Beyond variance reduction: Understanding the true impact of baselines on policy optimization

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Abstract

Policy gradients methods are a popular and effective choice to train reinforcement learning agents in complex environments. The variance of the stochastic policy gradient is often seen as a key quantity to determine the effectiveness of the algorithm. Baselines are a common addition to reduce the variance of the gradient, but previous works have hardly ever considered other effects baselines may have on the optimization process. Using simple examples, we find that baselines modify the optimization dynamics even when the variance is the same. In certain cases, a baseline with lower variance may even be worse than another with higher variance. Furthermore, we find that the choice of baseline can affect the convergence of natural policy gradient, where certain baselines may lead to convergence to a suboptimal policy for any stepsiz. Such behaviour emerges when sampling is constrained to be done using the current policy and we show how decoupling the sampling policy from the current policy guarantees convergence for a much wider range of baselines. More broadly, this work suggests that a more careful treatment of stochasticity in the updates—beyond the immediate variance—is necessary to understand the optimization process of policy gradient algorithms.

1 Introduction

Reinforcement learning algorithms aim to find a policy maximizing the total reward an agent collects through repeated interactions with the environment. Environments are usually cast in the Markov Decision Process (MDP) framework [Puterman, 2014]. An MDP is a set \( \{S, A, P, r, \rho\} \) where \( S \) and \( A \) are the set of states and actions, \( P \) is the environment transition function, \( r \) is the reward function, and \( \rho \) is the initial state distribution. A trajectory \( \tau = \{s_0, a_0, \ldots\} \) is a sequence of state-action pairs, and we denote by \( R(\tau) = \sum_{t=0}^{\infty} \gamma^t r(s_t, a_t) \) the discounted return of trajectory \( \tau \) for \( \gamma \in (0, 1) \), the discount factor. The goal of reinforcement learning algorithms is to find a policy \( \pi_\theta \), parameterized by \( \theta \), which maximizes that return. The policy \( \pi_\theta \) is a distribution over actions given the current state, but we can extend it to trajectories with \( \pi_\theta(\tau) = \rho(s_0) \prod_t \pi_\theta(a_t | s_t) P(s_{t+1} | s_t, a_t) \).

Policy gradient (PG) methods cast this problem as finding, by gradient ascent,

\[
\theta^* = \arg \max_\theta J(\theta) = \arg \max_\theta \int \tau R(\tau) \pi_\theta(\tau) \, d\tau ,
\]

where \( J(\theta) \) is the expected return for policy \( \pi_\theta \). The gradient of this function can be estimated using samples drawn from \( \pi_\theta \) since

\[
\nabla_\theta J(\theta) = \int \tau \pi_\theta(\tau) R(\tau) \nabla_\theta \log \pi_\theta(\tau) \, d\tau \tag{1}
\]
\[
\approx \frac{1}{N} \sum_i R(\tau_i) \nabla_\theta \log \pi_\theta(\tau_i) , \tau_i \sim \pi_\theta , \tag{2}
\]

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where the last line comes from using $N$ Monte-Carlo samples to estimate the expectation under $\pi_\theta$.

Since these methods rely on stochastic estimates of the true gradient, optimization theory predicts that their convergence speed will be affected by the variance of these estimates and by the geometry of the function $J$, represented by its curvature. Roughly speaking, the geometry dictates how effective true gradient ascent is at optimizing $J(\theta)$ while the variance can be viewed as a penalty, capturing how much slower the optimization process is by using noisy versions of this true gradient. More concretely, doing one gradient step with stepsize $\alpha$, using a stochastic estimate $g_t$ of the gradient, leads to

$$E[J(\theta_{t+1})] - J(\theta_t) \geq \alpha \|\nabla J(\theta_t)\|^2 - \frac{1}{2} \alpha^2 L \|g_t\|^2,$$

when $J$ is $L$-smooth, i.e. its gradients are $L$-Lipschitz [Bottou et al., 2018].

While most works in the optimization literature focus on improving the dependence on the curvature, research on policy gradient methods is more focused on reducing the noise of the updates. One common technique is the use of control variates [Greensmith et al., 2004; Hofmann et al., 2015], referred to as baselines in the context of reinforcement learning. These baselines $b$ are subtracted from the observed returns to obtain shifted returns, $R(\tau) - b$, and are typically state-dependent, and do not change the expectation of gradient. Previous work showed that the minimum variance baseline for policy evaluation was the expected reward [Bhatnagar et al., 2009], while the minimum variance baseline for policy gradient involves the norm of the gradient [Peters and Schaal, 2008; Weaver and Tao, 2013]. Reducing variance has been the main motivation for many previous works on baselines [e.g., Gu et al., 2016; Liu et al., 2017; Grathwohl et al., 2017; Wu et al., 2018; Cheng et al., 2020], but baselines’ influence on other aspects of the optimization process has hardly been studied. In this paper, we take a deeper look at the role of baselines and their effects on optimization.

Contributions

Our work demonstrates that baselines can impact the optimization process beyond variance reduction and lead to qualitatively different learning curves, even when the variance of the gradients is the same. For instance, given two baselines with the same variance, the smaller baseline promotes committal behaviour where a policy will quickly tend towards a deterministic one, while the larger baseline leads to non-committal behaviour, where the policy retains higher entropy for a longer period. We observe that these differences can have a significant impact on the empirical performance of tabular agents trained on simple MDPs, unexplained by the variance of the gradients.

