ii)
$$V^*(h) - V^{\tilde{\Pi}}(h) \stackrel{??}{=} O\left(\frac{\varepsilon}{(1-\gamma)^?}\right)$$
 where $\tilde{\Pi}(h) := \pi^*(s)$ (28)

is apparent. Here are some (weak) arguments why (28) is plausible:

- (1) Given that for fixed policy, Theorems 5 and 6 with approximately ϕ -uniform Q respectively V were similar, it seems a-priori plausible that (28) could hold.
- (2) For $\varepsilon = 0$ it immediately follows from Theorem 9, since in this case $\Pi(h) = \Pi^*(h)$. One might expect that some continuity argument allows to establish a bound for small $\varepsilon > 0$.
- (3) Theorem 8i&iii mostly carried over to Theorem 9, so a-priori it is not too implausible that Theorem 8ii carries over to (28). On the other hand, the proofs of (i) and (iii) of both theorems were sufficiently different, so the analogy argument is weak.
 - (4) Let $\tilde{a} := \tilde{\Pi}(h) := \pi^*(s)$ for $s = \phi(h)$. Then

$$\langle Q^*(h,\tilde{a})\rangle_B \overset{Thm.9i}{\geq} q^*(s,\tilde{a}) - \frac{3\varepsilon\gamma}{(1-\gamma)^2} \overset{(8)}{=} v^*(s) - \frac{3\varepsilon\gamma}{(1-\gamma)^2} \overset{(27)}{\geq} V^*(h) - \frac{3\varepsilon}{(1-\gamma)^2}$$

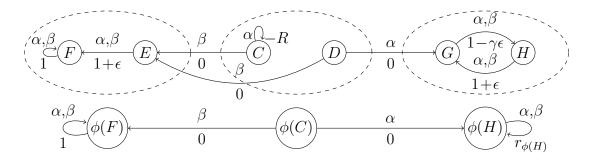
$$Q^*(h,\tilde{a}) \overset{(3)}{\leq} V^*(h)$$

For $\varepsilon = 0$ this pair of inequalities implies that $Q^*(h,\tilde{a})$ lower bounds its own expectation, therefore it must be constant and equal to $V^*(h)$ on each $\phi^{-1}(s)$ -partition. For $\varepsilon > 0$, with high probability $Q^*(h,\tilde{a})$ cannot be much smaller than $V^*(h)$. If it weren't for the probability qualifier we could now apply Lemma 7 to establish (28) (as in the proof of Theorem 8ii). Low probability events could invalidate this argument.

Indeed, (28) does not hold:

Theorem 10 ($\phi V*$) For any $0 \le \gamma < 1$ and any (arbitrarily large) C, there exist P, ϕ , and B with $\Pi^*(h) = \Pi^*(\tilde{h})$ and $|V^*(h) - V^*(\tilde{h})| \le \varepsilon$ for all $\phi(h) = \phi(\tilde{h})$ such that for p defined via (15) and (5) and $\tilde{\Pi}(h) := \pi^*(s)$ for $s = \phi(h)$, we have $V^*(h) - V^{\tilde{\Pi}}(h) \ge C$.

Proof. An (28) offending raw and aggregated MDP are depicted in the following diagram:



An arrow $(A) \xrightarrow{a} (B)$ denotes that action $a \in \mathcal{A} := \{\alpha, \beta\}$ leads with probability 1 and reward r' from state A to state B. R is a large positive reward. For the above raw MDP, we have $\Pi^*(C) = \Pi^*(D) = \beta$ and $\Pi^*(E) = \Pi^*(F) = \Pi^*(G) = \Pi^*(H) = \mathcal{A}$. Under this policy

$$\begin{array}{lll} V^*(F) & = & 1 + \gamma + \gamma^2 + \gamma^3 + \dots & = & \frac{1}{1 - \gamma} \\ V^*(E) & = & (1 + \varepsilon) + \gamma V^*(F) & = & \frac{1}{1 - \gamma} + \varepsilon \\ V^*(G) & = & (1 - \gamma \varepsilon) + \gamma V^*(H) & = & \frac{1}{1 - \gamma} & < & V^*(E) \\ V^*(H) & = & (1 + \varepsilon) + \gamma V^*(G) & = & \frac{1}{1 - \gamma} + \varepsilon \\ V^*(C) & = & V^*(D) & = & 0 + \gamma V^*(E) & = & \frac{\gamma}{1 - \gamma} + \gamma \varepsilon \end{array}$$

Now for ϕ aggregating the dashed-encircled states, and for stochastic inverse $B(F|\phi(F)) := 1$, and $B(H|\phi(H)) := 1/2$, and $B(C|\phi(C)) := 0$, the aggregated MDP is depicted in the lower part of the above diagram, where

$$r_{\phi(H)} := (1 - \gamma \varepsilon) B(G|\phi(H)) + (1 + \varepsilon) B(H|\phi(H))$$

$$= \frac{1}{2} (1 - \gamma \varepsilon) + \frac{1}{2} (1 + \varepsilon) = 1 + \frac{\varepsilon}{2} (1 - \gamma)$$

$$\Rightarrow v^*(\phi(H)) = \frac{r_{\phi(H)}}{1 - \gamma} = \frac{1}{1 - \gamma} + \frac{\varepsilon}{2} > \frac{1}{1 - \gamma} = v^*(\phi(F))$$

The optimal action in state $\phi(C)$ is therefore $\pi^*(\phi(C)) = \alpha = \tilde{\Pi}(C)$, hence $V^{\tilde{\Pi}}(C) = \frac{-R}{1-\gamma}$, hence $V^* - V^{\tilde{\Pi}}$ can be made arbitrarily large.

