Understanding the Curse of Horizon in Off-Policy Evaluation via Conditional Importance Sampling

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Abstract

We establish a connection between the importance sampling estimators typically used for off-policy policy evaluation in reinforcement learning and the extended conditional Monte Carlo method. We show with some examples that in the finite horizon case there is no strict ordering in general between the variance of such conditional importance sampling estimators: the variance of the per-decision or stationary variants may, in fact, be higher than that of the crude importance sampling estimator. We also provide sufficient conditions for the finite horizon case under which the per-decision or stationary estimators can reduce the variance. We then develop an asymptotic analysis and derive sufficient conditions under which there exists an exponential vs. polynomial gap (in terms of horizon $T$) between the variance of importance sampling and that of the per-decision or stationary estimators.

1 Introduction

Off-policy [Sutton and Barto 2018] policy evaluation is the problem of estimating the expected return of a given target policy from the distribution of samples induced by a different policy. Due in part to the growing sources of data about past sequences of decisions and their outcomes – from marketing to energy management to healthcare – there is increasing interest in developing accurate and efficient algorithms for off-policy policy evaluation.

For Markov Decision Processes, this problem was addressed (Precup et al., 2000) early on by importance sampling (IS) (Rubinstein, 1981), a method prone to large variance due to rare events (Glynn, 1994; L’Ecuyer et al., 2009). The per-decision importance sampling estimator of (Precup et al. 2000) tries to mitigate this problem by leveraging the temporal structure – earlier rewards cannot depend on later decisions – of the domain.

While neither importance sampling (IS) nor per-decision IS (PDIS) assumes the underlying domain is Markov, more recently, a new class of estimators (Hallak and Mannor 2017; Liu et al. 2018; Gelada and Bellemare 2019) has been proposed that leverages the Markovian structure. In particular, these approaches propose performing importance sampling over the stationary state-action distributions induced by the corresponding Markov chain for a particular policy. By avoiding the explicit accumulation of likelihood ratios along the trajectories, it is hypothesized that such ratios of stationary distributions could substantially reduce the variance of the resulting estimator, thereby overcoming the “curse of horizon” (Liu et al. 2018) plaguing off-policy evaluation. The recent flurry of empirical results shows significant performance improvements over the alternative methods on a variety of simulation domains. Yet so far there has not been a formal analysis of the accuracy of IS, PDIS, and stationary state-action IS which will strengthen our understanding of their properties, benefits and limitations.

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Because all three estimators are unbiased, their mean squared error accuracy is simply their variance. Therefore, the intuition from prior work suggests that stationary importance sampling should have the best accuracy, followed by per-decision IS and then (worst) the crude IS estimator. Surprisingly, we show that this is not always the case. In particular, we construct short-horizon MDP examples in Figure 1 that demonstrate that the crude IS can have a lower variance estimate than per-decision IS or stationary IS, and also show results for the other combinations.

We then describe how this observation is quite natural when we note that all three estimators are instances of a more general class of estimators: the extended (Bratley et al. [1987]) form of the conditional Monte Carlo estimators (Hammersley [1956], Dubi and Horowitz [1979], Granovsky [1981]). If \( X \) and \( Y \) are two well-defined random variables on the same probability space such that \( \theta = \mathbb{E}[Y] = \mathbb{E}[Y|X] \), then the conditional Monte Carlo estimator for \( \theta \) is \( \mathbb{E}[Y|x] \). By the law of total variance, the variance of the conditional Monte Carlo estimator cannot be larger than that of the crude Monte Carlo estimator \( y \). However when \( X \) and \( Y \) are sequences of random variables, and we want to estimate \( \mathbb{E} \left[ \sum_{t=1}^{T} Y_t \right] \), the variance of the so-called extended conditional Monte Carlo estimator \( \sum_{t=1}^{T} \mathbb{E}[Y_t|x_t] \) is not guaranteed to reduce variance due to covariance between the summands. In this paper, we show that per-decision and stationary importance sampling can be obtained by applying the extended conditional Monte Carlo method to crude importance sampling. We refer to the estimators resulting from this combination as “conditional importance sampling” estimators.

Building on these insights, we then provide a general variance analysis for conditional importance sampling estimators, as well as sufficient conditions for variance reduction in Section 5. In Section 4 we provide upper and lower bounds for the asymptotic variance of the crude, per-decision and stationary estimators. These bounds show, under certain conditions, that the per-decision and stationary importance sampling estimators can reduce the asymptotic variance to a polynomial function of the horizon compared to the exponential dependence of the per-decision estimator. Our proofs apply to general state spaces and use concentration inequalities for martingales. Importantly, these bounds characterize a set of common conditions under which the variance of stationary importance sampling can be smaller than that of per decision importance sampling, which in turn, can have a smaller variance than the crude importance sampling estimator. In doing so, our results provide concrete theoretical foundations supporting recent empirical successes in long-horizon domains.

## 2 Notation and Problem Setting

We consider Markov Decision Processes (MDPs) with discounted or undiscounted rewards and under a fixed horizon \( T \). An MDP is defined by a tuple \((S, A, P, p_1, r, \gamma, T)\), where \( S \subseteq \mathbb{R}^d \) is the state space and \( A \) is the action space, which we assume are both bounded compact Hausdorff spaces. We use the notation \( P(S|s,a) \) to denote the transition probability kernel where \( S \subseteq S, s \in S, a \in A \) and \( r_t(s,a) : S \times A \times [T] \rightarrow [0,1] \) for the reward function. The symbol \( \gamma \in [0,1] \) refers to the discount factor. For simplicity we write the probability density function associated with \( P \) as \( p(s'|s,a) \). Furthermore, our definition contains a probability density function of the initial state \( s_1 \) which we denote by \( p_1 \). We use \( \pi(a_t|s_t) \) and \( \mu(a_t|s_t) \) to denote the conditional probability density/mass functions associated with the policies \( \pi \) and \( \mu \). We call \( \mu \) the behavior policy and \( \pi \) the target policy. We are interested in estimating the value of \( \pi \), defined as:

\[
v^\pi = \mathbb{E}_\pi \left[ \sum_{t=1}^{T} \gamma^{t-1} r_t \right].
\]

Furthermore, we use the notation \( \tau_{1:T} \) to denote a \( T \)-step trajectory of the form: \( \tau_{1:T} = \{(s_t, a_t, r_t)\}_{t=1}^{T} \).

When appropriate, we use the subscript \( \pi \) or \( \mu \) to specify if \( \tau_{1:T} \) comes from the induced distribution of \( \pi \) or \( \mu \). We use the convention that the lack of subscript for \( \mathbb{E} \) is equivalent to writing \( \mathbb{E}_\mu \), but otherwise write

\[1\]Our analysis works for both discounted and undiscounted reward.
\( \mathbb{E}_\pi \) explicitly. We denote the 1-step likelihood ratio and the \( T \)-steps likelihood ratio respectively as:

\[
\rho_t = \frac{\pi(a_t|s_t)}{\mu(a_t|s_t)}, \quad \rho_{1:T} = \prod_{t=1}^T \rho_t .
\]

We define the \( T \)-step state distribution and stationary state distribution under the behavior policy as:

\[
d_t^\mu(s, a) = \Pr(s_t = s, a_t = a| s_1 \sim p_1, a_1 \sim \mu(a_t|s_t))
\]

\[
d_{\gamma,1:T}^\mu(s, a) = \sum_{t=1}^T \gamma^t d_t^\mu(s, a), \quad d_T^\mu = \lim_{T \to \infty} d_{\gamma,1:T}^\mu
\]

For simplicity of notation, we drop the \( \gamma \) in \( d_{\gamma,1:T}^\mu \) and \( d_T^\mu \) when \( \gamma = 1 \), and overload \( d^\mu \) to denote the marginal state distribution as well: i.e. \( d^\mu(s) = \int_a d^\mu(s, a)da \) (and similarly for \( d^\pi \)). We use \( c \) to denote the KL divergence of \( \mu \) and \( \pi \) and where the expectation is taken under \( d^\mu \) over the states: \( \mathbb{E}_{d^\mu} [D_{KL}(\mu||\pi)] \). We assume \( c > 0 \), otherwise \( \pi \) and \( \mu \) are identical and our problem reduces to on-policy policy evaluation.