Furthermore, we find that the choice of baseline can even impact the convergence of natural policy gradient, which cannot be accounted for by the variance. In particular, we construct a simple MDP where using the baseline minimizing the variance leads to convergence to a deterministic, sub-optimal policy for any positive stepsize, while there is another baseline with larger variance that guarantees convergence to the optimal policy.

As such a behaviour is impossible under the standard assumptions used in optimization, this result shows how these assumptions, used to prove the convergence of policy gradient methods, may be violated in practice. It also provides a counterexample to the convergence of natural policy gradient algorithms in general, a popular variant which has been proven to converge much faster than vanilla policy gradient when using the true gradient [Agarwal et al., 2019].

Lastly, we identify on-policy sampling as a key factor to these convergence issues as it induces a vicious circle where making bad updates can lead to worse policies, in turn leading to worse updates. A natural solution is to break the dependency between the sampling distribution and the updates through off-policy sampling. We show that ensuring that all actions are sampled with sufficiently large probability at each step is enough to guarantee convergence in the constructed counterexamples, regardless of the baseline chosen. We discuss this approach and contrast it to other potential solutions, such as entropy regularization and decreasing step sizes.

Overall, through the study of baselines in policy gradient methods, we find that baselines have complex effects on the optimization process and suggest that future research in policy gradient algorithms should consider stochastic updates more carefully, beyond their variance.
2 Baselines, learning dynamics and exploration

As the convergence speed of stochastic optimization algorithms depend on the variance of the gradient estimator, reducing the noise in the gradients has been the topic of many research papers [e.g., Le Roux et al., 2012; Wang et al., 2013; Reddi et al., 2015; Defazio et al., 2014; Johnson and Zhang, 2013]. In reinforcement learning, high variance has been identified as a key problem to address in policy gradient methods and reductions in variance usually lead to increases in performance [Williams, 1992; Sutton and Barto, 2018; Ilyas et al., 2018]. By introducing a baseline $b$, the resulting policy gradient estimate $(R(\tau_i) - b)\nabla \log \pi(\tau_i)$ may have reduced variance without introducing bias. While the choice of baseline is known to affect the variance, we show that baselines can also lead to qualitatively different behaviour of the optimization process, even when the variance is the same. This difference cannot be explained by the expectation or variance, quantities which govern the usual bounds for convergence rates [Bottou et al., 2018]. In this section, we show that even for estimators of the gradient with the same variance, we can observe different induced behaviors. One we call committal, where the agent tends to repeat the same action many times leading to a deterministic policy, and one we call non-committal, where the agent more often takes different actions and the policy retains higher entropy.

2.1 Committal and non-committal behaviours

To provide a complete picture of the optimization process, we analyze the evolution of the policy throughout optimization. We start by experimenting in a simple setting, a deterministic three-armed bandit, where informative visualizations are easier to produce.

To eliminate variance as a potential confounding factor, we consider different baselines with the same variance. We start by computing the baseline leading to the minimum-variance of the gradients, which is $b^* = \frac{\mathbb{E}[R(\tau)]\|\nabla \log \pi(\tau)\|_2^2}{\mathbb{E}[\|\nabla \log \pi(\tau)\|_2^2]}$, [Weaver and Tao, 2013; Greensmith et al., 2004; Peters and Schaal, 2008]. This baseline depends on the current policy and would usually be difficult to compute due to the weighted average over all trajectories, but it can be done analytically for this simple environment. As the variance is a quadratic function of the baseline, adding or subtracting the same constant $\epsilon$ to the minimum-variance baseline results in the same variance. Thus, we use these two perturbed baselines to demonstrate that there are phenomena in the optimization process that cannot be explained by variance.

Fig. 1 presents fifteen learning curves on the probability simplex, which represents the space of all possible policies for the three-armed bandit, when using vanilla policy gradient and a softmax parameterization. We consider baselines of the form $b = b^* + \epsilon$, where $b^*$ is the minimum-variance baseline. Choosing $\epsilon = \pm 1$ leads to two estimators with the same variance, which allows us to explain away the impact of the variance in the learning dynamics.

Figure 1: We plot 15 different trajectories of vanilla policy gradient on a 3-arm bandit problem with rewards $(1, 0.7, 0)$ and stepsize $\eta = 0.05$ when using various perturbations of the minimum-variance baseline $b = b^* + \epsilon$. The black dot is the initial policy and colors represent time, from purple to yellow. For $b^* + 1$, we find that the learning curves all travel near the center of the simplex, a path with policies of high entropy, while $b^* + 1$ results in curves that are more likely to take a path through regions of low entropy. Figure made with Ternary [Harper and Weinstein, 2015].
Inspecting the plots, we can see that the the learning curves for $\epsilon = -1$ and $\epsilon = 1$ are qualitatively different even though they share the same variance. For $\epsilon = -1$, we can see that the policies quickly reach a neighborhood of a corner of the probability simplex, a deterministic policy, which can be a suboptimal one, as indicated by the curves ending up at the deterministic policy choosing action 2. On the other hand, for $\epsilon = 1$, every learning curve ends up at the optimal policy, although the convergence might be slower. We reemphasize that these differences cannot be explained by the variance since the baselines result in identical variances.

Additionally, for $b = b^*$, we can see that the learning curves spread out further. Compared to $\epsilon = 1$, some get closer to the top corner of the simplex, suggesting that the minimum-variance baseline may be worse than other, larger baselines. In the next section, we theoretically substantiate this claim and show that, for the natural policy gradient, it is possible to converge to a suboptimal policy when using the minimum-variance baseline; but there are larger baselines that guarantee convergence to an optimal policy.