Discussion. Theorem 8ii is our main result. It implies that we can aggregate histories as much as we wish, as long as the optimal Q-value function and policy are still approximately representable as functions of aggregated states. Whether the reduced process P_{ϕ} is Markov or not is immaterial. We can use surrogate MDP p to find an ε -optimal policy for P.

All bounds in this sections can be shown to be tight by constructing appropriate example MDPs. Furthermore, all conditions of the theorems and lemmas can be

shown to be necessary by constructing counter-examples that violate one of the conditions and the conclusions in each theorem/lemma.

Most RL work, including on state aggregation, is formulated in terms of MDPs, i.e. the original process P is already an MDP. Let us call this the original or raw MDP. We could interpret the whole history as a raw state, which formally makes every P an MDP, but normally only observations are identified with raw states, i.e. P is a raw MDP iff P(o'r'|ha) = P(o'r'|oa). In this case, $V^*(h_t) = V^*(o_t)$ etc. depends on raw states only (which is well known or follows from Theorem 2 with $\phi(h_t) = o_t$). Since our results hold for all P, they clearly hold if P is a raw MDP and if $\phi(h_t) := \phi(o_t)$ maps raw states to aggregated states.

The remainder of this paper shows how much we can aggregate and how to develop RL algorithms exploiting these insights.

6 Extreme Aggregation

The results of Section 5 showed that histories can be aggregated and modeled by an MDP even if the true aggregated process is not an MDP. The only restrictions were that the (Q-)Value functions and Policies could still be (approximately) represented as functions of the aggregated states. We will see in this section that in theory this allows to represent any process P as a small finite-state MDP.

Extreme aggregation based on Theorem 8. Consider ϕ that maps each history to the vector-over-actions of optimal Q-values $Q^*(h,\cdot)$ discretized to some finite ε -grid:

$$\phi(h) := \left(\lfloor Q^*(h, a)/\varepsilon \rfloor \right)_{a \in \mathcal{A}} \in \left\{ 0, 1, \dots, \lfloor \frac{1}{\varepsilon(1 - \gamma)} \rfloor \right\}^{\mathcal{A}} =: \mathcal{S}$$
 (29)

That is, all histories with ε -close Q^* -values are mapped to the same state:

$$|Q^*(h,a) - Q^*(\tilde{h},a)| \le \varepsilon \quad \forall \phi(h) = \phi(\tilde{h}) \ \forall a$$

Now choose some B and determine p from P via (15) and (5). Find the optimal policy π^* of MDP p of size |S|. Define $\tilde{\Pi}(h) := \pi^*(\phi(h))$. By Theorem 8ii, $\tilde{\Pi}$ is an ε' -optimal policy of the original process P in the sense that

$$|V^{\tilde{\Pi}}(h) - V^*(h)| \leq \frac{2\varepsilon}{(1-\gamma)^2} =: \varepsilon'$$

The following theorem summarizes the considerations for the above choice of ϕ :

Theorem 11 (Extreme ϕ) For every process P there exists a reduction ϕ (29) and MDP p defined via (15) and (5) whose optimal policy π^* is an ε' -optimal policy $\tilde{\Pi}(h) := \pi^*(\phi(h))$ for P. The size of the MDP is bounded (uniformly for any P) by

$$|\mathcal{S}| \le \left(\frac{3}{\varepsilon'(1-\gamma)^3}\right)^{|\mathcal{A}|}$$

Proof. For S defined in (29) we have

$$|\mathcal{S}| = \left(\left\lfloor \frac{1}{\varepsilon(1-\gamma)} \right\rfloor + 1 \right)^{|\mathcal{A}|} = \left(\left\lfloor \frac{2}{\varepsilon'(1-\gamma)^3} \right\rfloor + 1 \right)^{|\mathcal{A}|} \le \left(\frac{3}{\varepsilon'(1-\gamma)^3} \right)^{|\mathcal{A}|}$$

where in the last inequality we have assumed $\varepsilon' \leq \frac{1}{1-\gamma}$. (For $\varepsilon' > \frac{1}{1-\gamma}$ the theorem is trivial, since any policy is ε' -optimal). The theorem now follows from the considerations in the paragraphs before the theorem.