In this paper, we define the estimator and discuss the variance over a single trajectory but of all our results carry to \( N \) trajectories by multiplying by a factor \( 1/N \). We define the \textit{crude} importance sampling (IS) estimator and the per-decision importance sampling (PDIS) from [Precup et al. (2000)] as:

\[
\hat{v}_{IS} = \rho_{1:T} \sum_{t=1}^T \gamma^{t-1} r_t, \quad \hat{v}_{PDIS} = \sum_{t=1}^T \gamma^{t-1} r_t \rho_{1:t}.
\]

The stationary importance sampling (SIS) estimator is defined as:

\[
\hat{v}_{SIS} = \sum_{t=1}^T \gamma^{t-1} r_t \frac{d_t^\mu(s_t, a_t)}{d_t^\pi(s_t, a_t)}.
\]

All three estimators are unbiased. Our definition of SIS is based on the importance ratio of the time-dependent state distributions (provided by an oracle) rather than the stationary distributions as in the prior work by [Liu et al. (2018); Hallak and Mannor (2017), but similar with Xie et al. (2019)]. This choice allows us to tackle both the finite horizon and infinite horizon more easily under the same general framework by taking \( T \to \infty \) when necessary. This is possible because the ratio \( \frac{d_t^\mu(s_t, a_t)}{d_t^\pi(s_t, a_t)} \) has the same asymptotic behavior as that of the stationary distribution ratio. Surprisingly, we show that even under perfect knowledge of the stationary ratio, it is generally non-trivial to guarantee a variance reduction for \( \hat{v}_{SIS} \).

The next standard assumptions helps us analyze our estimators in the asymptotic regime by relying on a central limit property for general Markov chains.

**Assumption 1** (Harris ergodic). The Markov chain of \( \{s_t, a_t\} \) under \( \mu \) is Harris ergodic. That is: the chain is aperiodic, \( \psi \)-irreducible, and positive Harris recurrent. See [Meyn and Tweedie (2012)] for more

**Assumption 2** (Drift property). There exist an everywhere-finite function \( B : \mathcal{S} \times \mathcal{A} \to [1, \infty) \), a constant \( \lambda \in (0, 1) \), \( b < \infty \) and a petite \( K \subset \mathcal{S} \times \mathcal{A} \) such that:

\[
\mathbb{E}_{s', a'|s, a} B(s', a') \leq \lambda B(s, a) + b 1((s, a) \in K).
\]

These are standard assumptions to describe the ergodic and recurrent properties of general Markov chains. Assumption 1 is typically used to obtain the existence of a unique stationary distribution [Meyn and Tweedie (2012)] and assumption 2 is used to measure the concentration property [Meyn and Tweedie (2012); Jones et al. (2004)].
Figure 1: Counterexamples. The labels for each edge are of the form (target policy probability, reward) where the first component is the transition probability induced by the given target policy, and the second component is the reward function for this transition. All examples assume deterministic transitions and the same initial state $s_1$. The square symbol represents a terminating state.

3 Counterexamples

It is tempting to presume that the root cause of the variance issues in importance sampling pertains entirely to the explicit multiplicative (Liu et al., 2018) accumulation of importance weights over long trajectories. The reasoning ensuing from this intuition is that the more terms one can drop off this product, the better the resulting estimator would be in terms of variance. In this section, we show that this intuition is misleading as we can construct small MDPs in which per-decision or stationary importance sampling does not necessarily reduce the variance of the crude importance sampling. We then explain this phenomenon in section 4 using the extended conditional Monte Carlo method and point out that the lack of variance reduction is attributable to the interaction of some covariance terms across time steps. However, all is not lost and section 6 shows that asymptotically ($T \to \infty$) stationary importance sampling achieves much lower variance than crude importance sampling or the per-decision variant.

In all examples, we use a two-steps MDP with deterministic transitions, undiscounted reward, and in which a uniform behavior policy is always initialized from the state $s_1$ (see figure 1). We then show that the ordering of the estimators based on their variance can vary by manipulating the target policy and the reward function so as to induce a different covariance structure between the reward and the likelihood ratio. We can then compute the exact variance (table 1) of each estimator manually (see appendix A). Example 1a shows that the per-decision estimator can have a larger variance than the crude estimator when stationary estimator improves on per-decision estimator. Example 1b shows an instance where the stationary estimator does not improve on the per-decision importance sampling, but per-decision importance sampling has a smaller variance than crude importance sampling. Finally, example 1c provides a negative example where the ordering goes against our intuition and shows that the stationary estimator is worse than the per-decision estimator, which in turn has a larger variance than the crude estimator. Note that the lack of variance reduction for stationary IS occurs even with perfect knowledge of the stationary ratio. We show in section 4 that the problem comes from the covariance terms across time steps.

|       | IS   | PDIS | SIS   |
|-------|------|------|-------|
| Example 1a | 0.12 | <0.2448 | >0.2 |
| Example 1b | 0.5424 | >0.4528 | <0.52 |
| Example 1c | 0.2304 | <0.2688 | <0.32 |

Table 1: Analytical variance of different estimators. See figure 1 for the problem structure.
4 Conditional Importance Sampling

The unbiasedness of crude importance sampling (IS) estimator follows from the fact that:

\[ E \left[ \rho_{1:T} \sum_{t=1}^{T} \gamma^{t-1} r_t \right] = E_{\pi} \left[ \sum_{t=1}^{T} \gamma^{t-1} r_t \right] = v^\pi, \]

Let \( G_T \) be the total (discounted) return \( \sum_{t=1}^{T} \gamma^{t-1} r_t \) and if \( \phi_T \) is some statistics such that \( \rho_{1:T} \) is conditionally independent with \( G_T \) given \( \phi_T \), then by the law of total expectation:

\[ E [\rho_{1:T} G_T] = E [E [\rho_{1:T} G_T | \phi_T, G_T]] \]
\[ = E [G_T E [\rho_{1:T} | \phi_T, G_T]] \]
\[ = E [G_T E [\rho_{1:T} | \phi_T]]. \]

Furthermore, by the law of total variance we have:

\[ \text{Var} (G_T E [\rho_{1:T} | \phi_T]) = \text{Var} (G_T \rho_{1:T}) - E [\text{Var}(G_T \phi_{1:T} | \phi_T, G_T)] \]
\[ = \text{Var} (G_T \rho_{1:T}) - E [G_T^2 \text{Var}(\rho_{1:T} | \phi_T)]. \]

Because the second term is always non-negative, it follows that \( \text{Var} (G_T E [\rho_{1:T} | \phi_T]) \leq \text{Var} (G_T \rho_{1:T}). \) This conditioning idea is the basis for the conditional Monte Carlo (CMC) as a variance reduction method.

In this paper, we use “conditional importance sampling” as well as the stationary variants \( \text{CMC} \) (Bratley et al. 1987). Assuming that \( r_t \) is conditionally independent with \( \rho_{1:T} \) given \( \phi_t \), then by the law of total expectation:

\[ v^\pi = E [G_T \rho_{1:T}] = \sum_{t=1}^{T} \gamma^{t-1} E [E [r_t \rho_{1:t} | \phi_t, r_t]] = E \left[ \sum_{t=1}^{T} \gamma^{t-1} r_t E \left[ \rho_{1:t} | \phi_t \right] \right]. \]

We refer to estimators in this form as “extended conditional importance sampling estimators”: a family of estimators encompassing both the per-decision importance sampling (PDIS) estimator of Precup et al. (2000) and as well as the stationary variants Hallak and Mannor (2017) Liu et al. (2018) Gelada and Bellemare (2019).

In this paper, we use “conditional importance sampling” to refer to all variants of importance sampling based on the conditional Monte Carlo method, in its “extended” form or not. To obtain the per-decision estimator in our framework, it suffices to define the stage-dependent statistics \( \phi_t \) to be the history \( \tau_{1:t} \) up to time \( t \):

\[ v^\pi = E \left[ \sum_{t=1}^{T} \gamma^{t-1} r_t E \left[ \rho_{1:t} | \tau_{1:t} \right] \right] = E \left[ \sum_{t=1}^{T} \gamma^{t-1} r_t \rho_{1:t} \right]. \]

In this last expression, \( E [\rho_{1:T} | \tau_{1:t}] = \rho_{1:t} \) follows from the fact that the likelihood ratio is a martingale (L’Ecuyer and Tuffin 2008). Similarly, the stationary importance sampling (SIS) estimator can be derived by conditioning on the state and action at time \( t \):

\[ v^\pi = E \left[ \sum_{t=1}^{T} \gamma^{t-1} r_t E \left[ \rho_{1:t} | s_t, a_t \right] \right] = E \left[ \sum_{t=1}^{T} \gamma^{t-1} r_t \frac{d\pi^T(s_t, a_t)}{d\pi}(s_t, a_t) \right]. \]

In this case, the connection between the expected importance sampling weights conditioned on \( (s_t, a_t) \) and the ratio of stationary distributions warrants a lengthier justification which we formalize in the following lemma (proved in appendix).

Bucklew (2004, 2005) also uses this expression to describe the “stochastic” definition of IS. Our work considers the extended form of the CMC method for Markov chains: a more general setting with very different variance properties.
Lemma 1. \( \mathbb{E}(\rho_{1:t}|s_t, a_t) = d_t^{(s,a)} \rho_{1:t|s_t,a_t} \).