To help explain these different behaviours, we look at the update rules more closely. When using a baseline $b$, the update of Eq. 2 becomes

$$\nabla_\theta J(\theta) \approx \frac{1}{N} \sum_i [R(\tau_i) - b]\nabla_\theta \log \pi_\theta(\tau_i), \tau_i \sim \pi_\theta.$$  

A sample of the gradient of the expected return is $[R(\tau_i) - b]\nabla_\theta \log \pi_\theta(\tau_i)$. Thus, if $R(\tau_i) - b$ is positive, which happens more often when the baseline $b$ is small, the update rule will increase the probability $\pi_\theta(\tau_i)$. This leads to an increase in the probability of taking the actions the agent took before, regardless of their quality. This is reflected in the results for the $\epsilon = -1$ case. Because the agent is likely to choose the same actions again, we call this committal behaviour.

While a smaller baseline leads to committal behaviour, a larger baseline makes the agent second-guess itself. If $R(\tau_i) - b$ is negative, which happens more often when $b$ is large, the parameter update decreases the probability $\pi_\theta(\tau_i)$ of the sampled trajectory $\tau_i$, reducing the probability the agent will re-take the actions it just took. While this might slow down convergence, this also makes it harder for the agent to get stuck. This is reflected in the $\epsilon = 1$ case, as all the learning curves end up at the optimal policy. We call this non-committal behaviour.

While the previous experiments used perturbed variants of the minimum-variance baseline to control for the variance, this baseline would usually be infeasible to compute in more complex MDPs. Instead, a more typical choice of baseline would be the value function [Sutton and Barto, 2018, Ch. 13], which we evaluate in Fig. 1. We see that choosing the value function as a baseline generated good results on this task, despite it not being the minimum variance baseline. The reason becomes clearer when we write the value function as $V^\pi = b^* - \frac{\text{Cov}(R, \|\nabla \log \pi\|^2)}{\text{Var} \|\nabla \log \pi\|^2}$. The term $\text{Cov}(R, \|\nabla \log \pi\|^2)$ typically becomes negative as the gradient becomes smaller on trajectories with high rewards during the optimization process, leading to the value function being an optimistic baseline, justifying a choice commonly made by practitioners.

### 2.2 Extension to multi-step MDPs

We now consider a more complex MDP: a 10x10 gridworld consisting of 4 rooms as depicted on Fig. 2a. We use a discount factor $\gamma = 0.99$. The agent starts in the upper left room and two adjacent rooms contain a goal state of value 0.6 or 0.3. However, the best goal (even discounted), with a value of 1, lies in the furthest room, so that the agent must learn to cross the sub-optimal rooms and reach the furthest one. We again train our agent with vanilla policy gradient. However, in this case, because we do not know the minimum variance baseline, we consider different fixed baselines rather than baselines with a fixed distance to the minimum variance one. In particular, we cannot in this example easily assess the relative variance of each gradient estimator.

In order to exhibit the committal vs non-committal behavior of the agent depending on the baseline, we monitor the entropy of the policy and the entropy of the stationary state distribution over time. Fig. 2b shows the average returns over time and Fig. 2c and 2d show the entropy of the policy in two ways. The first is the average entropy of the action distribution along the states visited in each trajectory, and the second is the entropy of the distribution of the number of times each state is visited up to that point in training. We observe that the action entropy for smaller baselines tends to decay faster compared to larger ones, indicating...
convergence to a deterministic policy. We see that this quick convergence is premature in some cases since the returns are not as high for the lower baselines. In Figure 2d, we observe that low baselines induce a drop in the entropy of state distribution for steps between $\sim 100$ and $\sim 1,000$. This is due to the fact that these baselines made the agent converge prematurely to a suboptimal solution, one in the adjacent rooms to the start, as we can see by the low returns. When the agent discovers there are longer paths that yield a higher return, the state entropy increases. Interestingly, we find that the best performing baseline is 0.5. This value underestimates the largest ($\approx 0.87$ after discounting) while being above most of the other returns. Intuitively, this choice may be advantageous since $R(\tau) - b$ will be positive when reaching the optimal goal—increasing the probability of sampling the same actions, but also discourage trajectories that reach suboptimal goals and achieve lower returns. In the next section, we support this intuition theoretically and prove that, in the three-armed bandit, a baseline which lies between the best and second-best reward will guarantee convergence to the optimal policy.

In the previous gridworld experiments, we utilized constant baselines to illustrate the committal and non-committal behaviours. These baselines do not share the same variance and, in this case, we cannot use the perturbed minimum-variance baseline since it is infeasible to compute. Nevertheless, we can still qualitatively observe the same two distinct behaviours. What is important is the sign of the shifted return, $R(\tau) - b$, regardless of how $b$ is computed. When $R(\tau) - b > 0$, we can expect committal behaviour and when $R(\tau) - b < 0$, non-committal behaviour. As these phenomena can be directly inferred from the policy gradient and the sign of the effective rewards $R(\tau) - b$, we posit that they extend to all MDPs. In particular, in complex MDPs, the first trajectories explored are likely to be suboptimal and a low baseline will increase their probability of being sampled again, requiring the use of techniques such as entropy regularization to prevent the policy from getting stuck too quickly.