Extreme aggregation based on (28). If (28) would hold, we could aggregate even better: Consider ϕ that maps each history to the optimal Value $V^*(h)$ discretized to some finite ε -grid and to the optimal action $\Pi^*(h)$:

$$\phi(h) := \left(\lfloor V^*(h)/\varepsilon \rfloor, \Pi^*(h) \right) \in \left\{ 0, 1, ..., \lfloor \frac{1}{\varepsilon(1-\gamma)} \rfloor \right\} \times \mathcal{A} =: \mathcal{S}$$
 (30)

That is, all histories with ε -close V^* -Values and same optimal action are mapped to the same state:

$$|V^*(h) - V^*(\tilde{h})| \le \varepsilon$$
 and $\Pi^*(h) = \Pi^*(\tilde{h})$ $\forall \phi(h) = \phi(\tilde{h})$

As before, determine p, find its optimal policy π^* , and define $\tilde{\Pi}(h) := \pi^*(\phi(h))$. If (28) holds, then $\tilde{\Pi}$ is an ε' -optimal policy of original process P in the sense that

$$|V^{\tilde{\Pi}}(h) - V^*(h)| = O\Big(\frac{\varepsilon}{(1-\gamma)^?}\Big) =: \varepsilon'$$

hence the size of the required MDP in Theorem 11 would only be linear rather than exponential in \mathcal{A} :

$$|\mathcal{S}| = O\left(\frac{|\mathcal{A}|}{\varepsilon'(1-\gamma)^{1+?}}\right) \tag{31}$$

Discussion. A valid question is of course whether Theorem 11 is just an interesting theoretical insight/curiosity or of any practical use. After all, ϕ depends on Q^* (or V^* and Π^*), but if we knew Q^* , Π^* would readily be available and the detour through p and π^* pointless.

Theorem 11 reaches relevance by the following observation: If we start with a sufficiently rich class of maps Φ that contains at least one ϕ approximately representing $Q^*(h,\cdot)$, and have a learning algorithm that favors such ϕ , then Theorems 5–9 tell us that we do not need to worry about whether P_{ϕ} is MDP or not; we "simply" use/learn MDP p instead. Theorem 11 tells us that this allows for extreme aggregation far beyond MDPs.

This program is in parts worked out in the next two sections, but more research is needed for its completion. Learning p from (real) P-samples is considered in Section 7 and learning ϕ in Section 8.

7 Reinforcement Learning

In RL, P and therefore p are unknown. We now show how to learn p from samples from P. For this we have to link B to the distribution over histories induced by P and to the behavior policy Π_B the agent follows. We still assume ϕ is given.

Behavior policy Π_B . Let $\Pi_B: \mathcal{H} \sim \mathcal{A}$ be the behavior policy of our RL agent, which in general is non-stationary due to learning, often stochastic to ensure exploration, and (usually) different from any policy considered so far $(\Pi^*, \pi^*, \tilde{\Pi}, \pi^0, \Pi, \pi)$. Note that a sequence of policies $\Pi_1, \Pi_2, ...$ where each Π_t is learnt from h_t and used at time t (or for some number of steps) is nothing but a single non-stationary policy $\Pi_B(h_t) = \Pi_t(h_t) \forall t, h_t$, so Π_B indeed includes the case of policy learning.

Choice of B. The interaction of agent Π_B with environment P stochastically generates some history h_t followed by action a_t with joint probability, say $P_B(h_t a_t)$. We use subscripts B and/or ϕ to indicate dependence on Π_B and/or ϕ . A natural choice for B(h|sa) in (14) would be to condition on P_B on $s_t a_t$. We now show that this does not work and how to fix the problem. We can get $P_{\phi B}(h_t|s_t a_t)$ from P_B and P_B and several other useful distributions by standard probability manipulations (conditioning, marginalization, product and chain rule) as follows:

$$P_{B}(h_{t+1}|h_{t}) = P(o_{t+1}r_{t+1}|h_{t}a_{t})\Pi_{B}(a_{t}|h_{t}) \qquad [h_{t+1} = h_{t}a_{t}o_{t+1}r_{t+1}]$$

$$P_{B}(h_{n}) = \prod_{t=0}^{n-1} P_{B}(h_{t+1}|h_{t}), \qquad P_{B}(h_{t}a_{t}) = \Pi_{B}(a_{t}|h_{t})P_{B}(h_{t})$$

$$P_{\phi B}(s_{t}a_{t}) = \sum_{h_{t}:\phi(h_{t})=s_{t}} P_{B}(h_{t}a_{t}), \qquad P_{\phi B}(h_{t}|s_{t}a_{t}) = \frac{P_{B}(h_{t}a_{t})}{P_{\phi B}(s_{t}a_{t})} \llbracket \phi(h_{t}) = s_{t} \rrbracket$$

$$P_{\phi B}(s_{t+1}r_{t+1}|s_{t}a_{t}) = \sum_{h_{t}:\phi(h_{t})=s_{t}} P_{\phi}(s_{t+1}r_{t+1}|h_{t}a_{t})P_{\phi B}(h_{t}|s_{t}a_{t}) \quad [\text{see (5) for def. of } P_{\phi}] (32)$$

$$P_{\phi B}(s_{t}a_{t}s_{t+1}r_{t+1}) = P_{\phi B}(s_{t+1}r_{t+1}|s_{t}a_{t})P_{\phi B}(s_{t}a_{t})$$

 $P_{\phi B}(h_t|s_t a_t)$ has the following properties:

$$P_{\phi B}(h_t|s_t a_t) \ge 0$$
 and $\sum_{h_t \in \mathcal{H}_t} P_{\phi B}(h_t|s_t a_t) = \sum_{h_t : \phi(h_t) = s_t} P_{\phi B}(h_t|s_t a_t) = 1 \quad \forall t, s_t, a_t \quad (33)$

This is close to the required condition (14) for B but crucially different. The sum in (14) is over histories of all lengths while in (33) the sum is limited to histories of length t. It is easy to miss this difference due to the compact notation. Technically P_B is a probability measure on infinite sequences \mathcal{H}_{∞} and $P_B(h_t)$ is short for $P_B(\Gamma_{h_t})$ where Γ_{h_t} is the set of infinite histories starting with h_t , i.e. $P_B(h_t)$ is the probability that the infinite history starts with h_t ($\sum_{h_t \in \mathcal{H}_t} P_B(h_t) = 1 \forall t$). On the other hand, B(h) is a probability distribution over finite histories of mixed length ($\sum_{h \in \mathcal{H}} B(h) = 1$); similarly for P_B and B conditioned on / parameterized by s and a.

