A comparative study of counterfactual estimators

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Abstract

We provide a comparative study of several widely used off-policy estimators (Empirical Average, Basic Importance Sampling and Normalized Importance Sampling), detailing the different regimes where they are individually suboptimal. We then exhibit properties optimal estimators should possess. In the case where examples have been gathered using multiple policies, we show that fused estimators dominate basic ones but can still be improved.

1. Introduction

The Reinforcement Learning (RL) theory gathers approaches that enable autonomous agents to learn how to evolve in an unknown environment through trial-and-error feedbacks. These algorithms optimize the behavior of an agent according to rewards received through past interactions with the world (Bertsekas & Tsitsiklis (1995); Sutton & Barto (1998)). In recent years, RL has had success with implementing agents which learned to control a remote helicopter or play several Atari games without any prior knowledge on the environment. Very recently, it was a key block in AlphaGo, the first algorithm able to beat a human world master at Go.

To interact with its environment, an autonomous agent follows a policy dictating the action to take, either deterministically or according to some prescribed distribution. The expected reward of a policy \( \pi \) is then defined as

\[
J(\pi) = \int_{\mathcal{T}} \pi(\tau) \bar{r}(\tau) \, d\tau.
\]

where \( \mathcal{T} \) is the set of all actions \( \tau \), \( \bar{r}(\tau) \) is the expected reward associated with \( \tau \) and \( \pi \) is the distribution prescribed by the policy.

A possible way to estimate \( J(\pi) \) is to sample from \( \pi \) and collect, for each rollout \( i \in \{1, \ldots, N\} \), the chosen action \( \tau_i \), and the reward \( r_i \) whose conditional expectation is \( \bar{r}(\tau_i) \). Then, noting \( D^N = \{ (\tau_i, r_i), \ldots, (\tau_N, r_N) \} \) the sequence of actions and collected rewards, we may use the classical Monte-Carlo estimator: \( \hat{J}_{MC}(D^N) = \frac{1}{N} \sum_{i=1}^{N} r_i \).

However, in many settings such as robotics or industrial applications, it can be crucial to estimate the expected reward of a policy \( \pi_{test} \) without sampling from it, as it may be too expensive (in time or money). Thus, the estimation of a new policy has to be based on data gathered with a previous policy \( \pi \), usually called the behavior policy in the RL community.

Offline methods were developed to use data from the behavior policy to evaluate the expected reward of a test policy (also called the target policy). This setting is known as off-policy evaluation (OPE) or counterfactual reasoning (see (Bottou et al., 2013) for a comprehensive study on the setting). Over the years, many estimators of the performances of a test policy have been developed, amongst which Basic Importance Sampling (BIS, Hammersley & Handscomb (1964)), Normalized Importance Sampling (NIS, Powell & Swann (1966)), Empirical Average (EA, Hirano et al. (2003)) and Capped Importance Sampling (CIS, Bottou et al. (2013)).

All these estimators achieve a different tradeoff between bias and variance and the standard way to compare them is through the use of the Mean Square Error (MSE), as mentioned by Thomas & Brunskill (2016). However, when faced with a particular setup, there are no guidelines to choose a good estimator and one is often left with the task of trying them all. Li et al. (2014) provided a first comparative study of basic importance sampling with the empirical average estimator but this was not extended to other popular estimators.

Even though these estimators were designed assuming all the examples were collected using a single policy \( \pi \), they can be extended to the case where each sample \( i \) has been collected using a different policy \( \pi_i \). In that setting, other estimators such as Fused Importance Sampling (FIS, Peshkin & Shelton (2002)) have been used but without additional guarantees compared to BIS.

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We study in section 2 the differences between the BIS, NIS and EA in the single policy case. In particular, we show that NIS may be seen as an interpolation between BIS, which we prove to be optimal when the rewards have high variance, and EA, which we prove to be optimal when the rewards are deterministic. We also make explicit desirable properties an estimator should have to achieve low MSE.

Further, in section 3, we prove that, when examples have been collected using multiple policies, FIS dominates BIS. We then show that FIS is the optimal unbiased estimator when the variance of the rewards is very large but that, in the low variance regime, better performing unbiased estimators exist.

Let us now introduce some notations. First of all, for simplicity we will assume that the set of actions $\mathcal{T}$ is finite, even though our results (apart from those concerning (EA)) extend to the infinite case. Every time we select action $\tau$, we observe a random reward $r(\tau)$ with (unknown) expectation $\hat{r}(\tau)$ and variance $V_r(\tau)$. The objective is to estimate the expected reward of the target policy $\pi_{\text{test}}$:

$$J(\pi_{\text{test}}) = \sum_{\tau \in \mathcal{T}} \pi_{\text{test}}(\tau) \hat{r}(\tau).$$

We consider we have collected $\{(\tau_i, r_i)\}_{i=1}^N$ where the sequence of actions $s = \{\tau_i\}_{i=1}^N$, that we call the sampled path, was generated by following the behavior policy $\pi$.

2. Examples collected with a single policy

In this section, we assume that all the examples were collected using the same behavior policy $\pi$. Further, we will assume most of the time that all actions have been selected at least once, so that EA is well defined.

We recall the formula for the estimators we consider:

$$\hat{J}_{\text{BIS}}(\pi_{\text{test}}, \pi, D^N) = \frac{1}{N} \sum_{i=1}^N \frac{\pi_{\text{test}}(\tau_i)}{\pi(\tau_i)} r_i,$$

$$\hat{J}_{\text{NIS}}(\pi_{\text{test}}, \pi, D^N) = \frac{1}{\sum_{i=1}^N \pi_{\text{test}}(\tau_i) \pi(\tau_i)} \sum_{i=1}^N \frac{\pi_{\text{test}}(\tau_i)}{\pi(\tau_i)} r_i,$$

$$\hat{J}_{\text{EA}}(\pi_{\text{test}}, \pi, D^N) = \sum_{\tau \in \mathcal{T}} \pi_{\text{test}}(\tau) \hat{r}(\tau),$$

where, for EA, $\hat{r}(\tau)$ is the empirical average\(^1\) of the rewards of action $\tau$. To exhibit the difference between these estimators, we rewrite them under the form

$$\hat{J}_z = \sum_{\tau \in \mathcal{T}} \omega_z(\tau, s) \pi_{\text{test}}(\tau) \hat{r}(\tau),$$

with

$$\omega_{\text{BIS}}(\tau, s) = \omega_{\text{BIS}}(\tau) = \frac{k(\tau, s)}{N \pi(\tau)}$$

$$\omega_{\text{NIS}}(\tau, s) = \frac{k(\tau, s)}{\pi(\tau) \sum_{j=1}^N \pi_{\text{test}}(\tau_j) / \pi(\tau_j)}$$

$$\omega_{\text{EA}}(\tau, s) = 1,$$

where, like for the EA estimator, $\hat{r}(\tau)$ is the empirical average of action $\tau$ and $k(\tau, s) = \sum_{\tau_i \in s} 1_{\tau_i = \tau}$ is the number of times action $\tau$ has been sampled in $s$.