Assuming that an unbiased estimator of the conditional weights \( \mathbb{E}[\rho_{1:t}|\phi_t] \) is available, the conditional importance sampling estimators are also unbiased. However, the law of total variance no longer implies a variance reduction because the variance is now over a sum of random variables of the form:

\[
\text{Var}\left( \sum_{t=1}^{T} r_t w_t \right) = \sum_{t=1}^{T} \text{Var}(r_t w_t) + \sum_{k \neq t} \text{Cov}(r_k w_k, r_t w_t). 
\]

where \( w_t = \mathbb{E}[\gamma^{-1} \rho_{1:t}|\phi_t] \). In general, there is no reason to believe that the sum of covariance terms interact in such a way as to provide a variance reduction. If stage-dependent conditioning of the importance weights need not reduce the variance in general, all we are left with is to “optimistically” \( \text{Bratley et al., 1987} \) suppose that the covariance structure plays in our favor. Over the next sections, we develop sufficient conditions for a variance reduction with the per-decision estimator while theorem 2 applies to the stationary importance sampling estimator. In section 6, we develop an asymptotic analysis of the variance when \( T \to \infty \). We show that under some mild assumptions, the variance of the crude importance sampling estimator is always exponentially large in the horizon \( T \). Nevertheless, we show that there are cases where the per-decision or stationary estimators can help reduce the variance to \( O(T^2) \).

5 Finite-Horizon Analysis

While the counterexamples of section 3 show that there is no consistent order in general between the different IS estimators and their variance, we are still interested in characterizing when a variance reduction can occur. In this section, we provide theorems to answer when \( \text{Var}(\hat{v}_{PDIS}) \leq \text{Var}(\hat{v}_{IS}) \) and when \( \text{Var}(\hat{v}_{SIS}) \) is guaranteed to be smaller than \( \text{Var}(\hat{v}_{PDIS}) \). We start by introducing a useful lemma to analyze the variance of the sum of conditional expectations.

Lemma 2. Let \( X_t \) and \( Y_t \) be two sequences of random variables. Then

\[
\text{Var}\left( \sum_t Y_t \right) - \text{Var}\left( \sum_t \mathbb{E}[Y_t|X_t] \right) \geq 2 \sum_{t<k} \mathbb{E}[Y_t Y_k] - 2 \sum_{t<k} \mathbb{E}\left[ \mathbb{E}[Y_t|X_t] \mathbb{E}[Y_k|X_k] \right].
\]

This lemma states that the variance reduction of the stage-dependent conditional expectation depends on the difference between the covariance of the random variables and that of their conditional expectations. The variance reduction analysis of PDIS and SIS in theorems 1 and 2 can be viewed as a consequence of this result. We develop in those cases some sufficient conditions to guarantee that the difference between the covariance terms is positive.

Theorem 1 (Variance reduction of PDIS). If for any \( 1 \leq t \leq k \leq T \) and initial state \( s \), \( \rho_{0:k}(\tau) \) and \( r_k(\tau)\rho_{0:k}(\tau) \) are positively correlated, \( \text{Var}(\hat{v}_{PDIS}) \leq \text{Var}(\hat{v}_{IS}) \).

This theorem guarantees the variance reduction of PDIS given a positive correlation between the likelihood ratio and the importance-weighted reward. The random variables \( \rho_{0:k}(\tau) \) and \( r_k(\tau)\rho_{0:k}(\tau) \) are positively correlated when for a trajectory with large likelihood ratio, the importance-weighted reward (which is an unbiased estimator of reward under the target policy \( \pi \)) is also large. Intuitively, a positive correlation is to be expected if the target policy \( \pi \) is more likely to take a trajectory with a higher reward. We expect that this property may hold in applications where the target policy is near the optimal value for example.

Theorem 2 (Variance reduction of SIS). If for any fixed \( 0 \leq t \leq k < T \),

\[
\text{Cov}(\rho_{1:t} r_t, \rho_{0:k} r_k) \geq \text{Cov}\left( d_t^{(s,a)} r_t, d_k^{(s,a)} r_k \right)
\]

then \( \text{Var}(\hat{v}_{SIS}) \leq \text{Var}(\hat{v}_{PDIS}) \).
This theorem implies that the relative order of variance between SIS and PDIS depends on the ordering of the covariance terms between time-steps. In the case when $T$ is very large, the covariance on the right is very close to zero, and if the covariance on the left is positive (which is true for many MDPs) the variance of SIS can be smaller than PDIS.

6 Asymptotic Analysis

We have seen in section 3 that a variance reduction cannot be guaranteed in the general case and we then proceeded to derive sufficient conditions. However, this section shows that the intuition behind per-decision and stationary importance sampling does hold under some conditions and in the limit of the horizon $T \to \infty$. Under the light of these new results, we expect those estimators to compare favorably to crude importance sampling for very long horizons: an observation also implied by the sufficient conditions derived in the last section.

In the following discussion, we consider the asymptotic rate of the variance as a function when $T \to \infty$. We show that under some mild assumptions, the variance of crude importance sampling is exponential with respect to $T$ and bounded from two sides. For the per-decision estimator, we provide conditions when the variance is at least exponential or at most polynomial with respect to $T$. Under some standard assumptions, we also show that the variance of stationary importance sampling can be polynomial with respect to $T$, indicating an exponential variance reduction. As a starting point, we prove a result characterizing the asymptotic distribution of the importance-weighted return.

**Theorem 3.** Under Assumption 1, for $\pi \neq \mu$, $\lim_T (\rho_{1:T})^{1/T} = e^{-c}$, $\lim_T |\hat{\psi}_{IS}|^{1/T} < e^{-c}$ a.s.

**Corollary 1.** Under the same condition as theorem 3, $\rho_{1:T} \to a.s. 0$, $\rho_{1:T} \sum_{t=1}^T \gamma^{t-1} r_t \to a.s. 0$

Although crude importance sampling is unbiased, this result shows that it also converges to zero almost surely. Theorem 3 further proves that it converges to an exponentially small term $\exp(-cT)$. This indicates that in most cases the return is almost zero, leading to poor estimates of $v^\pi$, and under some rare events the return can be very large and the expectation is $v^\pi > 0$.

Equipped with these results, we can now show that the variance of the crude importance sampling estimator is exponential with respect to $T$. To quantitatively describe the variance, we need the following assumptions so that $\log \rho_t$ is bounded:

**Assumption 3.** $|\log \rho_t| < \infty$

This assumption entails that $\rho_t$ is both upper-bounded (a common assumption) and lower-bounded. We only need the assumption on the lower bound of $\rho_t$ in the proof of a lower bound part in theorem 4 and 5. For the lower bound part, it essentially amounts to the event where all likelihood ratio terms on a trajectory are greater than zero. Then by the law of total variance, the original variance can only be larger than the variance of all returns conditioned on this event. Before we characterize the variance of the IS estimator, we first prove that the log-likelihood ratio is a martingale with bounded differences.

**Lemma 3.** Under Assumption 4, 5, and 6 there exists a function $\hat{f} : S \times A \to \mathbb{R}$ such that:

1. $\forall(s,a), |\hat{f}(s,a)| < c_1 \sqrt{B(s,a)}$ for constant $c_1$.

2. For any $T > 0$, $\log \rho_{1:T} + Tc - \hat{f}(s_1, a_1) + \hat{f}(s_{T+1}, a_{T+1})$ is a mean-zero martingale with respect to the sequence $\{s_i, a_i\}_{i=1}^T$ with martingale differences bounded by $2c_1 \sqrt{\|B\|_\infty}$.

We are now ready to give both upper and lower bounds on the variance of the importance sampling estimator using an exponential function of $T$ from both sides.

**Theorem 4 (Variance of IS estimator).** Under Assumption 7, 8, and 9 there exist $T_0 > 0$ such that for all $T > T_0$,

$$\text{Var}(\hat{\psi}_{IS}) \geq \frac{(v^\pi)^2}{4} \exp \left( \frac{Tc^2}{8c_1^2 \|B\|_\infty} \right) - (v^\pi)^2$$
where $B$ is defined in Assumption 2, $c_1$ is some constant defined in lemma 3, $c = \mathbb{E}_{\mu} [D_{KL} (\mu | \pi)]$. If $U_\rho = \sup_{s,a} \frac{\pi(a|s)}{\mu(a|s)} < \infty$, $\text{Var}(\hat{v}_{\text{IS}}) \leq TU_\rho^T - (v^\pi)^2$.

The lower bound part shows that the variance is at least an exponential function of the horizon $T$, and the rate depends on the distance between the behavior and target policies, as well as the recurrent property of the Markov chain associated with the behavior policy. This result differs from that of Xie et al. (2019), which is based on the CLT for i.i.d sequences, since our analysis considers more broadly a distribution of samples from a Markov chain.