We can fix this mismatch by introducing weights $w_t: \mathcal{S} \times \mathcal{A} \longrightarrow [0;1]$ and define

$$B(h_t|sa) := w_t(sa)P_{\phi B}(h_t|s_t = s, a_t = a) \ \forall t, \text{ where } \sum_{t=1}^{\infty} w_t(sa) = 1 \ \forall s, a \ (34)$$

which now satisfies (14) (due to $\sum_{h\in\mathcal{H}} = \sum_{t=1}^{\infty} \sum_{h_t\in\mathcal{H}_t}$). MDP p can now be represented as

$$p(s'r'|sa) = \sum_{t=1}^{\infty} w_t(sa) \sum_{h_t \in \mathcal{H}_t} P_{\phi}(s_{t+1} = s', r_{t+1} = r'|h_t, a_t = a) P_{\phi B}(h_t|s_t = s, a_t = a)$$

$$= \sum_{t=1}^{\infty} w_t(sa) P_{\phi B}^t(s'r'|sa)$$
(35)

That is, p is the w-weighted time-average of $P_{\phi B}^t$. The first equality follows from (15) and (34); the second one from (32). We also introduced the shorthand $P_{\phi B}^t(s'r'|sa) := P_{\phi B}(s_{t+1} = s', r_{t+1} = r'|s_t = s, a_t = a)$.

Choice of w_t . If $P_{\phi B}^t$ in (35) is stationary, i.e. independent of t, then $p(s'r'|sa) = P_{\phi B}^t(s'r'|sa)$ for all t, since the weights sum to one, and estimation is easy. Note that in general we cannot estimate non-stationary $P_{\phi B}^t$, since for each t we have only one sample available, but we will see that estimation of p is still possible. Assume we have observed h_n for some (fixed) n, and choose $w_t(sa)$ to average over all time steps t in which state s is obtained and action a is taken:

$$w_t(sa) := \begin{cases} \frac{1}{n(sa)} & \text{if } t \in T_n(sa), \\ 0 & \text{else.} \end{cases}$$
 $T_n(sa) := \{t \le n : s_t = s, a_t = a\}$ $n(sa) := \#T_n(sa)$ (36)

Inserting this into (35) gives

$$p(s'r'|sa) = \frac{1}{n(sa)} \sum_{t \in T_n(sa)} P_{\phi B}^t(s'r'|sa)$$
 (37)

We can estimate the right-hand-side as follows:

Law of large numbers. For $\tau = 1, 2, 3, ...$ let $X_{\tau} \in \{0, 1\}$ be binary random variables with expectation $\mathbb{E}[X_{\tau}]$. Define $N_1 = \sum_{\tau=1}^{N} X_{\tau}$ be the number of sampled 1s. The strong law of large numbers says that

$$\frac{N_1}{N} - \frac{1}{N} \sum_{\tau=1}^{N} \mathbb{E}[X_{\tau}] \xrightarrow{N \to \infty} 0 \quad \text{almost surely} \quad \text{under weak conditions}$$
 (38)

Note that the law holds far beyond i.i.d. random variables under a variety of conditions [Faz06, VGS05] which we collectively call 'weak conditions'. It is not even necessary for N_1/N to converge.

Estimation of p. Now fix some (s,a), and let $X_{\tau} := [s_{t+1} = s', r_{t+1} = r'] \equiv [s_t a_t s_{t+1} r_{t+1} = s a s' r']$, where $t = t_{\tau}^{sa}$ is the τ -th occurrence of sa in the history. Formally, $\tau = \#T_t(sa)$ and $s_t = s$ and $a_t = a$. (Here we assume that variables in h_t , hence also t_{τ}^{sa} , are random variables, while sas'r' are realizations.) Let N := n(sa) and

$$n(sas'r') := N_1 = \sum_{\tau=1}^{N} X_{\tau} = \#\{t \le n : s_t a_t s_{t+1} r_{t+1} = sas'r'\}$$

and $\mathbb{E}[X_{\tau}] = P(X_{\tau} = 1) = P_{\phi B}^{t}(s'r') = P_{\phi B}^{t}(s'r'|sa)$, with $t = t_{\tau}^{sa}$. The last equality holds, since $s_{t_{\tau}^{sa}} = s$ and $a_{t_{\tau}^{sa}} = a$. Using $\sum_{\tau=1}^{N} P_{\phi B}^{t_{\tau}^{sa}} = \sum_{t \in T_{n}(sa)} P_{\phi B}^{t}$, (38) implies

$$\frac{n(sas'r')}{n(sa)} - \frac{1}{n(sa)} \sum_{t \in T_n(sa)} P_{\phi B}^t(s'r'|sa) \xrightarrow{n(sa) \to \infty} 0 \quad \text{a.s. under weak conditions}$$
(39)

Theorem 12 (p-estimation) For B defined in (34) and (36), convergence (39) implies

$$\frac{n(sas'r')}{n(sa)} - p(s'r'|sa) \xrightarrow{n \to \infty} 0 \quad almost \ surely$$
 (40)

For example, if X_{τ} (for each sa) are stationary ergodic processes, then (39) hence (40) hold for all state-action pairs that matter (i.e. for those occurring infinitely often).