We shall compare these weights $\omega$ to the theoretical weights the estimator minimizing the MSE would have, which will now be computed.

2.1. Theoretical optimal weights

Since the samples are exchangeable, the dependency of the optimal weights $\omega^*(\tau, s)$ on $s$ is only limited to $(k(\tau, s))_{\tau \in \mathcal{T}} := k(s) \in \mathbb{N}^\mathcal{T}$, the list of all counts for a given path $s$. We also denote $\mathcal{K}$ the set of all possible such $k(s)$. Thus, we can rewrite the MSE as

$$MSE(\hat{J}) = \mathbb{E}_{R, s} \left[ \left( \hat{J} - J(\pi_{\text{test}}) \right)^2 \right]$$

$$= \sum_{\kappa \in \mathcal{K}} \sum_{s : k(s) = \kappa} \pi(s) \mathbb{E}_{R} \left[ \left( \hat{J} - J(\pi_{\text{test}}) \right)^2 \right].$$

As optimal weights only depend on $k(s)$, we can optimize independently each $\kappa \in \mathcal{K}$. Moreover, for every $\kappa \in \mathcal{K}$, $\mathbb{E}_{R} \left[ \left( \hat{J} - J(\pi_{\text{test}}) \right)^2 \right]$ is constant for all paths $s$ such that $k(s) = \kappa$. The problem therefore becomes

$$\omega^*(k_{1\kappa}) = \arg \min_{\omega} \mathbb{E}_{R} \left[ \left( \hat{J} - J(\pi_{\text{test}}) \right)^2 \right]$$

$$= \arg \min_{\omega} \mathbb{E}_{R} \left[ \left( \sum_{\tau \in \mathcal{T}} \omega(\tau, s) \pi_{\text{test}}(\tau) \hat{r}(\tau) - \sum_{\tau \in \mathcal{T}} \pi_{\text{test}}(\tau) \hat{r}(\tau) \right)^2 \right]$$

$$= \arg \min_{\omega} \left( \sum_{\tau} (\omega(\tau, s) - 1) \pi_{\text{test}}(\tau) \hat{r}(\tau) \right)^2 + \sum_{\tau} \omega^2(\tau, s) \pi_{\text{test}}^2(\tau) \frac{V_r(\tau)}{k(\tau)} .$$

These optimal weights can be computed analytically (the calculation is provided in the appendix) and are equal to

$$\omega^*(\tau, k(s)) = \frac{k_r \hat{r}(\tau)}{\pi_{\text{test}}(\tau) V_r(\tau)} \sum_{\tau'} \pi_{\text{test}}(\tau') \hat{r}(\tau') + \sum_{\tau'} \frac{k_r \hat{r}(\tau')^2}{V_r(\tau')}. $$

\(^1\)In most implementations, when action $\tau$ has never been sampled, $\hat{r}(\tau)$ is set to 0.
where we used the notation \( k_r = k(\tau, s) \) to simplify notations. We emphasize that these weights are only theoretical since \( \bar{r}(\tau) \) and \( V_r(\tau) \) are unknown.

In the case of a single action, this simplifies to

\[
\omega^*(\tau, k_r) = \frac{\bar{r}(\tau)^2}{\bar{r}(\tau)^2 + \frac{V_r(\tau)}{k_r}}. \tag{3}
\]

Moreover, in that case, an unbiased estimator requires \( E_{k_r}[\omega_Z(\tau, k_r)] = 1 \). We see that, when the variance \( V_r(\tau) \) is large, the optimal weight trades off variance for bias.

When \( V_r(\tau) = 0 \) we recover that the weights should be constant equal to one. Indeed in this case, the term appearing in the MSE is the bias term and the weights that are setting the bias to zero are constant and equal to one. These weights correspond to the empirical average weights.

When \( V_r(\tau)/\bar{r}^2(\tau) \) is high, we find that the optimal weight should depend on \( k_r \) and \( \bar{r}^2(\tau)/V_r(\tau) \). Intuitively, the bias should be higher when the variance of \( \bar{r}(\tau) \) is very high. This variance depends both on the intrinsic variance of the reward and the number of times the action was taken. That is why the optimal weight depend on \( k_r \) and \( \bar{r}(\tau) \).

### 2.2. Suboptimality of traditional counterfactual estimators

We now explore in which settings BIS, EA, NIS are suboptimal. To that extent, it is beneficial to realise from where the variance of these estimators come. There are two sources of variance in a counterfactual estimator. The first one comes from the variance of the rewards \( V_r(\tau) \) and the second one comes from the variance of the path induced by the behavior policy. These two components can be made explicit by computing the variance of any estimator using the law of total variance (detailed in the appendix):

\[
\mathbb{V}(\hat{J}_Z) = \mathbb{V}_{\text{int}}(\hat{J}_Z) + \mathbb{V}_{\text{path}}(\hat{J}_Z) \tag{4}
\]

with

\[
\mathbb{V}_{\text{int}}(\hat{J}_Z) = E_{s \sim \pi} \left[ \sum_\tau \omega_Z^2(\tau, s) \pi^2_{\text{test}}(\tau) \frac{V_r(\tau)}{k_r} \right] \tag{5}
\]

\[
\mathbb{V}_{\text{path}}(\hat{J}_Z) = \sum_\tau \omega_Z(\tau, s) \pi_{\text{test}}(\tau) \bar{r}(\tau). \tag{6}
\]

\( \mathbb{V}_{\text{path}} \) is equal to 0 when the weights \( \omega \) are independent of the path \( s \), as is the case with EA. \( \mathbb{V}_{\text{int}} \) is small when weights are small for actions with low variance on the empirical average. However, since the latter can only be obtained with weights which depend on \( s \), each estimator achieves a different tradeoff between \( V_{\text{path}} \) and \( V_{\text{int}} \).

#### 2.2.1. Basic Importance Sampling

We recall that \( \omega_{\text{BIS}}(\tau, s) = \frac{k_r}{\pi(\tau) N} \) and these weights are thus linear in \( k_r \). This linear relationship is the one found in the optimal weights of Eq. 3 when the variance \( V_r(\tau) \) is much larger than \( \bar{r}^2(\tau) \). Thus, in the case of high variance \( V_r(\tau) \), we expect BIS to be close to optimal. In particular, BIS has the desirable property that action that were sampled many times, and thus whose average reward is well estimated, have a higher weight in the final estimator than actions whose average reward are poorly estimated.

In the low variance regime, however, \( V_{\text{path}} \) dominates \( V_{\text{int}} \). Since this estimator does not take the sampled path into account to reduce \( V_{\text{path}} \), BIS is suboptimal in that low variance regime.