**Proof Sketch.** Let $Y$ be the IS estimator and $Z$ be indicator function $\mathbb{1}(Y > v^\pi/2)$. By the law of total variance, $\text{Var}(Y) \geq \text{Var}(\mathbb{E}(Y | Z))$. Since the expectation of $\mathbb{E}(Y | Z)$ is a constant, we only need to show that the second moment of $\mathbb{E}(Y | Z)$ is asymptotically exponential. To achieve this, we observe that $\mathbb{E}([\mathbb{E}(Y | Z)]^2) \geq \mathbb{E}(Y > v^\pi/2)(\mathbb{E}(Y | Y > v^\pi/2))^2$. We can then establish that $\mathbb{E}[Y|Y > v^\pi/2]$ is $\Omega(1/\mathbb{Pr}(Y > v^\pi/2))$ using the fact that the expectation of $Y$ is a constant. It follows that we can upper bound $\mathbb{Pr}(Y > v^\pi/2)$ by an exponentially small term. This can be done by a concentration inequality for martingales. The upper bound part is proved by bounding the absolute range of each variable.

Now we prove upper and lower bounds for the variance of the per-decision estimator as a function of $\gamma$, the expected reward at time $t \mathbb{E}_\pi [r_t]$ and other properties of MDP. We then give a sufficient condition for the variance of PDIS to have an exponential lower bound, and when it is at most polynomial.

**Theorem 5** (Variance of the PDIS estimator). Under Assumption 7, 5 and 3 $\exists T_0 > 0$ s.t. $\forall T > T_0$, $\text{Var}(\hat{v}_{\text{PDIS}})$ is at least:

$$\sum_{t=T_0}^{T} \frac{\gamma^{2t-2}(\mathbb{E}_\pi (r_t))^2}{4} \exp(\frac{tc^2}{8c_1^2 \|B\|_{\infty}}) - \left(\frac{v^\pi}{2}\right)^2$$

where $B$, $c_1$ and $c$ are same constants in theorem 4, and $C$ is some constant. If $U_\rho = \sup_{s,a} \frac{\pi(a|s)}{\mu(a|s)} < \infty$,

$$\text{Var}(\hat{v}_{\text{PDIS}}) \leq T \sum_{t=1}^{T} U_\rho \gamma^{2t-2}(\mathbb{E}_\mu (r_t))^2 - (v^\pi)^2$$

**Proof Sketch.** The proof of the lower bound part is similar to the proof of the last theorem where we first lower bound the square of the sum by a sum of squares. We then apply the proof techniques of theorem 4 for the time-dependent terms. The proof for the upper bound relies the Cauchy-Schwartz inequality on the square of sum and then upper bound each term directly.

Using theorem 5 we can now give sufficient conditions for the variance of the PDIS estimator to be at least exponential or at most polynomial.

**Corollary 2.** With theorem 5 holds, $\text{Var}(\hat{v}_{\text{PDIS}}) = \Omega(\exp \epsilon T)$ if the following conditions hold: 1) $\gamma \geq \exp\left(\frac{c^2}{16c_1^2 \|B\|_{\infty}}\right)$; 2) There exist a $\epsilon > 0$ such that

$$\mathbb{E}_\pi (r_t) = \Omega\left(\exp\left(-t \left(\frac{c^2}{16c_1^2 \|B\|_{\infty}} + \log \gamma - \epsilon/2\right)\right)\right)$$

This corollary says that if $\gamma$ is close enough to 1 and the expected reward under the target policy is larger than an exponentially decaying function, then the variance of $\hat{v}_{\text{PDIS}}$ is at least exponentially large. We note that the second condition is satisfied if $r_t(s,a)$ is a function that does not depends on $t$ and $\mathbb{E}_{\pi^c}(r(s,a)) > 0$. This is due to the fact that $\mathbb{E}_\pi (r_t) \rightarrow \mathbb{E}_{\mu} (r(s,a))$ as $t \rightarrow \infty$ and we obtain a constant which is larger than any exponentially decaying function.

**Corollary 3.** Let $U_\rho = \sup_{s,a} \frac{\pi(a|s)}{\mu(a|s)}$. If $U_\rho \gamma \leq 1$ or $U_\rho \gamma \lim_{T \rightarrow \infty} (\mathbb{E}_\pi [r_T])^{1/T} < 1$, $\text{Var}(\hat{v}_{\text{PDIS}}) = O(T^2)$. 8
This corollary says that when $\gamma$ and the reward $\mathbb{E}_\pi(r_t)$ decreases fast enough, the variance of PDIS is polynomial in $T$, indicating an exponential improvement over crude importance sampling for long horizons. We can now prove an upper bound on the variance of stationary importance sampling.

**Theorem 6** (Variance of the SIS estimator).

\[
\text{Var}(\hat{v}_\text{SIS}) \leq T \sum_{t=1}^{T} \gamma^{t-1} \left( \mathbb{E} \left[ \left( \frac{d^\pi_t(s_t, a_t)}{d^\mu_t(s_t, a_t)} \right)^2 \right] - 1 \right)
\]

The proof uses Cauchy-Schwartz to bound each covariance term. In this theorem, the left hand side, is very close to $O(T^2)$ but $\mathbb{E} \left[ \left( \frac{d^\pi_t(s_t, a_t)}{d^\mu_t(s_t, a_t)} \right)^2 \right]$ still depends on $t$ and is not constant. Intuitively, the assumption that the ratio of stationary distributions is bounded is enough for this to hold since $d^\mu_t$ and $d^\pi_t$ is close to $d^a$ and $d^\pi$ for large $t$. We formally show this idea in the next corollary. However, we first need to introduce a continuity definition for function sequences.

**Definition 1** (asymptotically equi-continuous). A function sequence $f_t : \mathbb{R}^d \mapsto \mathbb{R}$ is asymptotically equi-continuous if for any $\epsilon > 0$ there exist $n, \delta > 0$ such that for all $t > n$ and $\text{dist}(x_1, x_2) = \delta$, $|f_t(x_1) - f_t(x_2)| \leq \epsilon$.

**Corollary 4.** If $d^\mu_t(s_t)$ and $d^\pi_t(s_t)$ are asymptotically equi-continuous, $\frac{d^\pi(s)}{d^\mu(s)} \leq U_s$, and $\frac{\pi(a|s)}{\mu(a|s)} \leq U_\rho$, then $\text{Var}(\hat{v}_\text{SIS}) = O(T^2)$

This corollary implies that as long as the stationary ratio and one step ratios are bounded, the variance of stationary IS is $O(T^2)$. This bound matches the polynomial dependency on the horizon from [Xie et al. (2019)] but our proof considers general spaces with samples coming from a Markov chain. Our result is however predicated on having access to an oracle of $d^\pi_t/d^\mu_t$ because our results characterizes the variance reduction due to conditioning irrespective of the choice of estimators for $d^\pi_t/d^\mu_t$. This result, along with the lower bound for variance of PDIs and IS, suggests that for long-horizon problems SIS reduces the variance significantly, from exp$(T)$ to $O(T^2)$. Only when corollary 3 holds, which requires a much stronger assumption than this, PDIS yields $O(T^2)$ variance.

7 Related Work

This idea of substituting the importance ratios for their conditional expectations can be found in the thesis of [Hesterberg (1988)] under the name conditional weights and is presented as an instance of the conditional Monte Carlo method. Instead, we consider the class of importance sampling estimators arising from the extended conditional Monte Carlo method and under a more general conditional independence assumption than that of [Hesterberg (1988) p.48]. The “conditional” form of the per-decision and stationary estimators are also discussed in appendix A of [Liu et al. (2018)] where the authors hypothesize a potential connection to the more stringent concept of Rao-Blackwellization; our work shows that PDIS and SIS belong to the extended conditional Monte Carlo method and on which our conditional importance sampling framework is built.

The extended conditional Monte Carlo method is often attributed to [Bratley et al. (1987), Glasserman (1993)] studies the extended conditional Monte Carlo more generally under the name filtered Monte Carlo. The sufficient condition for variance reduction in section 5 is closely related to theorem 3.8 of [Glasserman (1993), theorem 12 of Glynn and Iglehart (1988), the main theorem of Ross (1988) on page 310 and exercise 2.6.3 of Bratley et al. (1987)]. Our results in section 6 use elements of the proof techniques of Glynn et al. (1996), Glynn and Olvera-Cravioto (2019) but in the context of importance sampling for per-decision and stationary methods rather than for derivative estimation. The multiplicative structure of the importance sampling ratio in our setting renders impossible a direct application of those previous results to our setting.

Prior work has shown worst-case exponential lower bounds on the variance of IS and weighted IS [Jiang and Li (2015), Guo et al. (2017)]. However, these results are derived with respect to specific MDPs while our
Theorem 4 provides general variance bounds. The recent work on stationary importance sampling\cite{Halla and Mannor (2017); Gelada and Bellemare (2019); Liu et al. (2018)} has prompted multiple further investigations. First, Xie et al. (2019) introduces the expression “marginalized” importance sampling to refer to the specific use of a stationary importance sampling estimator in conjunction with an estimate of an MDP model. This idea is related to both model-based reinforcement learning and the control variates method for variance reduction\cite{Bratley et al. (1987); L’Ecuyer (1994)}; our work takes a different angle based on the extended conditional Monte Carlo. Our Corollary 4 about the variance of the stationary estimator matches their $O(T^2)$ dependency on the horizon but our result holds for general spaces and does not rely on having an estimate of the reward function.