Proof. (39) trivially implies (40) by (37). For stationary ergodic X_{τ} , provided $N \to \infty$, (38) hence (39) hold by

$$\frac{N_1}{N} \equiv \frac{1}{N} \sum_{\tau=1}^{N} X_{\tau} \xrightarrow{\text{ergodicity}} \mathbb{E}[X_1] \stackrel{\text{stationarity}}{=} \frac{1}{N} \sum_{\tau=1}^{N} \mathbb{E}[X_{\tau}]$$

Discussion. Limit (40) shows that standard frequency estimation for p will converge to the true p under weak conditions. If P_{ϕ} is MDP, samples are conditionally i.i.d. and the 'weak conditions' are satisfied. But the law of large numbers and hence (40) holds far beyond the i.i.d. case [FK01, VGS05], e.g. for stationary ergodic processes. For instance, if the original process P is a stationary ergodic MDP, and ϕ aggregates raw states, the resulting process P_{ϕ} is (only) a Partially Observable MDP (POMDP). Still, for stationary Π_B , the POMDP is stationary and ergodic, hence p can be estimated by (40). Stationarity is actually not necessary, and indeed often does not hold due to a non-stationary environment P or a non-stationary behavior policy Π_B (or both).

A subtlety which we have glossed over is that implicitly $T_n(sa)$ also depends on h_n . Mathematically this means that T_n , w_t , and p are random variables, which requires some extra care in the derivation. Practically this means that p can depend on the realized history (data) h_n , which is no problem, since (40) is all that matters. Note that the estimation itself depends on the history, and p converges provided n(sas'r')/n(sa) converges. For time-independent $P_{\phi B}^t(s'r'|sa)$, p is independent of h_n .

Other choices for w_t are possible, e.g. $w_t(sa) := P_{\phi B}^t(sa) / \sum_{t=1}^n P_{\phi B}^t(sa)$ for $t \le n$ and 0 for t > n is independent of h_n and leads to very similar results under somewhat stronger conditions [Hut14]. We could also use any w for which $w_t(sa) = 0$ if $t \notin T_n(sa)$ and $\sum_{t=1}^n w_t(sa) = 1$. This leads to a w-weighted average estimator. For instance, functions $w_{t_\tau^{sa}}(sa)$ increasing with τ would weigh more recent observations higher in the estimation of p, which can be beneficial in non-stationary problems.

We estimate p in order to estimate q^* and ultimately π^* . This is model-based RL. We can also learn π^* model-free. For instance, condition (40) should be sufficient for Q-learning to converge to Q^* . Q-learning and other RL algorithms designed for MDPs have been observed to often (but not always) perform well even if applied to non-MDP domains. Our results appear to explain why, but this calls for further investigations.

8 Feature Reinforcement Learning

The idea of FRL is to $learn \ \phi$ [Hut09c]. FRL starts with a class of maps Φ , compares different $\phi \in \Phi$, and selects the most appropriate one given the experience h_t so far. Several criteria based on how well ϕ reduces P to an MDP have been devised [Hut09b, Hut09a] and theoretically [SH10] and experimentally [NSH11] investigated [Ngu13]. Theorems 5–9 show that demanding P_{ϕ} to be approximately MDP is overly restrictive. Theorem 11 suggests that if we relax this condition, much more substantial aggregation is possible, provided Φ is rich enough.

(F)RL deals with the case of unknown P. We first discuss learning ϕ for the unrealistic case of exact aggregation ($\varepsilon = 0$) and infinite sample size ($n = \infty$). This serves as a useful guide to work out its generalization to the realistic but significantly more complex case of approximate aggregation based on finite sample size. Finally we discuss a family of recent algorithms (BLB and extensions [Ngu13]) that appear to nearly have the right properties for our purpose. This section is more a collection of ideas and outlook towards algorithms exploiting and motivating the usefulness of the new insights obtained in the previous sections.

Search for exact ϕ based on infinite sample size.¹ Since we are now concerned with comparing different $\phi \in \Phi$, we subscribe quantities with ϕ when necessary. Consider the unrealistic case of infinite sample size $(n = \infty)$ and a search for exact reductions ϕ . We call a reduction $\phi : \mathcal{H} \to \mathcal{S}_{\phi}$ exact iff $Q^*(h,a) = q_{\phi}^*(s,a)$ for all $s = \phi(h)$ and a (cf. Theorem 8). The condition could be weakened to $V^*(h) = v_{\phi}^*(s)$ and $\Pi^*(h) = \pi_{\phi}^*(s)$ (cf. Theorem 9).

¹The definitions of the order relations \leq and \leq_{\times} in the published version [Hut16] were incomplete and have been updated. This is the only post-publication change.