We exhibit experiments in Figure 1 where on the three plots we can observe the suboptimality of BIS when \( V_r(\tau) \) is small.

#### 2.2.2. Empirical Average

We now recall that the weights of the EA estimator are \( \omega_{\text{EA}}(\tau, s) = 1 \). These weights are equal to the optimal weights of Eq. 3 when \( V_r(\tau) = 0 \). Indeed, if the rewards are deterministic, \( V_{\text{path}} \) dominates \( V_{\text{int}} \). Since the constant weights of EA induce \( V_{\text{path}} = 0 \), the EA estimator is optimal in that regime, provided each action was sampled at least once.

If, however, the variance of the rewards \( V_r(\tau) \) is large, then \( V_{\text{int}} \) dominates \( V_{\text{path}} \). Since it focuses on setting \( V_{\text{path}} \) to 0 at the expense of a larger \( V_{\text{int}} \), EA is suboptimal in that high variance regime. Instead, we would like to downweight the actions which have been rarely sampled and upweight those which have been sampled often.

In the three plots of Figure 1, we show experiments that proves this suboptimal behavior of EA when \( V_r(\tau) \) is large.

#### 2.2.3. Normalized Importance Sampling

We now focus our attention on NIS and show that this estimator may be seen as an interpolation between BIS and EA. First, we recall that the weights of the NIS estimator are

\[
\omega_{\text{NIS}}(\tau, s) = \frac{k_r}{\pi(\tau) \sum_{j=1}^N \frac{\pi_{\text{test}}(\tau_j)}{\pi(\tau_j)}}. \tag{1}
\]
which can be rewritten
\[
\omega_{\text{NIS}}(\tau, s) = \frac{k_{r}}{\pi(\tau)N} \sum_{\tau' \in \mathcal{T}} \pi_{\text{test}}(\tau') \frac{k_{r}}{\pi(\tau')N} \\
= \frac{1}{\pi_{\text{test}}(\tau)} \left( 1 + \frac{\sum_{\tau' \neq \tau} \pi_{\text{test}}(\tau') \frac{k_{r}}{\pi(\tau')N} \right) .
\] (8)

To simplify the analysis, we make the assumption that
\[
\sum_{\tau' \neq \tau} \pi_{\text{test}}(\tau') \frac{k_{r}}{\pi(\tau')N} \approx 1 - \pi_{\text{test}}(\tau) .
\] (9)

since \( \sum_{\tau' \neq \tau} \pi_{\text{test}}(\tau') \frac{k_{r}}{\pi(\tau')N} \) should concentrate faster around \( \frac{k_{r}}{\pi(\tau)N} \). Under this assumption,
\[
\omega_{\text{NIS}}(\tau, s) = \frac{1}{\pi_{\text{test}}(\tau)} \left( 1 + \frac{(1 - \pi_{\text{test}}(\tau))\pi(\tau)N}{\pi_{\text{test}}(\tau)k_{r}} \right) .
\] (10)

In Table 1, we compute the value of \( \omega_{\text{NIS}} \) for different value of \( \pi_{\text{test}}(\tau) \) based on this approximation.

| \( \pi_{\text{test}}(\tau) \) | \( \varepsilon \) | \( 0.5 \) | \( 1 - \varepsilon \) |
|--------------------------|--------------|-------|------|
| \( \omega_{\text{NIS}}(\tau) \) | \( \frac{k_{r}}{\pi(\tau)N} \) | \( \frac{k_{r}}{1 + \varepsilon \frac{\pi(\tau)N}{k_{r}}} \) | \( 1 \) |

Notice that when \( V_{c}(\tau) \) is low, the assumption we made to compute an approximation of the weights holds. Moreover, NIS is a better estimator than BIS since the corresponding weights are closer to 1, no matter the value of \( \pi_{\text{test}} \).

On the other side of the spectrum, when \( \pi_{\text{test}} \) is peaked, NIS achieve very similar performances than empirical average.

In the middle range, for instance when two main actions have probabilities close to 0.5, NIS interpolates between EA and BIS. Indeed, it uses weights similar to the harmonic average between EA and BIS weights. This tradeoff seems to depend on the value of \( \pi(\tau) \). Indeed, if \( \pi(\tau) \) is high, \( \pi(\tau)N \) will be more concentrated around one. Hence, in this case, \( \omega_{\tau} \) is close to one and NIS has the same behavior than empirical average. If \( \pi(\tau) \) is low, \( \frac{\pi(\tau)N}{k_{r}} \) dominates and NIS has a similar behavior to BIS.

We show in the first two plots of Figure 1 this dependence by varying the agreement between \( \pi_{\text{test}} \) and \( \pi \). We also show in the bottom plot that when \( \pi_{\text{test}} \) is very peaked, NIS has a very similar behavior to EA.

This study aimed at providing some intuition why

i) the empirical average estimator is optimal and normalized important sampling is better than basic importance sampling when \( V_{\text{int}} \) is low,

ii) basic importance sampling is better than empirical average when \( V_{\text{int}} \) is high

iii) NIS achieves a tradeoff between empirical average and normalized importance sampling.

We now present some experiments to show these different properties.

### 2.3. Experiments with one behavior policy

We consider an environment with \( K = 20 \) actions where each action yields rewards following a scaled Bernoulli distribution:
\[
r(\tau) = \begin{cases} 
\frac{1}{\sqrt{\pi}} & \text{with prob } \sqrt{\pi} Z(\tau) \vphantom{\sqrt{\pi}} \\
0 & \text{otherwise} \end{cases}
\]

with \( p \in [0, 1] \). Indexing the actions from 1 to \( K \), we consider a symmetric reward defined as \( Z(i) = (i + 1)/K \) for \( i = 1 : K/2 \) and \( Z(i) = K(K - i) \) for \( i = K/2 : K \) and \( \pi(i) = \frac{2i}{K(K + 1)} \). Thus, symmetric actions have the same \( V(\tau) \) but the action whose index is superior to \( K/2 \) is sampled more times than the action whose index is inferior to \( K/2 \).

In the first two figures, \( \pi_{\text{test}} \) is a peaked distribution, choosing two actions with equal probability 0.475 and the remaining actions with equal probability \( \frac{0.05}{K/2} \).

Since \( \bar{Z}^2(\tau) = Z^2(\tau) \) and \( V_{c}(\tau) = \bar{Z}^2(\tau) \), varying \( p \) from 0 to 1 changes the ratio \( \bar{Z}^2(\tau)/(\bar{Z}^2(\tau) + V_{c}(\tau)) \).

The first plot of Fig. 1 shows the MSE of the estimators as a function of \( p \) when the two actions chosen with high probability by \( \pi_{\text{test}} \) are \( K = 20 \) and \( K = 10 \).