## 3 Convergence to suboptimal policies

We empirically saw that policy gradient algorithms can reach suboptimal policies and that the choice of baseline can affect the likelihood of this occurring. In this section, we support this finding theoretically and prove that converging to a suboptimal policy is indeed possible when using natural policy gradient, even in the simplest RL setting—bandits. We discuss how this finding fits with existing convergence results and why standard assumptions are not satisfied in these counterexamples.

### 3.1 A simple example

Standard convergence results assume access to the true policy gradient [e.g., Agarwal et al. 2019] or, in the stochastic case, that the variance of the updates is uniformly bounded for all parameter values [e.g., Bottou et al. 2018]. These assumptions are in fact quite strong and are violated in a simple MDP when using natural policy gradient: a two-armed bandit problem with fixed rewards. Here there is only one state and two actions. Pulling the optimal arm gives a reward of $r_1 = +1$, while pulling the suboptimal arm leads
α = 0.05.  
α = 0.1.  
α = 0.15.

Figure 3: Learning curves for 100 runs of 200 steps, on the two-armed bandit, with baseline $b = -1$ for three different step sizes $\alpha$. Blue: Curves converging to the optimal policy. Red: Curves converging to a suboptimal policy. Black: Average performance. The number of runs that converged to the suboptimal solution are 5%, 14% and 22% for the three step sizes respectively. Larger step sizes are more prone to getting stuck at a suboptimal solution but settle on a deterministic policy more quickly.

to a reward of $r_0 = 0$. We use the sigmoid parameterization and call $p_t = \sigma(\theta_t)$ the probability of sampling the optimal arm at time $t$.

Our stochastic estimator of the natural gradient is therefore

$$ g_t = \begin{cases} 
\frac{1 - b}{p_t}, & \text{with probability } p_t \\
\frac{b}{1 - p_t}, & \text{with probability } 1 - p_t,
\end{cases} $$

where $b$ is a baseline that does not depend on the action sampled at time $t$ but may depend on $\theta_t$. By computing the variance of the updates, $\text{Var}[g_t] = \frac{(1 - p_t - b^2)}{p_t(1 - p_t)}$, we notice it is unbounded when the policy becomes deterministic, i.e. $p_t \to 0$ or $p_t \to 1$, violating the assumption of uniformly bounded variance, unless $b = 1 - p_t$, which is the optimal baseline. Note that using the vanilla (non-natural) policy gradient would, on the contrary, yield a bounded variance. In fact, we later present a convergence result in its favour. For the natural policy gradient, the following proposition establishes potential convergence to a suboptimal arm and we demonstrate this empirically in Fig. 3.

**Proposition 1.** Consider a two-armed bandit with rewards 1 and 0 for the optimal and suboptimal arms, respectively. Suppose we use natural policy gradient starting from $\theta_0$, with a fixed baseline $b < 0$, and fixed stepsize $\alpha > 0$. If the policy samples the optimal action with probability $\sigma(\theta_t)$, then the probability of picking the suboptimal action forever and having $\theta_t$ go to $-\infty$ is strictly positive. Additionally, if $\theta_0 \leq 0$, we have

$$ P(\text{suboptimal action forever}) \geq (1 - e^{\theta_0})(1 - e^{\theta_0 + \alpha b}) - \frac{\alpha}{\pi} $$

**Proof.** All the proofs may be found in the appendix.

By inspecting the updates, we can gain some intuition as to why there is convergence to a suboptimal policy. The overall issue is the committal nature of the baseline, i.e. choosing an action leads to an increase of that action’s probability, even if it is a poor choice. In detail, we see that choosing the suboptimal arm leads to a decrease in $\theta$ by $\frac{\alpha b}{1 - p_t}$, thus increasing the probability the same arm is drawn again and decreasing $\theta$ further. By checking the probability of this occurring forever, $P(\text{suboptimal arm forever}) = \prod_{t=1}^{\infty} (1 - p_t)$, we find that $1 - p_t$ converges quickly enough to 1 that the infinite product is nonzero, indicating that it is possible to get trapped choosing the wrong arm forever (Proposition 1), and $\theta_t \to -\infty$ as $t$ grows.

One could guess that this issue could be solved by picking a baseline with lower variance. This is true, as the minimum-variance baseline $b = 1 - p_t$ leads to 0 variance and both possible updates are equal to $+\alpha$, guaranteeing that $\theta \to +\infty$, thus convergence. In fact, any baseline $b \in (0, 1)$ would suffice since both updates would be positive and greater than $\alpha \min(b, 1 - b)$. Appendix B.2 contains a more detailed analysis for the perturbed minimum-variance baseline. While reducing variance helps in this example, in the next section we show this is not always the case.
3.2 Reducing variance through baselines can be detrimental

As we saw with the two-armed bandit, the direction of the updates is important in assessing convergence. More specifically, problems can arise when the choice of baseline induces committal behaviour. We now show a different MDP where committal behaviour happens even when using the minimum-variance baseline, thus leading to convergence to a suboptimal policy. Furthermore, we design a better baseline which ensures all updates move the parameters towards the optimal policy. This cements the idea that the quality of parameter updates must not be analyzed in terms of variance but rather in terms of the probability of going in a bad direction, since a baseline that induces higher variance leads to convergence while the minimum-variance baseline does not. The following theorem summarizes this.

**Theorem 1.** There exists an MDP where using the stochastic natural gradient, on a softmax-parameterized policy, with the minimum-variance baseline, can lead to convergence to a suboptimal policy with probability \( \rho > 0 \); but there is a different baseline (with larger variance) which results in convergence to the optimal policy with probability 1.