Voloshin et al. (2019) also observed empirically that stationary importance sampling can yield a less accurate estimate than the crude importance sampling estimator or PDIS. Our analysis also considers how IS and PDIS might also vary in their accuracy, but focuses more broadly on building a theoretical understanding of those estimators and provide new variance bounds. Finally, parallel work by Kallus and Uehara (2019b) studies and analyzes incorporating control variates with stationary importance sampling by leveraging ideas of “double” machine learning\cite{Kallus and Uehara (2019a); Chernozhukov et al. (2016)} from semi-parametric inference. In contrast to that work, we provide a formal characterization of the variance of important sampling without control variates, and our results do not make the assumptions of a consistent value function estimator which is necessary for analysis in Kallus and Uehara (2019b).

8 Conclusion

Our analysis sheds new light on the commonly held belief that the stationary importance sampling estimators necessarily improve on their per-decision counterparts. As we show in section 5 in short-horizon settings, there exist MDPs in which the stationary importance sampling estimator is provably worse than the per-decision one and both are worse than the crude importance sampling estimator. Furthermore, this increase in the variance occurs even if the stationary importance sampling ratio is given as oracle. To better understand this phenomenon, we establish a new connection between the per-decision and stationary estimators to the extended conditional Monte Carlo method. From this perspective, the potential lack of variance reduction is no longer surprising once we extend previous theoretical results from the simulation community to what we call “conditional importance sampling”. This formalization help us derive sufficient conditions for variance reduction in theorems 1 and 2 for the per-decision and stationary settings respectively.

We then reconcile our theory with the known empirical success of stationary importance sampling through the theorems of section 6. We show that under some assumptions, the intuition regarding PDIS and SIS does hold asymptotically and their variance can be polynomial in the horizon (corollary 3 and 4 respectively) rather than exponential for the crude importance sampling estimator (theorem 1). Furthermore, we show through corollary 2 and corollary 4 that there exist conditions under which the variance of the stationary estimator is provably lower than the variance of the per-decision estimator.

In summary, the proposed framework of conditional importance sampling estimator both helps us understand existing estimators for off-policy policy evaluation and may lead to interesting future work by conditioning on different statistics. In general, there may also be other statistics such as the history of reward, state abstractions, and others that better leverage the specific structure of an MDP.

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A Details of Counterexamples

In this section we provide details of computing the variance in Figure 1. For each MDP, there are totally four possible trajectories (product of two actions and two steps), and the probabilities of them under behavior policy are all 1/4. We list the return of different estimators for those four trajectories, then compute the variance of the estimators.

| Path | IS | PDIS | SIS | IS | PDIS | SIS | IS | PDIS | SIS |
|------|----|------|-----|----|------|-----|----|------|-----|
| $a_1, a_1$ | 0.25 | 1.44 | 1.2 | 0 | 0 | 0 | 0 | 0 | 0 |
| $a_1, a_2$ | 0.25 | 1.92 | 2.16 | 2.0 | 1.44 | 1.44 | 1.2 | 0.96 | 0.96 | 0.8 |
| $a_2, a_1$ | 0.25 | 0.96 | 0.8 | 0.8 | 0.64 | 0.8 | 0.8 | 0.96 | 0.8 | 0.8 |
| $a_2, a_2$ | 0.25 | 1.28 | 1.44 | 1.6 | 1.92 | 1.76 | 2.0 | 1.28 | 1.44 | 1.6 |

Expectation: 1.4 1.4 1.4 1.0 1.0 1.0 0.8 0.8 0.8
Variance: 0.12 0.2448 0.2 0.5424 0.4528 0.52 0.2304 0.2688 0.32

Table 2: Importance sampling returns and the variance. See figure 1 for the problem structure.

B Proof of Lemma 1

Proof. In this proof, we use $\tau$ to denote the trajectory without reward: $\tau_{1:t} = \{s_k, a_k\}_{k=1}^t$. Since $\mathbb{E}(\rho_{1:t}|s_t, a_t) = \mathbb{E}(\rho_{1:t-1}|s_{t-1}, a_{t-1})\rho_t$, we only need to prove that $\mathbb{E}(\rho_{1:t-1}|s_t, a_t) = \frac{d\pi(s_t)}{d\mu(s_t)}$.

$$\mathbb{E}(\rho_{1:t-1}|s_t, a_t) = \int \prod_{k=1}^{t-1} \frac{\pi(s_k, a_k)}{\mu(s_k, a_k)} p_\mu(\tau_{1:t-1}|s_{t-1}, a_{t-1}) d\tau_{1:t-1}$$

(1)

$$= \frac{p_\pi(\tau_{1:t-1})}{p_\mu(\tau_{1:t-1})} \int p_\mu(\tau_{1:t-1}|s_{t-1}, a_{t-1}) d\tau_{1:t-1}$$

(2)

$$= \frac{p_\pi(\tau_{1:t-1})}{p_\mu(\tau_{1:t-1})} \int p_\mu(\tau_{1:t-1}) p(s_t|s_{t-1}, a_{t-1}) \mu(a_t|s_t) d\tau_{1:t-1}$$

(3)

$$= \frac{p_\pi(\tau_{1:t-1})}{p_\mu(\tau_{1:t-1})} \int d_\pi(s_t) \mu(a_t|s_t) d\tau_{1:t-1}$$

(4)

$$= \frac{1}{d_\mu(s_t)} \int p(s_t|s_{t-1}, a_{t-1}) p_\pi(\tau_{1:t-1}) d\tau_{1:t-1}$$

(5)

$$= \frac{1}{d_\mu(s_t)} \int p(s_t|\tau_{1:t-1}) d\tau_{1:t-1}$$

(6)

$$= \frac{d_\pi(s_t)}{d_\mu(s_t)}$$

(7)
C Proofs for Finite Horizon Case

C.1 Proof of Lemma 2

Proof. Since $E \left( \sum_t \mathbb{E}(Y_t|X_t) \right) = \mathbb{E} \left( \sum_t Y_t \right)$, we just need to compute the difference between the second moment of $\sum_t Y_t$ and $\sum_t \mathbb{E}(Y_t|X_t)$:

$$E \left( \sum_t \mathbb{E}(Y_t|X_t) \right)^2 = E \left( \sum_t \mathbb{E}(Y_t|X_t)^2 + 2 \sum_{t<k} \mathbb{E}(Y_t|X_t)\mathbb{E}(Y_k|X_k) \right)$$

(8)

$$= \sum_t E(\mathbb{E}(Y_t|X_t))^2 + 2 \sum_{t<k} E(\mathbb{E}(Y_t|X_t)\mathbb{E}(Y_k|X_k))$$

(9)

$$\leq \sum_t E(\mathbb{E}(Y_t^2|X_t)) + 2 \sum_{t<k} E(\mathbb{E}(Y_t|X_t)\mathbb{E}(Y_k|X_k))$$

(10)

$$= \sum_t E(Y_t^2) + 2 \sum_{t<k} E(\mathbb{E}(Y_t|X_t)\mathbb{E}(Y_k|X_k))$$

(11)

Thus we finished the proof by taking the difference between $E \left( \sum_t Y_t \right)^2$ and $E \left( \sum_t \mathbb{E}(Y_t|X_t) \right)^2$. \qed

C.2 Proof of Theorem 1

Proof. Let $\tau_{1:t}$ be the first $t$ steps in a trajectory: $(s_1, a_1, r_1, \ldots, s_t, a_t, r_t)$, then $\rho_t r_t = \mathbb{E}(\rho_{1:T} r_{1:t})$. To prove the inequality between the variance of importance sampling and per decision importance sampling, we apply Lemma 2 to the variance, letting $Y_t = r_t \rho_{1:T}$ and $X_t = \tau_{1:t}$. Then it is sufficient to show that for any $1 \leq t < k \leq T$,

$$E(r_t r_k \rho_{1:T} \rho_{1:k}) = E(Y_k Y_t) \geq E(E(Y_t|X_t)E(Y_k|X_k)) = E(r_t r_k \rho_{1:T} \rho_{1:k})$$

(14)

To prove that, it is sufficient to show $E(r_t r_k \rho_{1:T} \rho_{1:T} \tau_{1:t}) \geq E(r_t r_k \rho_{1:T} \rho_{1:T} \tau_{1:t})$. Since

$$E(r_t r_k \rho_{1:T} \rho_{1:k} \tau_{1:t}) = r_t \rho_{1:T} \mathbb{E}(r_k \rho_{1:k} \tau_{1:t})$$