The second plot shows the MSE of the estimators as a function of \( p \) when the two actions chosen with high probability by \( \pi_{\text{test}} \) are \( K = 10 \) and \( K = 1 \).

In the bottom plot of Fig. 1, \( \pi_{\text{test}} \) is choosing the middle action \( (K = 10) \) with probability 0.95 and is uniform on other actions.

When the rewards are close to deterministic (right part of each plot), we see the optimality of EA and the strong dependence of BIS on \( V_{\text{path}} \). The gap we observe between the MSE of EA and the MSE of BIS in the right part of the plots corresponds to \( V_{\text{path}} \).

When \( V_{c}(\tau)/\bar{Z}^2(\tau) \) is high, BIS and NIS achieve a lower MSE than EA since the weights of empirical average do not depend on \( k_{r} \) and suffer from a high \( V_{\text{int}} \).

With the first two plots, we show the dependence of NIS on the agreement between \( \pi_{\text{test}} \) and \( \pi \). This agreement defines if NIS is similar to EA or BIS. Finally, in the final plot, when the target policy is very peaked, NIS has the same
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3. Examples collected with multiple policies

We now extend our analysis to the case where different policies might have been used to collect examples. Formally, we consider a family of behavior policies \( \{ \pi_i \}_{i \in [1,N]} \) such that action \( \tau_i \) was sampled according to \( \pi_i \).

We first show that, in this context, BIS is dominated by another estimator called Fused Importance Sampling (FIS, Peshkin & Shelton (2002)). We then study how both of these estimators are suboptimal. Additionally, we provide a new unbiased estimator which theoretically outperforms the Fused estimator. Finally, we detail why, in some cases, when several policies were implemented, one must be careful when using the EA estimator.

3.1. BIS and FIS in the context of multiple policies

In the case of multiple policies, most importance sampling techniques can still be used by considering the importance weights corresponding to the policy used at the time data were collected. The corresponding estimators may be written

\[
\hat{J}_{BIS}(\pi_{test}, \{ \pi_i \}, D^N) = \frac{1}{N} \sum_{i=1}^{N} \int_{\tau} \pi_{test}(\tau) \pi_i(\tau) r_i(\tau) \, d\tau
\]

where \( \alpha_{BIS}^i(\tau, s) = \frac{1}{N} \). Since the formulation is not the same as Eq. 2, we denote the weights by \( \alpha_Z \) instead of \( \omega_Z \).

FIS uses another formulation for the weights, namely

\[
\alpha_{FIS}^i(\tau, s) = \frac{\pi_i(\tau)}{\frac{1}{N} \sum_{j=1}^{N} \pi_j(\tau)} .
\]

FIS is usually preferred to BIS but, until now, there was no theoretical justification for this choice. Lemma 3.1 proves that FIS dominates BIS.

**Lemma 3.1 (FIS dominates BIS).** Let us assume we are given \( N \) policies \( \pi_1, \ldots, \pi_N \), each of them sampling an action \( \tau_i \) and receiving a random reward \( r_i(\tau_i) \), and that we are trying to assess the average reward obtained using a test policy \( \pi_{test} \). Let us define the two estimators, Basic Importance Sampling and Fused Importance Sampling, as follows:

\[
\hat{J}_{BIS} = \frac{1}{N} \sum_{i=1}^{N} \int_{\tau} \frac{\pi_{test}(\tau)}{\pi_i(\tau)} r_i(\tau) 1_{\tau_i=\tau} \, d\tau
\]

\[
\hat{J}_{FIS} = \sum_{i=1}^{N} \int_{\tau} \frac{\pi_{test}(\tau)}{\frac{1}{N} \sum_{j=1}^{N} \pi_j(\tau)} r_i(\tau) 1_{\tau_i=\tau} \, d\tau
\]

Then we have

\[
\forall(\hat{J}_{FIS}) \leq \forall(\hat{J}_{BIS})
\]
Further, since both estimators are unbiased, \( \hat{J}_{\text{FIS}} \) dominates \( \hat{J}_{\text{BIS}} \).

**Proof.** The proof is in the Appendix. \( \square \)

The intuition behind this result is the following. Consider a fixed action \( \tau \) and assume that this action has been sampled several times, at stage \( n_1, n_2, \ldots, n_k \). The overall weight put by BIS is of the order of

\[
\frac{1}{N} \left( \frac{\pi_{\text{test}}(\tau)}{\pi_{n_1}(\tau)} + \frac{\pi_{\text{test}}(\tau)}{\pi_{n_2}(\tau)} + \cdots + \frac{\pi_{\text{test}}(\tau)}{\pi_{n_k}(\tau)} \right)
\]

while the weight put by FIS would be of the order of

\[
\frac{k \pi_{\text{test}}(\tau)}{\sum_{j=1}^{N} \pi_j(\tau)}
\]

If by any chance, one of the \( \pi_{n_i} \) is really small (but not the other ones), then the weight put on BIS can be pretty huge while the one of FIS would remain reasonably small. Looking at the details of the proof, the key argument when comparing the variances is how different means (Cesaro vs harmonic means) compare with each other.

### 3.2. The optimal unbiased estimator

Even though FIS dominates BIS, it is not optimal. We now provide a new estimator which achieves a lower MSE than FIS.

**Lemma 3.2 (Optimal unbiased estimator).** Let us consider the family of estimators that can be written under the form:

\[
\hat{J}_Z(\pi_{\text{test}}, \{\pi_i\}, D^N) = \frac{1}{N} \sum_{i=1}^{N} \sum_{\tau \in \mathcal{T}} \pi_Z^i(\tau) \frac{\pi_{\text{test}}(\tau)}{\pi_i(\tau)} r_\tau 1_{\tau_i = \tau}
\]

with:

\[
\forall \tau \in \mathcal{T}, \sum_{i=1}^{N} \alpha^i_Z(\tau) = N
\]

Amongst this family, the weights of the estimator that minimizes the MSE can be written as:

\[
\alpha^i_{\text{opt}}(\tau) = \frac{\pi_i(\tau)}{\sum_{j=1}^{N} \pi_j(\tau) [1 - \pi_i(\tau)] + V_\tau(\tau)}
\]

with \( \tilde{r}(\tau) \) and \( V_\tau(\tau) \) as defined in the introduction.

**Proof.** As we impose the unbiasedness of the estimator, we only need to minimize the variance of \( \hat{J}_Z(\pi_{\text{test}}, \{\pi_i\}, D^N) \) with respect to \( \{\alpha^i_Z(\tau)\}_{i \in [N], \tau} \).

Since we are free to choose the weights for each action independently, we focus on minimizing the MSE computed on one action \( \tau \).