The MDP used in this theorem is the same three-armed bandit as in the previous section. This theorem supports the empirical finding we saw before in Fig. 1 and we have repeated it for the natural policy gradient, whose plots can be found in the appendix. In this example, the key is that the minimum-variance baseline can be lower than the second best reward; so pulling the second arm will increase its probability and induce committal behaviour. This can cause the agent to prematurely commit to the second arm and converge to the wrong policy. On the other hand, using any baseline whose value is between the optimal reward and the second best reward, which we term a *gap* baseline, will always increase the probability of the optimal action at every step, no matter which arm is drawn. Since the updates are sufficiently large at every step, this is enough to ensure convergence with probability 1, despite the higher variance compared to the minimum variance baseline. The key to this example is that whether a baseline underestimates or overestimates the second best reward can affect the convergence of the algorithm and is more critical than the resulting variance of the gradient estimates.

As such, more than lower variance, good baselines seem to be those that can assign positive effective returns to the good trajectories and negative effective returns to the others. These results cast doubt on whether finding baselines which minimize variance is a meaningful goal to pursue. As we saw, the baseline can affect optimization in subtle ways, beyond variance, and further study is needed to identify the true causes of some improved empirical results observed in previous works on baselines. This importance of the sign of the returns, rather than their exact value, echoes with the cross-entropy method [De Boer et al., 2005], which maximizes the probability of the trajectories with the largest returns, regardless of their actual value.

To address these convergence issues, one could consider reducing the step sizes, with the hope that the policy would not converge as quickly towards a suboptimal deterministic policy and would eventually leave that bad region. Indeed, if we are to use the vanilla policy gradient in the two-armed bandit example, instead of the natural policy gradient, this effectively reduces the step size by a factor of \( \sigma(\theta)(1 - \sigma(\theta)) \) (the Fisher information). In this case, we are able to show convergence in probability to the optimal policy. See Proposition 7 in appendix for details and proof.

Empirically, we find that, when using the vanilla policy gradient, the policy may still remain stuck near a suboptimal policy when using a negative baseline, similar to Fig. 2. While the previous proposition guarantees convergence eventually, the rate may be very slow, which remains problematic in practice. There is theoretical evidence that following even the true vanilla policy gradient may result in slow convergence [Schaul et al., 2019], suggesting that the problem is not necessarily due to noise.

An alternative solution would be to add entropy regularization to the objective. By doing so, the policy would be prevented from getting too close to deterministic policies. While this might prevent convergence to a suboptimal policy, it would also exclude the possibility of fully converging to the optimal policy, though the policy may remain near it. Other works have also developed provably convergence policy gradient algorithms using different mechanisms, such as exploration bonuses or ensembles of policies [Cai et al., 2019, Efroni et al., 2020, Agarwal et al., 2020].
4 Off-policy sampling

So far, we have seen that committal behaviour can be problematic as it can cause convergence to a suboptimal policy. This can be especially problematic when the agent follows a near-deterministic policy as it is unlikely to receive different samples which would move the policy away from the closest deterministic one, regardless of the quality of that policy.

As discussed previously, one could adjust step sizes or add entropy regularization to address these issues, but here we consider a different aspect of the algorithm. Up to this point, we assumed that actions were sampled according to the current policy, a setting known as on-policy. This setting couples the updates and the policy and is a root cause of the committal behaviour: the update at the current step changes the policy, which affects the distribution of rewards obtained and hence the next updates. However, we know from the optimization literature that, since our gradient estimate is unbiased, bounding its variance will lead to convergence. As the variance becomes unbounded when the probability of drawing some actions goes to 0, a natural solution to avoid these issues is to sample actions from a behaviour policy that selects every action with sufficiently high probability. Such a policy would make it impossible to choose the same, suboptimal action forever. We emphasize that we assume here that we can choose our sampling policy, contrary to what most works on off-policy learning assume.

4.1 Convergence guarantees with importance sampling

Since we change the behaviour policy, we introduce importance sampling corrections to preserve the unbiased updates \cite{Kahn:1951, Precup:2000}. These simple modifications are enough to guarantee convergence for all baselines, as outlined in the following proposition.

Proposition 2. Let us consider a two-armed bandit with stochastic rewards with bounded support. We define \( q_t \) to be the behavior policy, where \( q_t \) is the probability of sampling the optimal arm at time \( t \). Then, for \( \epsilon_t = \min\{q_t, 1 - q_t\} \), and for any finite baseline, if \( \lim_{t \to \infty} \epsilon_t^2 = +\infty \), then the target policy \( p_t \) converges to the optimal policy almost surely when using natural policy gradient.

The condition on \( q_t \) imposes a cap on how fast the behaviour policy can become deterministic: no faster than \( t^{-1/2} \). Intuitively, this ensures each action is sampled sufficiently often and prevents premature convergence to a suboptimal policy. The condition is satisfied for any sequence of behaviour policies which assign at least \( \epsilon_t \) probability to each action at each step, such as \( \epsilon \)-greedy policies. It also holds if \( \epsilon_t \) decreases over time at a sufficiently slow rate. By choosing as behaviour policy \( \mu \) a linear interpolation between \( \pi \) and the uniform policy, \( \mu(a) = (1 - \gamma)\pi(a) + \frac{\gamma}{2}, \gamma \in (0, 1) \), where \( K \) is the number of arms, we recover the classic EXP3 algorithm for bandits \cite{Auer:2002, Seldin:2012}.