(15)

$$= r_t \rho_{1:T} \mathbb{E}(r_k \rho_{1:T} \tau_{1:t})$$

(16)

$$= r_t \rho_{1:T} \mathbb{E}(r_k \rho_{1:T} \tau_{1:t}) \mathbb{E}(\rho_{1:T} \tau_{1:t})$$

(17)

Given $\tau_{1:t}$, $r_k$ and $\rho_{1:T}$ can be viewed as $r_{k-t+1}$ and $\rho_{1:T-t+1}$ on a new trajectory. Then according to the statement of theorem, $r_{k-t+1} \rho_{1:T-t+1}$ and $\rho_{1:T-t+1}$ are positively correlated. Now we can upper bound $E(r_t r_k \rho_{1:T} \rho_{1:k} \tau_{1:t})$ by:

$$r_t \rho_{1:T} \mathbb{E}(r_k \rho_{1:T} \tau_{1:t}) \mathbb{E}(\rho_{1:T} \tau_{1:t}) \leq r_t \rho_{1:T} \mathbb{E}(r_k \rho_{1:T} \rho_{1:T} \tau_{1:t})$$

(19)

$$= E(r_t r_k \rho_{1:T} \rho_{1:T} \tau_{1:t})$$

(20)

This implies $E(r_t r_k \rho_{1:T} \rho_{1:T}) \geq E(r_t r_k \rho_{1:T} \rho_{1:k})$ by taking expectation over $\tau_{1:t}$, and finish the proof. \qed
C.3 Proof of Theorem 1

Proof. Using lemma 2 by $Y_t = \rho_{t+1} r_t$ and $X_t = s_t, a_t, r_t$ , we have that the variance of $\hat{v}_{SIS}$ is smaller than the variance of $\hat{v}_{PDIS}$ if for any $t < k$:

\[
E[\rho_{t+1}, \rho_{k:t} r_t] \geq E(\rho_{t+1} | s_t, a_t)E(\rho_{k:t} | s_t, a_t) r_t
\]

\[
= E \left[ \frac{d_T^T(s, a) d_T^T(s, a)}{d_T^T(s, a) d_T^T(s, a) r_t} \right]
\]

The second line follows from Lemma 1 to simplify $E(\rho_{t+1} | s_t, a_t)$. To show that, we will transform the above equation into a an expression about two covariances. To proceed we subtracting $E(\rho_{t+1} r_t)E(\rho_{k:t} r_t)$ from both sides, and note that the resulting left hand side is simply the covariance:

\[
\text{Cov} [\rho_{t+1}, \rho_{k:t} r_t] = E[\rho_{t+1}, \rho_{k:t} r_t] - E(\rho_{t+1} r_t)E(\rho_{k:t} r_t)
\]

\[
\geq E \left[ \frac{d_T^T(s, a) d_T^T(s, a)}{d_T^T(s, a) d_T^T(s, a) r_t} \right] - E(\rho_{t+1} r_t)E(\rho_{k:t} r_t)
\]

We now expand the second term in the right hand side

\[
E(\rho_{t+1} r_t)E(\rho_{k:t} r_t) = E(r_t E(\rho_{t+1} | s_t, a_t))E(r_t E(\rho_{k:t} | s_t, a_t))
\]

\[
= E \left[ \frac{d_T^T(s, a)}{d_T^T(s, a) r_t} \right] E \left[ \frac{d_T^T(s, a)}{d_T^T(s, a) r_t} \right]
\]

This shows that both sides of (23) are covariances. The result then follows under the assumption of the proof.

D Proofs for infinite horizon case

D.1 Proof of Theorem 3

Proof. We can write the log of likelihood ratio as sum of random variables on a Markov chain,

\[
\log \rho_{1:T} = \sum_{t=1}^{T} \log \rho_t = \sum_{t=1}^{T} \log \left( \frac{\pi(a_t | s_t)}{\mu(a_t | s_t)} \right)
\]

By the strong law of large number on Markov chain [Breiman 1960]:

\[
\frac{1}{T} \log \rho_{1:T} = \frac{1}{T} \sum_{t=1}^{T} \log \left( \frac{\pi(a_t | s_t)}{\mu(a_t | s_t)} \right) \rightarrow_{a.s.} E_{d^o} \log \left( \frac{\pi(a_t | s_t)}{\mu(a_t | s_t)} \right) = -c
\]

If $\pi \neq \mu$, the strict concavity of log function implies that:

\[
c = E_{d^o} \log \left( \frac{\pi(a | s)}{\mu(a | s)} \right) < \log E_{d^o} \left( \frac{\pi(a | s)}{\mu(a | s)} \right) = 0
\]

Thus $\frac{1}{T} \log \rho_{1:T} \rightarrow_{a.s.} c$ and $\rho_{1:T}^{1/T} \rightarrow_{a.s.} e^{-c}$. Since $r_t \leq 1$, $|\rho_{1:T} \sum_{t=1}^{T} \gamma^{t-1} r_t|^{1/T} \leq \rho_{1:T}^{1/T} T^{1/T}$. Since $T^{1/T} \rightarrow 1$, $\lim_{T \rightarrow \infty} |\rho_{1:T} \sum_{t=1}^{T} \gamma^{t-1} r_t|^{1/T} = 0 < e^{-c}$.

D.2 Proof of Corollary 1

Proof. $\rho_{1:T} \rightarrow_{a.s.} 0$ directly follows from $\rho_{1:T}^{1/T} \rightarrow_{a.s.} e^{-c}$ in Theorem 3. For $\rho_{1:T} \sum_{t=1}^{T} \gamma^{t-1} r_t$, if there exist $\epsilon > 0$ such that $\rho_{1:T} \sum_{t=1}^{T} \gamma^{t-1} r_t > \epsilon$ for any $T$, then:

\[
\lim_{T \rightarrow \infty} \left| \rho_{1:T} \sum_{t=1}^{T} \gamma^{t-1} r_t \right|^{1/T} \geq \lim_{T \rightarrow \infty} \epsilon^{1/T} = 1
\]
This contradicts $e^{-c} > \lim_T |\rho_{1:T} \sum_{t=1}^T \gamma^{t-1} r_t|^{1/T}$ So $\lim_T \rho_{1:T} \sum_{t=1}^T \gamma^{t-1} r_t \leq 0$, which implies that $\rho_{1:T} \sum_{t=1}^T \gamma^{t-1} r_t \to a.s. 0$

D.3 Proof of Lemma 3

Proof. Let $f(s, a) = \log \frac{\pi(s, a)}{p(s, a)}$. According to Assumption 3 $|f(s, a)| < \infty$. Since $B(s, a) \geq 1$, $\frac{|f(s, a)|}{\sqrt{B(s, a)}} < \infty$. Since $f^2$ and $B$ are both finite, $E_{d^r} f^2 < \infty$ and $E_{d^r} B < \infty$. Now we satisfy the condition of Lemma 3 in Glynn et al. (1996), we have that there exist a solution $\hat{f}$ satisfying

$$f(\hat{t}, a) - E_{s,a} f(s', a') = f(s, a) - E_{d^r} f(s, a)$$

satisfying $|\hat{f}(s, a)| < c_1 \sqrt{B(s, a)}$ for some constant $c_1$. Following from the Poisson’s equation we have:

$$\log \rho_{1:T} + Tc = \sum_{t=1}^T (f(s_t, a_t) - E_{d^r} f(s, a))$$

$$= \sum_{t=1}^T \left( \hat{f}(s_t, a_t) - E_{s',a'|s_t,a_t} \hat{f}(s', a') \right)$$

$$= \hat{f}(s_1, a_1) - \hat{f}(s_{T+1}, a_{T+1}) + \sum_{t=2}^{T+1} \left( \hat{f}(s_t, a_t) - E_{s',a'|s_t-1,a_t-1} \hat{f}(s', a') \right)$$

$$\left( \hat{f}(s_t, a_t) - E_{s',a'|s_t-1,a_t-1} \hat{f}(s', a') \right)$$

are martingale differences. The absolute value of difference is upper bounded by $2\|\hat{f}\|_{\infty} \leq 2c_1 \sqrt{\|B\|_{\infty}}$. □

D.4 Proof of Theorem 4

Proof. Define $Y = \rho_{1:T} \sum_{t=1}^T \gamma^{t-1} r_t$ and $Z = 1(Y > v^\pi/2)$, then $v^\pi = E(Y)$. By the law of total variance,

$$\text{Var}(Y) = \text{Var}(E(Y|Z)) + E(\text{Var}(Y|Z))$$

$$\geq \text{Var}(E(Y|Z))$$

$$= E(\text{Var}(Y|Z))$$

$$= E(E(Y|Z)^2 - (v^\pi)^2)$$

$$\geq \Pr(Y > v^\pi/2)(E(Y|Y > v^\pi/2)^2 - (v^\pi)^2)$$

Now we are going to lower bound $E(Y|Y > v^\pi/2)$. We can rewrite $E(Y) = v^\pi$ as:

$$v^\pi = E(Y) = E(E(Y|Z))$$

$$= \Pr(Y > v^\pi/2)E(Y|Y > v^\pi/2) + \Pr(Y \leq v^\pi/2)E(Y|Y \leq v^\pi/2)$$

$$\leq \Pr(Y > v^\pi/2)E(Y|Y > v^\pi/2) + 1 \times v^\pi/2$$

So $E(Y|Y > v^\pi/2) \geq \frac{v^\pi}{2\Pr(Y > v^\pi/2)}$. Substitute this into the RHS of Equation 36

$$\text{Var}(Y) \geq \frac{(v^\pi)^2}{4\Pr(Y > v^\pi/2)} - (v^\pi)^2$$

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Now we are going to upper bound $\Pr(Y > v^\pi/2)$. Recall that we define $c = \mathbb{E}_\mu D_{KL}(\mu∥\pi) = -\mathbb{E}_\mu \log \left( \frac{\pi(a|s)}{\mu(a|s)} \right)$.