For a given action \( \tau \), the estimator is the sum of \( N \) independent random variables. Focusing on the variance for one sample, we have

\[
\text{Var}\left[\hat{J}_Z(\tau_i, r(\tau))\right] = \text{Var}\left[\frac{\alpha^i(\tau) \pi_{\text{test}}(\tau)}{\pi_i(\tau)} r(\tau) 1(\tau = \tau_i)\right].
\]

We can use the law of total variance and compute:

\[
\text{Var}\left[\hat{J}_Z(\tau_i = \tau, r(\tau))\right] = \mathbb{E}_\tau \left[\text{Var}_r\left[\frac{\alpha^i(\tau) \pi_{\text{test}}(\tau)}{\pi_i(\tau)} r(\tau) 1(\tau = \tau_i)\right]\right]
\]

\[
= \mathbb{E}_\tau \left[\frac{\alpha^i(\tau) \pi_{\text{test}}(\tau)}{\pi_i(\tau)} r(\tau) 1(\tau = \tau_i)\right] + \mathbb{E}_\tau \left[\frac{\alpha^i(\tau) \pi_{\text{test}}(\tau)}{\pi_i(\tau)} r(\tau) 1(\tau = \tau_i)\right]
\]

\[
= (\tilde{r}(\tau) \alpha^i(\tau))^2 \pi_{\text{test}}(\tau) \left(\frac{1}{\pi_i(\tau)} - 1\right) + \frac{(\alpha^i(\tau) \pi_{\text{test}}(\tau))^2}{\pi_i(\tau)} V_\tau(\tau).
\]

Since the unbiasedness requires \( \sum_{i=1}^{N} \alpha^i(\tau) = N \), we compute the Lagrangian:

\[
\mathcal{L}(\alpha^i(\tau), \lambda) = \left(\tilde{r}(\tau) \alpha^i(\tau)\right)^2 \pi_{\text{test}}(\tau) \left(\frac{1}{\pi_i(\tau)} - 1\right) + \frac{(\alpha^i(\tau) \pi_{\text{test}}(\tau))^2}{\pi_i(\tau)} V_\tau(\tau)
\]

\[
+ \lambda \left(\sum_{i=1}^{N} \alpha^i(\tau) - 1\right)
\]

Then we find:

\[
\alpha^i_{\text{opt}}(\tau) = \frac{\pi_i(\tau)}{\sum_{j=1}^{N} \pi_j(\tau) [1 - \pi_i(\tau)] + V_\tau(\tau)}
\]

This concludes the proof. \( \square \)

In the sequel, we call this estimator the *Optimal Unbiased Importance Sampling estimator (OUIS)*.

We first remark that there exists a trade-off between \( \tilde{r}^2(\tau) \) and \( V_\tau(\tau) \). When \( \frac{V_\tau(\tau)}{\tilde{r}^2(\tau)} \) is small, the optimal weights depend on \( \pi_i(\tau)/(1 - \pi_i(\tau)) \). They are different from the weights corresponding to the fused distribution which were linear in \( \pi_i(\tau) \). They are particularly different when the collecting policies are peaked.

However, when \( \frac{V_\tau(\tau)}{\tilde{r}^2(\tau)} \) is high, we recover the weights corresponding to the fused distribution. We proved that the weights of the fused distribution are the unbiased weights with no dependence on the sampled path that are minimizing \( V_{\text{int}} \).
We also remark that when the rewards are deterministic, the optimal weights are equal to:

\[
\omega^*_j(\tau) = \frac{\pi_i(\tau)}{1 - \pi_i(\tau)} \frac{1}{\sum_{j=1}^{N} \frac{\pi_j(\tau)}{1 - \pi_j(\tau)}}
\]

(15)

In this case, we do not need to compute some estimates of \( \tilde{r}(\tau) \) and \( V_\pi(\tau) \) to be able to use the weights.

### 3.3. Caveat on EA in the context of multiple policies

The empirical average estimator can also be considered in the context of multiple policies by computing for each action its empirical average \( \hat{r}_\gamma \).

However, if there exists a relationship between the different sampling policies, the empirical average could be a biased estimate of the expected reward.

A good example is to consider a sequence of policies that were gathered by implementing a policy learning algorithm that were maximizing the reward of the agent. If the agent received a very low reward the first time he explored an action, the policy optimisation algorithm will take time to consider a policy that is playing this action with high probability. At the end of the data collection, the empirical average might underestimate the true action reward.

Hence, in the case of multiple policies, even if all the actions were sampled, the empirical average estimator could be biased.

### 3.4. Experiments with multiple policies

#### 3.4.1. Cartpole environment

To compare the estimators’ performances in the case of multiple policies, we first test them on the Cartpole\(^2\) environment. We consider stochastic linear policies where at each time step the cart moves right with probability \( \sigma(x^T\theta) \) where \( x \) represents the state of the environment and \( \theta \) the parameter of the model. To optimize the reward of the agent, we use the PoWER algorithm (Kober & Peters, 2009) and consider the policies that were used to collect data in the optimisation process. To test our estimators, we estimated the expected reward of the final policy reached by the optimisation algorithm with the data collected by the 10 previous implemented policies. In each experiment, we use 300 rollouts (30 rollout per policy) to compute the estimators.

We use the per-decision version of all estimators as defined by Precup (2000). We compute the RMSE of each estimator by running this process 400 times. We compute confidence intervals by bootstrapping and give the value of the 5th, 50th, and 95th percentiles.

For the capped estimators, we use 10 as capping parameter. We also tested the Normalized fused importance sampling estimator as defined by Shelton (2001).

#### Table 2: RMSE of the different estimators (confidence intervals computed with 400 runs)

|          | RMSE (5th) | RMSE (mean) | RMSE(95th) |
|----------|------------|-------------|------------|
| BIS      | 122.32     | 236.73      | 321.40     |
| BCIS     | 84.65      | 87.30       | 90.24      |
| NBIS     | 39.34      | 43.22       | 47.52      |
| NBCIS    | 31.02      | 32.77       | 34.63      |
| FIS      | 23.10      | 25.38       | 27.91      |
| OUIS     | 23.13      | 25.82       | 28.77      |
| NFIS     | 7.06       | 7.91        | 8.66       |

Our optimal unbiased estimator has similar performance to the Fused Importance Sampling estimator. Indeed, the probability of most of the rollouts (except path of size one and 2) is tiny and \( \pi_i(\tau)/(1 - \pi_i(\tau)) \) is almost equal to \( \pi_i(\tau) \). Thus, the fused weights are very close to the optimal unbiased weights and the two estimators are achieving similar performances.

#### 3.4.2. Blackjack environment

We implemented the same type of experiments with a blackjack environment.

We use a policy iteration algorithm in order to maximize the reward of the agent. The algorithm is a Monte-Carlo policy iteration algorithm that plays epsilon-greedy according to the current Q function.

As in the Cartpole example, we select several policies that were considered in the optimisation process. We run the policy iteration algorithm 5000 times and consider 10 policies that correspond respectively to the time steps multiple of 500. The task is to compute the expected reward of the final policy based on 1000 rollouts (100 rollouts per policy).