Even for $n=\infty$, P hence Q^* needed for Π^* is (usually) not estimable (from h_∞). On the other hand, for each $\phi \in \Phi$, $p=p_\phi$ can be determined (exactly) by (40) (under weak conditions). From p_ϕ we can determine q_ϕ^* and π_ϕ^* via (8) and (9). The solution always satisfies the reduced Bellman equations exactly, even for very bad reductions, e.g. single state $\phi(h) \equiv 0 \,\forall h$. So the reduced problem is not sufficient to judge the quality of ϕ . An alternative to assuming $n=\infty$ is to assume that P is known, which also allows to determine p_ϕ , etc. So what follows applies to stochastic planning as well.

Coarsening and refining reductions ϕ : Let us now coarsen ϕ , i.e. further merge some partitions $\phi^{-1}(s)$. In the simplest case we just merge two states into one. In general, consider coarsening $\chi: \mathcal{S}_{\phi} \to \mathcal{S}_{\psi}$ and coarser reduction $\psi: \mathcal{H} \to \mathcal{S}_{\psi}$ such that $\psi(h) = \chi(\phi(h))$. We also call \mathcal{S}_{ϕ} a refinement of \mathcal{S}_{ψ} . For example, U-trees [McC96, UV98] and Kd-trees have been used in RL [EGW05], where expanding a leaf corresponds to splitting a state. Or in ϕ DBN, $\mathcal{S}_{\phi} = \{0,1\}^d$ is a binary feature vector, where removing one component corresponds to pairwise combining 2^d states to 2^{d-1} states [Hut09a].

Ordering reductions in Φ : We can partially order Φ as follows:

$$\psi \preceq \phi : \Leftarrow q_{\phi}^*$$
 is constant on all $s_{\phi} \in \chi^{-1}(s_{\psi})$ for all s_{ψ} and $a \Leftrightarrow q_{\phi}^*(s_{\phi}, a) = q_{\psi}^*(s_{\psi}, a)$ for all $s_{\psi} = \chi(s_{\phi})$ and a .

 $\psi \leq \phi$ means ψ is a better reduction than ϕ , since it leads to the same optimal q-value and therefore policy as ψ does, but is more parsimonious (coarser) than ϕ . If q_{ϕ}^* is not constant on ψ -partitions, coarsening ϕ to ψ and using ψ (potentially) leads worse to solutions. We capture this by

$$\phi \preceq \psi$$
 : \Leftarrow q_{ϕ}^* is *not* constant on all $s_{\phi} \in \chi^{-1}(s_{\psi})$ for all s_{ψ} and a \Leftrightarrow $q_{\phi}^*(s_{\phi}, a) \neq q_{\psi}^*(s_{\psi}, a)$ for some $s_{\psi} = \chi(s_{\phi})$ and a .

Note that \leq is a partial order, so this reverse definition is not redundant. As common, we also define $\psi \succeq \phi$ iff $\phi \preceq \psi$ iff ψ is worse than ϕ . ψ and ϕ are isomorphic iff $\psi \simeq \phi$ iff $\psi \preceq \phi$ and $\phi \preceq \psi$ iff χ is a bijection iff $q_{\phi}^* \equiv q_{\psi}^*$.

Enriching the order \preceq : \preceq is a transitive but 'very' partial order. Two maps are incomparable if neither is a refinement or coarsening of the other. We can enrich order \preceq as follows: For any two maps $\psi \not\simeq \psi'$, the map $\phi(h) := (\psi(h), \psi'(h)) \in \mathcal{S}_{\phi} \subseteq \mathcal{S}_{\psi} \times \mathcal{S}_{\psi'}$ refines both. We could define $\psi \preceq_{\times} \psi'$ iff $\psi \preceq \phi \preceq \psi'$, which is still equivalent to \preceq , but enables a natural extension: Case $\psi \preceq \phi \succeq \psi'$: This is only possible if q^* of ψ and ψ' (and ϕ) coincide in the sense that there exists a (finest common coarsening) ρ with $\rho \preceq \psi$ and $\rho \preceq \psi'$. A secondary criterion based on the relative complexity of ψ and ψ' could decide the case, e.g. $\psi \preceq_{\times} \psi'$ iff $|\mathcal{S}_{\psi}| \leq |\mathcal{S}_{\psi'}|$. Case $\psi \succeq \phi \preceq \psi'$: This is only possible if ϕ is neither ψ -uniform nor ψ' -uniform, hence strictly better than both $(\phi \preceq \psi \text{ and } \phi \preceq \psi')$, so assuming $\phi \in \Phi$, we can order ψ and ψ' at will, e.g. again

w.r.t. size. It is therefore natural to define an extended order as

$$\psi \preceq_{\times} \psi' : \Leftrightarrow [\psi \preceq \phi \preceq \psi'] \quad \text{or} \quad [\psi \preceq \phi \succeq \psi' \text{ and } |\mathcal{S}_{\psi}| \leq |\mathcal{S}_{\psi'}|]$$

or $[\phi \in \Phi \text{ and } \psi \succ \phi \prec \psi' \text{ and } |\mathcal{S}_{\psi}| < |\mathcal{S}_{\psi'}|]$

If Φ is closed under Cartesian product refinement (i.e. the above ϕ is always in Φ), then \leq_{\times} is a total order, otherwise it may (still) only be a partial order.