On the other hand, we can check that this condition is not satisfied for the example in Section 3.1. There, \( p_t \) could decrease exponentially fast since the tails of the sigmoid function decay exponentially and the parameters move by at least a constant at each step. In this case, \( \epsilon_t = \Omega(e^{-t}) \), resulting in \( \lim_{t \to \infty} te^{-2t} = 0 \), so Proposition 2 does not apply.

4.2 Importance sampling, baselines and variance

As we have seen, using a separate behaviour policy that samples all actions sufficiently often may lead to stronger convergence guarantees, even if it increases the variance of the gradient estimates in most of the space, as what matters is what happens in the high variance regions, which are usually close to the boundaries. Figure 4 shows the ratios of gradient variances between on-policy policy gradient without baseline, on-policy policy gradient with the minimum variance baseline, and off-policy policy gradient using importance sampling (IS) where the sampling distribution is \( \mu(a) = \frac{1}{2}\pi(a) + \frac{1}{2} \), i.e. a mixture of the current policy \( \pi \) and the uniform distribution. While using the minimum variance baseline decreases the variance on the entire space compared to not using a baseline, IS actually increases the variance when the current policy is close to uniform. However, IS does a much better job at reducing the variance close to the boundaries of the simplex, where it actually matters to guarantee convergence.

This suggests that convergence of policy gradient methods is not so much governed by the variance of the gradient estimates in general, but rather by the variance in the worst regions, usually near the boundary.
Figure 4: Comparison between the variance of different methods on a 3-armed bandit. Each plot depicts the log of the ratio between the variance of two approaches. For example, Figure (a) depicts $\log \frac{\text{Var}_{\text{vanilla}}}{\text{Var}_{\text{IS}}}$, the log of the ratio between the variance of the gradients of vanilla PG and PG with importance sampling (IS).

The triangle represents the probability simplex with each corner representing a deterministic policy on a specific arm. The method written in blue (resp. red) in each figure has lower variance in blue (resp. red) regions of the simplex. The sampling policy $\mu$, used in the PG method with IS, is a linear interpolation between $\pi$ and the uniform distribution, $\mu(a) = \frac{1}{2}\pi(a) + \frac{1}{6}$. Note that this is not the minimal variance sampling distribution and it leads to higher variance than Vanilla PG in some parts of the simplex.

While baselines can reduce the variance, they generally cannot prevent the variance in those regions from exploding, leading to the policy getting stuck. Thus, good baselines are not the ones reducing the variance across the space but rather those that can prevent the learning from reaching these regions altogether. Large values of $b$, such that $R(\tau) - b$ is negative for most trajectories, achieve precisely that. On the other hand, due to the increased flexibility of sampling distributions, importance sampling can limit the nefariousness of these critical regions, offering better convergence guarantees despite not reducing the variance everywhere.

One important point is that, although importance sampling is usually used in reinforcement learning to correct for the distribution of past samples [e.g., Munos et al. 2016], we advocate here for expanding the research on designing appropriate sampling distributions, a line of work which has a long history in statistics [Liu 2008].

5 Conclusion

We presented results that dispute common beliefs about baselines, variance, and policy gradient (PG) methods in general. As opposed to the common belief that baselines only provide benefits through variance-reduction, we showed that they can significantly affect the optimization process in ways that cannot be explained by the variance and that lower variance can be detrimental.

Different baselines can give rise to very different learning dynamics, even when they reduce the variance of the gradients equally. They do that by either making a policy quickly tend towards a deterministic one (committal behaviour) or by maintaining high-entropy for a longer period of time (non-committal behaviour).

Looking deeper, we found that committal behaviour can be problematic and lead to convergence to a suboptimal policy. Specifically, we showed that stochastic natural policy gradient does not always converge to the optimal solution due to the unusual situation in which the iterates converge to the optimal policy in expectation but not almost surely. Moreover, by showing that reducing variance through baselines can promote committal behaviour, we were able to show that using lower-variance can sometimes be detrimental to optimization, highlighting the limitations of using variance to analyze the convergence properties of these methods. In the process, we found that standard convergence guarantees for PG methods do not apply to some settings because of the assumption of bounded variance of the gradients is violated.

The aforementioned convergence issues are also caused by the problematic coupling between the algorithm’s updates and its sampling distribution since one directly impacts the other. As a potential solution, we showed
that off-policy sampling can sidestep these difficulties by ensuring we use a sampling distribution that is different than the one induced by the agent’s current policy. This supports the hypothesis that on-policy sampling can be problematic as observed in previous work [Schaul et al., 2019]. Nevertheless, importance sampling in RL is generally seen as problematic [van Hasselt et al., 2018] due to instabilities it introduces to the learning process. Moving from an imposed policy, using past trajectories, to a chosen sampling policy reduces the variance of the gradients for near-deterministic policies and can lead to much better behaviour. Such an observation might guide future developments in the field.

Finally, we would like to open the discussion on the meaning of exploration for policy gradient methods. Exploration is often defined as a way to reduce sample complexity. When defined in a prescriptive manner, however, it is often linked to properties of the current policy, for instance its stochasticity, and encouraged as such, for instance by using $\epsilon$-greedy. We believe the observations made in this work should instead make us think of exploration as a property of the learning dynamics. For instance, one could view it as a mechanism to ensure iterates will converge to similar solutions regardless of the trajectories sampled, thus countering the committal effect of negative baselines where trajectories are unlikely to intersect. While encouraging the policies to have high entropy, as done by entropy regularization, might be a way, we believe blindly enforced stochasticity is not the only, nor the best, way to yield efficient policy gradient methods.