If the policies considered are similar,

\[
\forall i, j, \forall \tau, \pi_i(\tau) \approx \pi_j(\tau),
\]

all the considered estimators are similar. To avoid this case, we play on the exploration rate in the policy iteration algorithm. An exploration rate that is decreasing slowly will lead to non-similar policies. We tested two different schemes to decrease the exploration rate:

- \( \epsilon_1^2 = \frac{2}{\pi^2 \log \tau} \)
- \( \epsilon_1^2 = 1 - \frac{0.95\tau}{\tau_{iter}} \)

where \( \tau_{iter} \) is the number of iterations of the policy iteration algorithm. The policies used in the estimator must be

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\(^2\)https://gym.openai.com/
more different in the second case than in the first case and we should observe a higher difference between the fused importance sampling estimator and the optimal unbiased estimator.

We have not implemented the capped estimators since the weights are not very high.

The confidence intervals are computed by bootstrapping based on 500 runs of the experiment. The results are gathered in Tables 3 and 3:

Table 3. Average MSE of the different estimators (2000 runs) with an exploration defined with $\epsilon_1$

|       | MSE (5th) | MSE (mean) | MSE(95th) |
|-------|-----------|------------|-----------|
| BIS   | 0.1251    | 0.1255     | 0.1261    |
| FIS   | 0.1249    | 0.1254     | 0.1258    |
| OUIS  | 0.1250    | 0.1253     | 0.1258    |
| NBIS  | 0.0427    | 0.0438     | 0.0450    |
| NFIS  | 0.0347    | 0.0354     | 0.0363    |
| NOUIS | 0.0363    | 0.0374     | 0.0383    |

Table 4. Average MSE of the different estimators (800 runs) with an exploration defined with $\epsilon_2$

|       | MSE (5th) | MSE (mean) | MSE(95th) |
|-------|-----------|------------|-----------|
| BIS   | 0.0905    | 0.0910     | 0.0915    |
| FIS   | 0.0870    | 0.0875     | 0.0880    |
| OUIS  | 0.0855    | 0.0860     | 0.0865    |
| NBIS  | 0.0523    | 0.0535     | 0.0546    |
| NFIS  | 0.0429    | 0.0441     | 0.0453    |
| NOUIS | 0.0458    | 0.0468     | 0.0479    |

In the first case of exploration parameter, the policies used to compute the estimator are very similar and we cannot observe a difference between OUIS and FIS. When policies are sufficiently different, we can observe a significant difference between the two estimators and OUIS achieves a lower MSE than FIS as expected. We also tested a normalized estimator based on the weights of OUIS but this estimator has higher MSE than NFIS. Having better weights in the unbiased case is not a guarantee to build a better normalized estimator.

4. Conclusion

Our work provides some key elements for understanding in which cases the different usual counterfactual estimators are suboptimal and why we can see normalized importance sampling as an interpolation between empirical average and basic importance sampling. In the case of multiple policies, we proved that fused importance sampling dominates basic importance sampling and then exhibited a new
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A. Proof: Law of total variance for deriving the estimators variance

We prove that when:

\[ \hat{J}_Z(D^N) = \sum_{\tau} \omega_Z(\tau, s)\pi_{test}(\tau)\hat{r}(\tau). \]

the variance can be written as:

\[ \mathbb{V}(\hat{J}_Z(D^N)) = \mathbb{E}_{s \sim \pi} \left[ \sum_{\tau} \omega^2_Z(\tau, s)\pi^2_{test}(\tau) \frac{V_r(\tau)}{k_{\tau}} \right] \]

\[ + \mathbb{V}_{s \sim \pi} \left[ \sum_{\tau} \omega_Z(\tau, s)\pi_{test}(\tau)\hat{r}(\tau) \right]. \]

with \( s \) the sampled path.

\[ \mathbb{E} \left[ \mathbb{V}[\hat{J}_Z(D^N)]|s\right] = \mathbb{E}_{s \sim \pi} \left[ \mathbb{V} \left[ \sum_{\tau} \omega_Z(\tau, s)\pi_{test}(\tau)\hat{r}(\tau)\right]|s\right] \]

\[ = \mathbb{E}_{s \sim \pi} \left[ \sum_{\tau} \mathbb{V} \left[ \omega_Z(\tau, s)\pi_{test}(\tau)\hat{r}(\tau)\right]|s\right] \]

\[ = \mathbb{E}_{s \sim \pi} \left[ \sum_{\tau} \omega^2_Z(\tau, s)\pi^2_{test}(\tau)\mathbb{V}[\hat{r}(\tau)|s]\right] \]

\[ = \mathbb{E}_{s \sim \pi} \left[ \sum_{\tau} \omega^2_Z(\tau, s)\pi^2_{test}(\tau) \frac{V_r(\tau)}{k_{\tau}} \right]. \]

\[ \mathbb{V} \left[ \mathbb{E}[\hat{r}(D^N)]|s\right] = \mathbb{V}_{s \sim \pi} \left[ \mathbb{E} \left[ \sum_{\tau} \omega_Z(\tau, s)\pi_{test}(\tau)\hat{r}(\tau)\right]|s\right] \]

\[ = \mathbb{V}_{s \sim \pi} \left[ \sum_{\tau} \omega_Z(\tau, s)\pi_{test}(\tau)\hat{r}(\tau) \right]. \]

\[ \square \]

B. Proof: Optimal weights with one collecting policy

We show how to compute the weights \( \{\omega_{opt}(\tau, s)\} \) which minimizes:

\[ MSE(\hat{J}(D^N)) = \left( \sum_{\tau} (\omega(\tau, s) - 1)\pi_{test}(\tau)\hat{r}(\tau) \right)^2 + \sum_{\tau} \omega^2(\tau, s)\pi^2_{test}(\tau) \frac{V_r(\tau)}{k_{\tau}} \]
They are equal to:
\[
\omega_{opt}(\tau, s) = \frac{k_{\tau}\bar{r}(\tau)}{V_{\tau}(\tau)\pi_{test}(\tau)} \sum_{\tau'} \pi_{test}(\tau')\bar{r}(\tau') + 2\omega(\tau, s)\pi_{test}^2(\tau) \frac{V_{\tau}(\tau)}{k_{\tau}}
\]

Proof. The MSE is quadratic in \(\omega(\tau, s)\):
\[
\frac{\partial \text{MSE}(\tilde{J}(D^N))}{\partial \omega(\tau, s)} = 2\pi_{test}(\tau)\bar{r}(\tau) \left( \sum_{\tau} (\omega(\tau', s) - 1)\pi_{test}(\tau')\bar{r}(\tau') \right) + 2\omega(\tau, s)\pi_{test}^2(\tau) \frac{V_{\tau}(\tau)}{k_{\tau}}
\]

and
\[
\omega_{opt}(\tau, s) = -k_{\tau}\bar{r}(\tau) \frac{V_{\tau}(\tau)\pi_{test}(\tau)}{1 + \sum_{\tau'} k_{\tau'}\bar{r}(\tau')^2 \frac{V_{\tau'}(\tau')}{V_{\tau}(\tau')}} \sum_{\tau'} (\omega_{opt}(\tau', s) - 1)\pi_{test}(\tau')\bar{r}(\tau')
\]