Now we define $c(T) = -\mathbb{E}_\mu \log \left( \frac{\pi(a|s)}{\mu(a|s)} \right) = -\frac{1}{T} \mathbb{E}_\mu [\log \rho_{1:T}]$.

\[
\Pr(Y > v^\pi/2) = \Pr(\rho_{1:T} \sum_{t=1}^{T} \gamma^{t-1} r_t > v^\pi/2) \leq \Pr(\rho_{1:T} > v^\pi/2) \leq \Pr(\log \rho_{1:T} > \log v^\pi - \log(2T)) \leq \Pr(\log \rho_{1:T} > \log v^\pi - \log(2T) + \hat{f}(s_{T+1}, a_{T+1}) - \hat{f}(s_1, a_1) > c) \leq \exp \left( -\frac{Tc^2}{8c_1^2 \|B\|_\infty} \right)
\]

Since $\log v^\pi$ is a constant, $\hat{f}(s_{T+1}, a_{T+1}) - \hat{f}(s_1, a_1)$ could be upper bounded by constant $2c_1 \sqrt{\|B\|_\infty}$, and $\lim_{T \to \infty} \frac{\log(2T)}{T} = 0$, we know that $\lim_{T \to \infty} \log v^\pi - \log(2T) + \hat{f}(s_{T+1}, a_{T+1}) - \hat{f}(s_1, a_1) = 0$. So there exists a constant $T_0 > 0$ such that for all $T > T_0$,

\[
\log v^\pi - \log(2T) + \hat{f}(s_{T+1}, a_{T+1}) - \hat{f}(s_1, a_1) > -\frac{c}{2}
\]

Therefore for all $T > T_0$:

\[
\Pr(Y > v^\pi/2) \leq \Pr \left( \frac{\log \rho_{1:T}}{T} + c + \frac{\hat{f}(s_{T+1}, a_{T+1}) - \hat{f}(s_1, a_1)}{T} > c/2 \right)
\]

According to Lemma 3 and Azuma’s inequality, we have:

\[
\Pr(Y > v^\pi/2) \leq \exp \left( -\frac{Tc^2}{8c_1^2 \|B\|_\infty} \right)
\]

Thus we can lower bound the variance of importance sampling estimator $Y$:

\[
\text{Var}(Y) \geq \frac{(v^\pi)^2}{4} \exp \left( -\frac{Tc^2}{8c_1^2 \|B\|_\infty} \right) - (v^\pi)^2
\]

If the one step likelihood ratio is upper bounded by $U_\rho$, then the variance of importance sampling estimator can be upper bounded by:

\[
\text{Var}(\tilde{v}_{IS}) = \mathbb{E}[Y^2] - (v^\pi)^2 \leq T U_\rho T - (v^\pi)^2
\]
D.5 Proof of Theorem 5

Proof. Let $Y_t = \rho_{t:t+1} \gamma_t r_t$. For the upper bound:

\[
\text{Var}(\hat{v}_{\text{PDIS}}) = \mathbb{E} \left( \left( \sum_{t=1}^{T} Y_t \right)^2 \right) - (v^\pi)^2
\]

\[
\leq \mathbb{E} \left( T \sum_{t=1}^{T} Y_t^2 \right) - (v^\pi)^2
\]

\[
= T \sum_{t=1}^{T} \mathbb{E}(Y_t^2) - (v^\pi)^2
\]

\[
\leq T \sum_{t=1}^{T} \mathbb{E}(U_t^2 \gamma_t^{2t-2}(\mathbb{E}_\mu(r_t))^2) - (v^\pi)^2
\]

\[
\leq T \sum_{t=1}^{T} U_t^2 \gamma_t^{2t-2}(\mathbb{E}_\mu(r_t))^2 - (v^\pi)^2
\]

For the lower bound, we notice that $Y_t \geq 0$ for any $t$, then:

\[
\mathbb{E} \left( \left( \sum_{t=1}^{T} Y_t \right)^2 \right) \geq \mathbb{E} \left( \sum_{t=1}^{T} Y_t^2 \right) = \sum_{t=1}^{T} \mathbb{E}(Y_t^2)
\]

For each $t$, we will follow a similar proof as how to lower bound part in Theorem 4:

\[
\mathbb{E}(Y_t^2) = \mathbb{E}(\mathbb{E}(Y_t^2 | I(Y_t > \gamma_t \mu_{\pi}(r_t) / 2)))
\]

\[
\geq \mathbb{E}(\mathbb{E}(Y_t | I(Y_t > \gamma_t \mu_{\pi}(r_t) / 2)))^2
\]

\[
\geq \mathbb{P}(Y_t > \gamma_t \mu_{\pi}(r_t) / 2) (\mathbb{E}(Y_t | I(Y_t > \gamma_t \mu_{\pi}(r_t) / 2)))^2
\]

Notice that $\mathbb{E}(Y_t) = \gamma_t \mu_{\pi}(r_t)$,

\[
\gamma_t \mu_{\pi}(r_t) = \mathbb{E}(Y_t)
\]

\[
= \mathbb{P}(Y_t > \gamma_t \mu_{\pi}(r_t) / 2) \mathbb{E}(Y_t | I(Y_t > \gamma_t \mu_{\pi}(r_t) / 2)) + \mathbb{P}(Y_t \leq \gamma_t \mu_{\pi}(r_t) / 2) \mathbb{E}(Y_t | I(Y_t \leq \gamma_t \mu_{\pi}(r_t) / 2)
\]

\[
\leq \mathbb{P}(Y_t > \gamma_t \mu_{\pi}(r_t) / 2) \mathbb{E}(Y_t | I(Y_t > \gamma_t \mu_{\pi}(r_t) / 2) + \gamma_t \mu_{\pi}(r_t) / 2
\]

So we can lower bound the $\mathbb{E}(Y_t^2)$:

\[
\mathbb{E}(Y_t | I(Y_t > \gamma_t \mu_{\pi}(r_t) / 2) \geq \frac{\gamma_t \mu_{\pi}(r_t)}{2 \mathbb{P}(Y_t > \gamma_t \mu_{\pi}(r_t) / 2)}
\]

\[
\mathbb{E}(Y_t^2) \geq \frac{\gamma_t^{2t-2} (\mu_{\pi}(r_t))^2}{4 \mathbb{P}(Y_t > \gamma_t \mu_{\pi}(r_t) / 2)}
\]
Now we are going to upper bound the tail probability \( \Pr(Y_t > \gamma^{t-1}E_\pi(r_t)/2) \):

\[
\Pr \left( Y_t | Y_t > \frac{\gamma^{t-1}E_\pi(r_t)}{2} \right) = \Pr \left( \rho_{t:t} \gamma^{t-1} r_t > \frac{\gamma^{t-1}E_\pi(r_t)}{2} \right) \leq \Pr \left( \rho_{t:t} > \frac{E_\pi(r_t)}{2} \right) = \Pr (\log \rho_{t:t} > \log E_\pi(r_t) - \log 2)
\]

\[
= \Pr (\frac{1}{t} \log \rho_{1:t} > \frac{E_\pi(r_t) - \log 2}{t}) = \Pr (\frac{1}{t} \log \rho_{1:t} + c + \frac{\hat{f}(s_{t+1}, a_{t+1}) - \hat{f}(s_1, a_1)}{T} > c + \frac{E_\pi(r_t) - \log 2 + \hat{f}(s_{t+1}, a_{t+1}) - \hat{f}(s_1, a_1)}{t})
\]

Since \( |E_\pi(r_t) - \log 2 + \hat{f}(s_{t+1}, a_{t+1}) - \hat{f}(s_1, a_1)| \) is bounded, there exist some \( T_0 > 0 \) such that if \( t > T_0 \), we can lower bound the right hand side in the probability by \( c/2 \). Then for \( t > T_0 \), by Azuma’s inequality (Azuma 1967),

\[
\Pr \left( Y_t | Y_t > \frac{\gamma^{t-1}E_\pi(r_t)}{2} \right) \leq \exp \left( \frac{-tc^2}{8c^2 \|B\|_\infty} \right)
\]

So we have that for \( t > T_0 \):

\[
E(Y_t^2) \geq \frac{\gamma^{2t-2}E_\pi(r_t)}{4} \exp \left( \frac{tc^2}{8c^2 \|B\|_\infty} \right)
\]

For \( 0 < t \leq T_0 \), \( E(Y_t^2) \geq 0 \) completes the proof.