Search for ϕ : Assume Φ contains at least one exact reduction ϕ_0 . Then the \preceq -minimal elements in Φ smaller than ϕ_0 are exactly the maximally coarse exact $\phi \in \Phi$. If Φ is closed under arbitrary coarsening, then there is a unique minimizer (modulo isomorphism). The same holds for \preceq_{\times} . This implies that any exhaustive search for a \preceq_{\times} -minimum in Φ will give an exact ϕ with minimal number of states, say ϕ_{min} . Now Theorem 8 tells us that $q_{\phi_{min}}^*$ (and hence $\pi_{\phi_{min}}^*$) are the optimal value and policy also of the original process P, irrespective of whether $P_{\phi_{min}}$ is Markov or not. So while the conditions of Theorem 8 cannot be verified in practice, the theorem justifies a search procedure based on q_{ϕ}^* that ignores the (non-)Markov structure of P_{ϕ} .

Search for approximate ϕ based on finite sample size. The principle approach in the previous paragraph is sound, but needs to be generalized in various ways before it can be used: Real sample size is finite, which means we only have access to approximations \hat{q}_{ϕ}^* and $\hat{\pi}_{\phi}^*$ via estimation \hat{p}_{ϕ} of p_{ϕ} . The criterion for exact equality $q_{\phi}^* = q_{\psi}^*$ in \leq needs to be replaced by a suitable $\hat{q}_{\phi}^* \approx \hat{q}_{\psi}^*$, which should be done anyway, since real-word problems seldom allow for exact reductions. \approx should be chosen so as to come with statistical guarantees; e.g. Kolmogorov-Smirnov tests have been used in [McC96]. A suitable $\hat{\pi}_{\phi}^* \approx \hat{\pi}_{\psi}^*$ requires more effort (see outlook). For large Φ this also requires appropriate regularization, i.e. penalizing complex ϕ [Hut09c]. To ensure $\hat{q}^* \to q^*$ for $n \to \infty$, we need proper exploration strategies [SLL09]. Finally, we want an efficient search procedure in Φ , rather than exhaustive search. This will be heuristic or will require strong assumptions on Φ [Ngu13]. All but the last point raised above have or should have general solutions (see next paragraph).

Utilizing existing algorithms. The BLB algorithm [MMR11] and its extensions IBLB [NMRO13] and improvements OMS [NOR13] solve most of the problems above and can (nearly) readily be used for our purpose.

The BLB family uses the same basic FRL setup from [Hut09c] used also here. The authors consider a countable class Φ assumed to contain at least one ϕ such that P_{ϕ} is an MDP (6). They consider average reward, rather than discounting, and analyze regret, which (in general) requires some assumption on the mixing rate or 'diameter' of the MDP. They prove that the total regret grows with $\tilde{O}(n^{1/2...2/3})$, depending on the algorithm.

Their algorithms and analyses rely on UCRL2 [JOA10], an exploration algorithm for finite-state MDPs. Going through the BLB proofs, it appears that the condition that P_{ϕ} is an MDP can be removed if p (15) is used instead, modulo the analysis of UCRL2 itself. The proofs for the bounds for UCRL2 exploit that s', r' conditioned on

s,a are i.i.d., which is true if P_{ϕ} is Markov but not in general. Asymptotic versions should remain valid under the 'weak conditions' alluded to in (40). With some stronger assumptions that guarantee good convergence rates, the regret analysis of UCRL2 should remain valid too. Formally, the use of Hoeffding's inequality for i.i.d. need to be replaced by comparable bounds with weaker conditions, e.g. Azuma's inequality for martingales.

There is one serious gap in the argument above. BLB uses average reward while our theorems are for discounted reward. It is often possible to adapt algorithms and proofs which come with regret bounds for average reward to PAC bounds for discounted reward or vice versa. This would have to be done first: either a PAC version of BLB by combining MERL [LHS13] with UCRL γ [LH14b], or average reward versions of the bounds derived in this paper.

9 Action Permutation Instead of Policy Condition

We can rename actions without changing the underlying problem: Let $A: \mathcal{A} \to \tilde{\mathcal{A}}$ be a bijection, and define $\tilde{P}(o'r'|h\tilde{a}) := P(o'r'|ha)$, where $\tilde{a} := A(a)$. Clearly, all results for P also hold for \tilde{P} if a is replaced by \tilde{a} everywhere, in particular $\tilde{\Pi}(h) := A(\Pi(h))$. In general, this is of little use. Things become more interesting if we allow the bijection A to be history-dependent, which we can do since our results hold for any, even non-stationarity, \tilde{P} . This allows us to devise an $A: \mathcal{A} \times \mathcal{H} \to \tilde{\mathcal{A}}$ such that $A(\Pi(h);h) = constant$ for the policy Π of interest. For example, for $\tilde{\mathcal{A}} := \mathcal{A}$, this is achieved by a permutation that swaps action $a = \Pi(h)$ with some arbitrary but fixed action $a^1 \in \mathcal{A}$, and leaves all other actions unchanged:

$$A(a;h) := \begin{cases} a^1 & \text{if} & \Pi(h) = a \\ \Pi(h) & \text{if} & \Pi(h) \neq a = a^1 \\ a & \text{else} \end{cases}$$

Since $\tilde{\Pi}(h) \equiv A(\Pi(h);h) \equiv a^1$ is constant, the ϕ -uniformity condition for $\tilde{\Pi}$ in Theorems 5, 6 and 9 becomes vacuous. While this transformation is of theoretical interest, it only becomes practically useful if we can somehow learn the function A without knowledge of Π , and in particular of Π^* . We could also allow non-bijective A that merge actions that have (approximately) the same (optimal) Q-value.