We note \(\lambda = \sum_{\tau'} \omega_{opt}(\tau', s)\pi_{test}(\tau')\bar{r}(\tau')\). We have:
\[
\omega_{opt}(\tau, s) = \frac{k_{\tau}\bar{r}(\tau)}{V_{\tau}(\tau)\pi_{test}(\tau)} \lambda
\]

By summing these expressions over \(\tau\), we reach:
\[
\sum_{\tau'} \omega_{opt}(\tau', s)\pi_{test}(\tau')\bar{r}(\tau') = \omega_{opt}(\tau, s)\pi_{test}(\tau)\bar{r}(\tau') + \sum_{\tau'} \omega_{opt}(\tau', s)\pi_{test}(\tau')\bar{r}(\tau')
\]

We have:
\[
\omega_{opt}(\tau, s) = \frac{k_{\tau}\bar{r}(\tau)}{V_{\tau}(\tau)\pi_{test}(\tau)} \lambda
\]

and
\[
\lambda = -\sum_{\tau'} \frac{k_{\tau'}\bar{r}(\tau')^2}{V_{\tau'}(\tau')} \left( \lambda - \sum_{\tau'} \pi(\tau')\bar{r}(\tau') \right)
\]

By summing these expressions over \(\tau\), we reach:
\[
\sum_{\tau'} \omega_{opt}(\tau', s)\pi_{test}(\tau')\bar{r}(\tau') = \omega_{opt}(\tau, s)\pi_{test}(\tau)\bar{r}(\tau') + \sum_{\tau'} \omega_{opt}(\tau', s)\pi_{test}(\tau')\bar{r}(\tau')
\]

Thus:
\[
\omega_{opt}(\tau, s) = \frac{k_{\tau}\bar{r}(\tau)}{V_{\tau}(\tau)\pi_{test}(\tau)} \sum_{\tau'} \pi_{test}(\tau')\bar{r}(\tau') + \sum_{\tau'} \frac{k_{\tau'}\bar{r}(\tau')^2}{V_{\tau'}(\tau')} \sum_{\tau'} \pi_{test}(\tau')\bar{r}(\tau')
\]

C. Proof: FIS dominates BIS

The basic importance sampling (BIS) estimator can be written
\[
\tilde{J}_{\text{BIS}}(D^N) = \frac{1}{N} \sum_{i=1}^{N} \int_{\tau} \frac{\pi_{test}(\tau)}{\bar{r}_i(\tau)} \pi_i(\tau) r_i(\tau) \, d\tau
\]

where \(r_i(\tau)\) is drawn from a distribution with mean \(\bar{r}(\tau)\) and variance \(V_\tau(\tau)\). Similarly, the fused importance sampling (FIS) estimator can be written
\[
\tilde{J}_{\text{FIS}}(D^N) = \frac{1}{N} \sum_{i=1}^{N} \int_{\tau} \frac{\pi_{test}(\tau)}{\pi_i(\tau)} r_i(\tau) \, d\tau
\]

We know that both estimators are unbiased so we focus on their variance. Using the law of total variance, we have that
\[
\text{Var}[	ilde{J}_{\text{BIS}}] = \text{Var}_R[R_{\text{BIS}}] + \text{Var}_R[R_{\text{BIS}}] \cdot \text{Var}_R[R_{\text{FIS}}]
\]

Let us start with the second term. Given the rewards, the expectation of the estimator is to be taken over the draws. We get:
\[
\text{E}[\tilde{J}_{\text{BIS}}|R] = \frac{1}{N} \sum_{i=1}^{N} \int_{\tau} \frac{\pi_{test}(\tau)}{\pi_i(\tau)} r_i(\tau) \pi_i(\tau) \, d\tau
\]

and the variance of this estimator is
\[
\text{Var}_R[R_{\text{BIS}}] = \frac{1}{N} \int_{\tau} \pi_{test}^2(\tau) V_\tau(\tau) \, d\tau
\]

Doing the same for FIS, we get
\[
\text{E}[\tilde{J}_{\text{FIS}}|R] = \frac{1}{N} \sum_{i=1}^{N} \int_{\tau} \frac{\pi_{test}(\tau)}{\pi_i(\tau)} r_i(\tau) \pi_i(\tau) \, d\tau
\]

and the variance of this estimator is
\[
\text{Var}_R[R_{\text{FIS}}] = \frac{1}{N} \int_{\tau} \pi_{test}^2(\tau) V_\tau(\tau) \sum_{i} \pi_i^2(\tau) \, d\tau
\]

We now focus on the first term of the total variance. Since both BIS and FIS are averages over \(i\), we compute the variance for each \(i\) then average them.
\[
\text{Var}[\tilde{J}_{\text{BIS}}] = \int_{\tau} \frac{\pi_{test}^2(\tau)}{\pi_i^2(\tau)} r_i^2(\tau) \pi_i(\tau) \, d\tau
\]

where
\[
\text{Var}[\tilde{J}_{\text{FIS}}] = \int_{\tau} \frac{\pi_{test}^2(\tau)}{\pi_i(\tau)} r_i^2(\tau) \, d\tau
\]