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Appendix

A Other experiments

A.1 3-armed bandits with natural policy gradient

We start by repeating the experiment in Section 2 with natural policy gradient instead of the vanilla policy gradient to emphasize that, although the theoretical results differ in both settings, empirical results are similar.

![Figure 5](image)

Figure 5: We plot 15 different trajectories of natural policy gradient, when using various baselines, on a 3-arm bandit problem with rewards $(1, 0.7, 0)$. The black line is the trajectory when following the true gradient (which is unaffected by the baseline), the other colors represent time. Different values of $\epsilon$ denote different perturbations to the minimum-variance baseline. We see some cases of convergence to a suboptimal policy for both $\epsilon = -1$ and $\epsilon = 0$. This does not happen for the larger baseline ($\epsilon = 1$). On the other hand, converging trajectories for $\epsilon = -1$ move faster toward the optimum than when using larger baselines. Using the value function as a baseline again reliably leads to convergence.

A.2 Simple gridworld

As a simple MDP with more than one state, we experiment using a 5x5 gridworld with two goal states, the closer one giving a reward of 0.8 and the further one a reward of 1. We ran the vanilla policy gradient with a fixed stepsize and discount factor of $0.99$ multiple times for several baselines. Fig. 6 displays individual learning curves with the index of the episode on the x-axis, and the fraction of episodes where the agent reached the reward of 1 up to that point on the y-axis. To match the experiments for the four rooms domain in the main text, Fig. 7 shows returns and the entropy of the actions and state visitation distributions for multiple settings of the baseline. Once again, we see a difference between the smaller and larger baselines. In fact, the difference is more striking in this example since some learning curves get stuck at suboptimal policies. Overall, we see two main trends in this experiment: a) The larger the baseline, the more likely the agent converges to the optimal policy, and b) Agents with negative baselines converge faster, albeit sometimes to a suboptimal behaviour. We emphasize that a) is not universally true and large enough baselines will lead to an increase in variance and a decrease in performance.

A.3 Additional results on the 4 rooms environment

For the four-rooms gridworld discussed in the main text, we extend the experiments and provide additional details. The environment is a 10x10 gridworld consisting of 4 rooms as depicted on Fig. 2a with a discount factor $\gamma = 0.99$. The agent starts in the upper left room and two adjacent rooms contain a goal state of value 0.6 (discounted, $\approx 0.54$) or 0.3 (discounted, $\approx 0.27$). However, the best goal, with a value of 1 (discounted, $\approx 0.87$), lies in the furthest room, so that the agent must learn to cross the sub-optimal rooms and reach the furthest one. We again train our agent with vanilla policy gradient and consider different fixed baselines.
Figure 6: Learning curves for a 5x5 gridworld with two goal states where the further goal is optimal. Trajectories in red do not converge to an optimal policy.

Figure 7: We plot the returns, the entropy of the policy over the states visited in each trajectory, and the entropy of the state visitation distribution averaged over 100 runs for multiple baselines for the 5x5 gridworld. The shaded regions denote one standard error and are close to the mean curve. Similar to the four rooms, the policy entropy of lower baselines tends to decay faster than for larger baselines, and smaller baselines tend to get stuck on suboptimal policies, as indicated by the returns plot.

In Fig. 2 of the main text, we saw that lower baselines lead to the action entropy decreasing more quickly and possibly converging to worse solutions. We consider an alternative visualization. Figures 8b, 8c and 8d depict similar plots to the ones of Fig. 1. Each point in the simplex is a policy, and the position is an estimate, computed with 1,000 Monte-Carlo samples, of the probability of the agent reaching each of the 3 goals. We observe that the starting point of the curve is equidistant to the 2 sub-optimal goals but further from the best goal, which is coherent with the geometry of the MDP. Because we have a discount factor of $\gamma = 0.99$, the agent first learns to reach the best goal in an adjacent room to the starting one, and only then it learns to reach the globally optimal goal fast enough for its reward to be the best one. All the returns therefore have values between 0 and $\gamma^{14} \approx 0.87$, as it takes 14 steps to reach the optimal goal.

In these plots, we can see differences between $b = -1$ and $b = 1$. For the lower baseline, we see that trajectories are much more noisy, with some curves going closer to the bottom-right corner, corresponding to the worst goal. This may suggest that the policies exhibit committal behaviour by moving further towards bad policies. On the other hand, for $b = 1$, every trajectory seems to reliably move towards the top corner before converging to the bottom-left, an optimal policy.

**B Two-armed bandit theory**

In this section, we expand on the results for the two-armed bandit. First, we show that there is some probability of converging to the wrong policy when using natural policy gradient with a constant baseline. Next, we consider all cases of the perturbed minimum-variance baseline ($b = b^* + \epsilon$) and show that some cases lead to convergence to the optimal policy with probability 1 while others do not. In particular there is a difference between $\epsilon < -1$ and $\epsilon > 1$, even though these settings can result in the same variance of the gradient estimates. Additionally, we prove that the vanilla policy gradient results in convergence in
Figure 8: We plot 10 different trajectories of policy gradient using different baselines on a 4 rooms MDP with goal rewards \((1, 0.6, 0.3)\). The color of each trajectory represents time and each point of the simplex represents the probability that a policy reaches one of the 3 goals.

contrast to the natural policy gradient. Finally, we show that using importance sampling with natural policy gradient also leads to convergence to the optimal policy with as long as the behaviour policy does not become deterministic too quickly.