10 Discussion

Summary. Our results show that RL algorithms for finite-state MDPs can be utilized even for problems P that have arbitrary history dependence and history-to-state reductions/aggregations ϕ that induce P_{ϕ} that are also neither stationary nor MDP. The only condition to be placed on the reduction is that the quantities

of interest, (Q-)Values and (optimal) Policies, can approximately be represented. This considerably generalizes previous work on feature reinforcement learning and MDP state aggregation and allows for extreme state aggregations beyond MDPs. The obtained tight results may also explain why RL algorithms designed for MDPs sometimes perform well beyond MDPs.

Outlook. As usual, lots remain to be done. A list of the more interesting remaining tasks and open questions follows:

- While the approximate ϕ -uniformity condition on Q^* in Theorem 8 is very weak compared to bisimilarity, uniformity of V^* in Theorem 9 is even weaker (Hypothetical Bound (31) compared to Theorem 11 shows how much of a difference this can make). The discussion before Theorem 10 indicates that weaker forms of (31) in expectation or with high probability or so may hold.
- An algorithm learning ϕ beyond MDPs that comes with regret or PAC guarantees has yet to be developed. This could be done by generalizing the partial order \leq_{\times} to $n < \infty$, or by adapting the class and proofs of BLB algorithms, or by integrating MERL with UCRL γ .
- The trick to use an a-dependent Q^* as a-independent map ϕ in Section 6 was to vectorize Q^* in a. Unfortunately this leads to a state-space size exponential in \mathcal{A} . Are there better ways of dealing with actions? Are there other extreme aggregations ϕ , or are a-dependent ϕ possible?
- Are average-reward total-regret versions of our discounted reward results possible, under suitable mixing rate conditions?
- For small discrete action spaces typical for many board games, the exact conditions on Π are met. For continuous action spaces as in robotics, we can simply discretize the action space, introducing another ε -error, but action-continuous versions of our results would be nicer. Any interesting generalization should replace the exact by approximate ϕ -uniformity conditions on Π .
- Our theorems and/or proof ideas should allow to extend existing convergence theorems for RL algorithms such as Q-learning and others from MDPs to beyond MDPs.
- The bisimulation conditions of classical state aggregation results are for reward and transition probabilities. It would be interesting to derive explicit weaker conditions for them that still imply our conditions on (Q-)Values.

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A List of Notation

General notation

```
[R] = 1 if R=true and =0 if R=false (Iverson bracket)
```

 $\#\mathcal{X}$ size of set \mathcal{X}

 ε,δ small non-negative real numbers

 ϵ empty string

|z| largest integer $\leq z$

Original history-based process

 $\mathcal{O}, \mathcal{R}, \mathcal{A}$ = finite observation, reward, action spaces.

 $o_t r_t a_t \in \mathcal{O} \times \mathcal{R} \times \mathcal{A} = \text{observation, reward, action at time } t$

 $t \le n \in \mathbb{N}$ = any time \le sample size

 P,Q,V,Π = Probability, (Q-)Value, Policy of original history-based Process

 $\Pi^*, \tilde{\Pi}, \Pi_B$ = optimal, approximately optimal, behavior Policy

 $h \in \mathcal{H}$ = $(\mathcal{O} \times \mathcal{R} \times \mathcal{A})^* \times \mathcal{O} \times \mathcal{R}$ = possible histories of any length

 $h' = hao'r' = \text{successor history of } h \in \mathcal{H}$

 $h_t = o_1 r_1 a_1 \dots o_t r_t = \text{history up to time } t$

 \mathcal{H}_t = $(\mathcal{O} \times \mathcal{R} \times \mathcal{A})^{t-1} \times \mathcal{O} \times \mathcal{R}$ = history of length t

P(o'r'|ha) = probability of next observation&reward given history&action

Reduction/aggregation from history to states

 S_{ϕ} = finite state space induced by ϕ (range of ϕ)

 $\phi: \mathcal{H} \to \mathcal{S}_{\phi} = \text{reduction/map/aggregation from histories to states}$

 $s_t = \phi(h_t) \in \mathcal{S} = \text{state at time } t$

 $P_{\phi}(s'r'|ha) = \text{marginalized } P\text{-probability over state\&reward given history\&action}$

B(h|sa) = dispersion probability. Stochastic "inverse" of ϕ

 $\langle Q(h,a)\rangle_B = B$ -average over $\{\tilde{h}: \phi(\tilde{h}) = \phi(h)\}$

 $w_t(sa)$ = non-negative weight function $\sum_{t=1}^{\infty} w_t(sa) = 1 \ \forall sa$

 $P_B(h)$ = probability of h from P interacting with Π_B

 $P_{\phi B}()$ = (partially) ϕ -reduced, marginalized, conditionalized P_B

 $\preceq, \preceq_{\times}$ = (extended) ordering of ϕ w.r.t. quality $(n = \infty \text{ so far only})$

Finite state Markov decision process (MDP)

S = finite state space

 p,q,v,π = probability, (q-)value, policy of MDP

s,a,s',r' = stat, action, successor state, reward

n(sas'r') = number of times sas'r' appears in h_{n+1}

 $\gamma \in [0;1)$ = discount factor