### Conclusion

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Thus, the variance of the global estimator is
\[
\mathbb{V}[\hat{J}_{\text{BIS}}|R] = \frac{1}{N^2} \sum_{i} \int_{\tau} \frac{\pi_{\text{test}}^2(\tau)}{\pi_{\text{i}}(\tau)} r_i^2(\tau) \, d\tau - \frac{1}{N^2} \sum_{i} \left( \int_{\tau} \pi_{\text{test}}(\tau) r_i(\tau) \, d\tau \right)^2.
\]
Taking the expectation over \( r_i(\tau) \) yields
\[
\mathbb{E}_R[\mathbb{V}[\hat{J}_{\text{BIS}}|R]] = \frac{1}{N^2} \int_{\tau} \pi_{\text{test}}^2(\tau) \left( \bar{r}^2(\tau) + V_r(\tau) \right) \sum_{i} \frac{1}{\pi_{\text{i}}(\tau)} \, d\tau - \frac{1}{N} \left( \int_{\tau} \pi_{\text{test}}(\tau) \bar{r}(\tau) \, d\tau \right)^2.
\]
Summing both terms for BIS, we get
\[
\mathbb{V}[\hat{J}_{\text{BIS}}] = \frac{1}{N^2} \int_{\tau} \pi_{\text{test}}^2(\tau) \left( \bar{r}^2(\tau) + V_r(\tau) \right) \sum_{i} \frac{1}{\pi_{\text{i}}(\tau)} \, d\tau - \frac{1}{N} \left( \int_{\tau} \pi_{\text{test}}(\tau) \bar{r}(\tau) \, d\tau \right)^2.
\]
Let us know compute the conditional variance of FIS for one sample.
\[
\mathbb{V}[\hat{J}_{\text{FIS}}|R] = \frac{1}{N} \int_{\tau} \frac{\pi_{\text{test}}^2(\tau)}{\sum_{j} \pi_{j}(\tau)} \bar{r}^2(\tau) \pi_{\text{i}}(\tau) \, d\tau - \left( \int_{\tau} \frac{\pi_{\text{test}}(\tau)}{\sum_{j} \pi_{j}(\tau)} r_i(\tau) \pi_{\text{i}}(\tau) \, d\tau \right)^2.
\]
Taking the expectation over \( R \) yields
\[
\mathbb{E}_R[\mathbb{V}[\hat{J}_{\text{FIS}}|R]] = \left[ \frac{1}{N^2} \int_{\tau} \frac{\pi_{\text{test}}^2(\tau)}{\sum_{j} \pi_{j}(\tau)} \left( \bar{r}^2(\tau) + V_r(\tau) \right) \pi_{\text{i}}(\tau) \, d\tau \right] - \left( \int_{\tau} \frac{\pi_{\text{test}}(\tau)}{\sum_{j} \pi_{j}(\tau)} \bar{r}(\tau) \pi_{\text{i}}(\tau) \, d\tau \right)^2.
\]
Summing over \( i \) yields
\[
\mathbb{E}_R[\mathbb{V}[\hat{J}_{\text{FIS}}|R]] = \frac{1}{N^2} \sum_{j} \int_{\tau} \frac{\pi_{\text{test}}^2(\tau)}{\sum_{j} \pi_{j}(\tau)} \left( \bar{r}^2(\tau) + V_r(\tau) \right) \, d\tau - \sum_{i} \left( \int_{\tau} \sum_{j} \frac{\pi_{\text{test}}(\tau)}{\pi_{j}(\tau)} \bar{r}(\tau) \pi_{\text{i}}(\tau) \, d\tau \right)^2 - \int_{\tau} \sum_{j} \frac{\pi_{\text{i}}^2(\tau)}{\sum_{j} \pi_{j}(\tau)} \bar{V}_r(\tau) \, d\tau.
\]
Summing both terms for FIS, we get
\[
\mathbb{V}[\hat{J}_{\text{FIS}}] = \int_{\tau} \frac{\pi_{\text{test}}^2(\tau)}{\pi_{\text{i}}(\tau)} \left( \bar{r}^2(\tau) + V_r(\tau) \right) \, d\tau - \sum_{i} \left( \int_{\tau} \sum_{j} \frac{\pi_{\text{test}}(\tau)}{\pi_{j}(\tau)} \bar{r}(\tau) \pi_{\text{i}}(\tau) \, d\tau \right)^2.
\]
We may now compute the difference of the two variances:
\[
\mathbb{V}[\hat{J}_{\text{BIS}}] - \mathbb{V}[\hat{J}_{\text{FIS}}] = \int_{\tau} \frac{\pi_{\text{test}}^2(\tau)}{\pi_{\text{i}}(\tau)} \left( \bar{r}^2(\tau) + V_r(\tau) \right) \sum_{i} \frac{1}{\pi_{\text{i}}(\tau)} \, d\tau - \frac{1}{N} \left( \int_{\tau} \pi_{\text{test}}(\tau) \bar{r}(\tau) \, d\tau \right)^2
\]
\[
- \int_{\tau} \sum_{j} \frac{\pi_{\text{test}}(\tau)}{\pi_{j}(\tau)} \left( \bar{r}^2(\tau) + V_r(\tau) \right) \, d\tau + \sum_{i} \left( \int_{\tau} \sum_{j} \frac{\pi_{\text{test}}(\tau)}{\pi_{j}(\tau)} \bar{r}(\tau) \pi_{\text{i}}(\tau) \, d\tau \right)^2.
\]
We prove the positivity of the first term through a lemma:

**Lemma C.1.** Let \( a_1, \ldots, a_N \) \( N \) strictly positive numbers. Then
\[
\frac{1}{N^2} \sum_{i} \frac{1}{a_i} \geq \frac{1}{\sum_{i} a_i}.
\]

**Proof.** Since both sides of the equation are strictly positive, we instead prove that the ratio of the two quantities is
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greater than 1.

\[
\sum_i \frac{1}{a_i} \sum_j a_j = \frac{1}{N^2} \sum_i \sum_j a_j a_i
\]

\[
= \sum_i \frac{a_i}{a_i} + \sum_i \sum_{j>i} \left( \frac{a_j}{a_i} + \frac{a_i}{a_j} \right)
\]

\[
= N + \sum_i \sum_{j>i} 2
\]

\[
= N + 2 \frac{N(N - 1)}{2}
\]

\[
= N^2.
\]

This concludes the proof. \(\square\)

Using \(a_i = \pi_i(\tau)\) and the positivity of \(\pi^2_{\text{test}}(\tau) (\bar{r}^2(\tau) + V_r(\tau))\), this proves the positivity of the first term.

To prove the negativity of the second term, we define a new random variable

\[
z_i = \int_\tau \frac{\pi_{\text{test}}(\tau)}{\sum_j \pi_j(\tau)} \bar{r}(\tau) \pi_i(\tau) \, d\tau
\]

where \(i\) is taken uniformly at random in \([1, N]\). The variance of \(z\) is:

\[
V[z] = \frac{1}{N} \sum_i \left( \int_\tau \frac{\pi_{\text{test}}(\tau)}{\sum_j \pi_j(\tau)} \bar{r}(\tau) \pi_i(\tau) \, d\tau \right)^2 - \left( \frac{1}{N} \sum_i \int_\tau \frac{\pi_{\text{test}}(\tau)}{\sum_j \pi_j(\tau)} \bar{r}(\tau) \pi_i(\tau) \, d\tau \right)^2
\]

\[
= \frac{1}{N} \sum_i \left( \int_\tau \frac{\pi_{\text{test}}(\tau)}{\sum_j \pi_j(\tau)} \bar{r}(\tau) \pi_i(\tau) \, d\tau \right)^2 - \frac{1}{N^2} \left( \int_\tau \pi_{\text{test}}(\tau) \bar{r}(\tau) \, d\tau \right)^2.
\]

Since \(V[z]\) is positive, the second term of Eq. 20 is negative. Thus, \(V[\hat{J}_\text{BIS}] - V[\hat{J}_\text{FIS}]\) is positive and FIS dominates BIS.