**D.6 Proof of Corollary**

**Proof.** First, \( \gamma \geq \exp \left( \frac{-c^2}{16c^2 \|B\|_\infty} \right) \) indicate \( \left( \frac{c^2}{8c^2 \|B\|_\infty} + 2 \log \gamma \right) > 0 \). This is necessary for the second condition to hold since \( r_t < 1 \). The second condition \( E_\pi(r_t) = \Omega \left( \exp \left( \frac{-tc^2}{8c^2 \|B\|_\infty} - 2t \log \gamma + ct/2 \right) \right) \) implies that there exist a \( T_1 > 0 \) and a constant \( C > 0 \) such that \( (E_\pi(r_t))^2 \geq C \left( \exp \left( \frac{-tc^2}{8c^2 \|B\|_\infty} - 2t \log \gamma + ct \right) \right) \), for any \( t > T_1 \). Then let \( T > \max \{T_1, T_0\} \), where \( T_0 \) is the constant in Theorem 4.

\[
\text{Var} \left( \sum_{t=T_0}^{T} \rho_t \gamma^{t-1} r_t \right) \geq \sum_{t=1}^{T} \gamma^{2t-2} \frac{E_\pi(r_t)^2}{4} \exp \left( \frac{tc^2}{8c^2 \|B\|_\infty} \right) - (\nu^\pi)^2
\]

\[
\geq \gamma^{2T-2} E_\pi(r_T)^2 \frac{Tc^2}{4} \exp \left( \frac{tc^2}{8c^2 \|B\|_\infty} \right) - (\nu^\pi)^2
\]

\[
\geq \gamma^{2T-2} C \exp(\epsilon T) - (\nu^\pi)^2 = \Omega(\exp \epsilon T)
\]
D.7 Proof of Corollary 3

Proof. If $U_\rho^\gamma \leq 1$, $U_\rho^\gamma - 1 \mathbb{E}_\pi (r_t) \leq 1/\gamma$ for any $t$ since $r_t \in [0, 1]$. If $U_\rho^\gamma \lim (\mathbb{E}_\mu (r_T))^{1/T} < 1$, let $\delta = 1 - U_\rho^\gamma \lim (\mathbb{E}_\rho (r_T))^{1/T} > 0$. There exist a $T_0 > 0$ such that for all $t > T_0$, $U_\rho^\gamma (\mathbb{E}_\pi (r_t))^{1/\gamma} \leq U_\rho^\gamma (\lim (\mathbb{E}_\mu (r_T))^{1/T} + \delta/2 (U_\rho^\gamma)) = 1 - \delta/2 < 1$. Therefore in both case, for all $T > T_0$, $U_\rho^\gamma - 1 \mathbb{E}_\mu (r_T) \leq 1/\gamma$:

$$\operatorname{Var}(\sum_{t=1}^T \rho_1 \cdot \gamma^{-1} r_t) \leq T \sum_{t=1}^T U_\rho^\gamma - 1 \mathbb{E}_\mu (r_T) \leq T \sum_{t=1}^T U_\rho^\gamma - 1 \mathbb{E}_\mu (r_T) + T \sum_{t=T_0+1}^T U_\rho^\gamma - 1 \mathbb{E}_\mu (r_T) \quad (73)$$

$$\leq TT_0 \frac{U_\rho^T}{U_\rho - 1} + 2T^2 \frac{1}{\gamma} \quad (74)$$

Since $T_0$ is a constant, the variance is $O(T^2)$.

D.8 Proof of Corollary 6

Proof.

$$\operatorname{Var} \left( \sum_{t=1}^T \frac{d^T_t (s_t, a_t)}{d^T_t (s_t, a_t)} \gamma^{-1} r_t \right) \quad (75)$$

$$= \sum_{t=1}^T \operatorname{Var} \left( \frac{d^T_t (s_t, a_t)}{d^T_t (s_t, a_t)} \gamma^{-1} r_t \right) + 2 \sum_{t<k} \operatorname{Cov} \left( \frac{d^T_t (s_t, a_t)}{d^T_t (s_t, a_t)} \gamma^{-1} r_t, \frac{d^T_k (s_k, a_k)}{d^T_k (s_k, a_k)} \gamma^{-1} r_k \right) \quad (76)$$

$$\leq \sum_{t=1}^T \operatorname{Var} \left( \frac{d^T_t (s_t, a_t)}{d^T_t (s_t, a_t)} \gamma^{-1} r_t \right) + 2 \sum_{t<k} \left( \operatorname{Var} \left( \frac{d^T_t (s_t, a_t)}{d^T_t (s_t, a_t)} \gamma^{-1} r_t \right) \gamma^{-1} - \operatorname{Var} \left( \frac{d^T_k (s_k, a_k)}{d^T_k (s_k, a_k)} \gamma^{-1} r_k \right) \right) \quad (77)$$

$$= T \sum_{t=1}^T \gamma^{2t-2} \operatorname{Var} \left( \frac{d^T_t (s_t, a_t)}{d^T_t (s_t, a_t)} r_t \right) \quad (79)$$

$$\leq T \sum_{t=1}^T \gamma^{2t-2} \left( \frac{d^T_t (s_t, a_t)}{d^T_t (s_t, a_t)} \right) \quad (80)$$

$$= T \sum_{t=1}^T \gamma^{-1} \left( \mathbb{E} \left( \frac{d^T_t (s_t, a_t)}{d^T_t (s_t, a_t)} \right)^2 - 1 \right) \quad (81)$$

D.9 Proof of Corollary 4

Lemma 4. If $d^\mu_t (s_t)$ and $d^\pi_t (s_t)$ are asymptotically equi-continuous, $d^\mu_t (s_t, a_t) \leq U_\mu$ and $d^\pi_t (s_t, a_t) \leq U_\pi$, then,

$$\lim \mathbb{E}_{s_t, a_t \sim d^\mu_t} \left( \frac{d^\pi_t (s_t, a_t)}{d^\mu_t (s_t, a_t)} \right)^2 = \mathbb{E}_{s_t, a_t \sim d^\mu} \left( \frac{d^\pi (s_t, a_t)}{d^\mu (s_t, a_t)} \right)^2$$

Proof. According to the law of large number on Markov chain [Breiman (1960)], the distribution of $d^\mu_t$ converge to the stationary distribution $d^\mu$ in distribution. By the Theorem 1 in [Boos et al. (1985)], $d^\mu_t (s, a)$ converge to $d^\mu (s, a)$ pointwisely, $d^\pi_t (s, a)$ converge to $d^\pi (s, a)$ pointwisely. So $\frac{d^\pi_t (s, a)}{d^\mu_t (s, a)}$ converge to $\frac{d^\pi (s, a)}{d^\mu (s, a)}$ pointwisely.
Lemma 4, there exist constant, and \(d\) proof.

\[
\text{Proof.} \quad T > T_0 \text{ such that for all } \pi, \mu, \text{ the right hand side of equation above converge to zero, which completes the proof.} \]

Proof of Corollary 4

Proof. Since \(\frac{d^\pi(s,a)}{d^\mu(s,a)}\) is bounded by \(U_\rho U_s\) and then \(E_{s,a \sim d^\mu} \left( \frac{d^\pi(s,a)}{d^\mu(s,a)} \right)^2\) is bounded by \(U_\rho^2 U_s^2\). Following from Lemma 4, there exist \(T_0 > 0\) such that for all \(t > T_0, E_{s_1, a_1 \sim d^\mu} \left( \frac{d^\pi(s_t,a_t)}{d^\mu(s_t,a_t)} \right)^2 \leq 2E_{s,a \sim d^\mu} \left( \frac{d^\pi(s,a)}{d^\mu(s,a)} \right)^2 \leq 2U_\rho^2 U_s^2.\) Then by Theorem 6 for \(T > T_0\)

\[
\Var \left( \sum_{t=1}^{T} \frac{d^\pi(s_t,a_t)}{d^\mu(s_t,a_t)} \gamma^{t-1} r_t \right) \leq T \sum_{t=1}^{T} \gamma^{t-1} E \left( \frac{d^\pi(s_t,a_t)}{d^\mu(s_t,a_t)} \right)^2 \\
\leq T \sum_{t=1}^{T_0} \gamma^{t-1} E \left( \frac{d^\pi(s_t,a_t)}{d^\mu(s_t,a_t)} \right)^2 + 2T(T - T_0) U_\rho^2 U_s^2 \\
= O(T^2)
\]