Notations:
- Our objective is \(J(\theta) = \mathbb{E}_{\pi_{\theta}}[R(\tau)]\), the expected reward for current parameter \(\theta\).
- \(p_t = \sigma(\theta_t)\) is the probability of sampling the optimal arm (arm 1).
- \(P_1\) is the distribution over rewards than can be obtained from pulling arm 1. Its expected value is \(\mu_1 = \mathbb{E}[r_1 \sim P_1][r_1]\). Respectively \(P_0, \mu_0\) for the suboptimal arm.
- \(g_t\) is a stochastic unbiased estimate of \(\nabla_\theta J(\theta_t)\). It will take different forms depending on whether we use vanilla or natural policy gradient and whether we use importance sampling or not.
- For \(\{\alpha_t\}_t\) the sequence of stepsizes, the current parameter \(\theta_t\) is a random variable equal to \(\theta_t = \sum_{i=1}^t \alpha_i g_i + \theta_0\) where \(\theta_0\) is the initial parameter value.
- We call non-singular importance sampling any importance sampling distribution so that the probability of each action is bounded below by a strictly positive constant.

For many convergence proofs, we will use the fact that the sequence \(\theta_t - \mathbb{E}[\theta_t]\) forms a martingale. In other words, the noise around the expected value is a martingale, which we define below.

**Definition 1** (Martingale). A discrete-time martingale is a stochastic process \(\{X_t\}_{t \in \mathbb{N}}\) such that

- \(\mathbb{E}[|X_t|] < +\infty\)
- \(\mathbb{E}[X_{t+1} | X_t, \ldots, X_0] = X_t\)

**Example 1.** For \(g_t\) a stochastic estimate of \(\nabla \theta J(\theta_t)\) we have \(X_t = \mathbb{E}[\theta_t] - \theta_t\) is a martingale. As \(\theta_t = \theta_0 + \sum_i \alpha_i g_i\), \(X_t\) can also be rewritten as \(X_t = \mathbb{E}[\theta_t - \theta_0] = (\theta_t - \theta_0) + \sum_{i=0}^t \alpha_i (\mathbb{E}[g_i | \theta_0] - g_i)\).

We will also be making use of Azuma-Hoeffding’s inequality to show that the iterates stay within a certain region with high-probability, leading to convergence to the optimal policy.

**Lemma 1** (Azuma-Hoeffding’s inequality). For \(\{X_t\}\) a martingale, if \(|X_t - X_{t-1}| \leq c_t\) almost surely, then we have \(\forall t, \epsilon \geq 0\)

\[
P(X_t - X_0 \geq \epsilon) \leq \exp\left(-\frac{\epsilon^2}{2 \sum_{i=1}^t c_i^2}\right)
\]
B.1 Convergence with a constant baseline

For the proofs in this subsection, we assume that the step size is constant i.e. $\alpha_t = \alpha$ for all $t$.

**Proposition 1.** Consider a two-armed bandit with rewards 1 and 0 for the optimal and suboptimal arms, respectively. Suppose we use natural policy gradient starting from $\theta_0$, with a fixed baseline $b < 0$, and fixed stepsize $\alpha > 0$. If the policy samples the optimal action with probability $\sigma(\theta)$, then the probability of picking the suboptimal action forever and having $\theta_t$ go to $-\infty$ is strictly positive. Additionally, if $\theta_0 \leq 0$, we have

$$P(\text{suboptimal action forever}) \geq (1 - e^{\theta_0})(1 - e^{\theta_0 + \alpha b})^{-\frac{1}{\alpha}}$$

**Proof.** First, we deal with the case where $\theta_0 < 0$.

Next, we use the bound $1 - x \geq \exp(\frac{-x}{2})$. This bound can be derived as follows:

$$1 - u \leq e^{-u}$$
$$1 - e^{-u} \leq u$$
$$1 - \frac{1}{y} \leq \log y, \quad \text{substitute } u = \log y \text{ for } y > 0$$
$$\frac{-x}{1 - x} \leq \log(1 - x), \quad \text{substitute } y = 1 - x \text{ for } x \in [0, 1)$$

$$\exp\left(\frac{-x}{1 - x}\right) \leq 1 - x.$$

Continuing with $x = \exp(\theta_0 - \alpha bt)$, the bound holds when $x \in [0, 1)$, which is satisfied assuming $\theta_0 \leq 0$.

$$1 - \sigma(\theta_0 - \alpha bt) \geq \exp\left(\frac{-1}{e^{-\theta_0 + \alpha bt} - 1}\right)$$

For now we ignore $t = 0$ and we will just multiply it back in at the end.

$$\prod_{t=1}^{\infty}[1 - \sigma(\theta_0 - \alpha bt)] \geq \prod_{t=1}^{\infty}\exp\left(\frac{-1}{e^{-\theta_0 + \alpha bt} - 1}\right)$$
$$= \exp\left(\sum_{t=1}^{\infty}\frac{-1}{e^{-\theta_0 + \alpha bt} - 1}\right)$$
$$\geq \exp\left(-\int_{t=1}^{\infty}\frac{1}{e^{-\theta_0 + \alpha bt} - 1}dt\right)$$

The last line follows by considering the integrand as the right endpoints of rectangles approximating the area above the curve.

Solving this integral by substituting $y = -\theta_0 + \alpha bt$, multiplying the numerator and denominator by $e^y$ and substituting $u = e^y$, we get:

$$= \exp\left(\frac{1}{\alpha b} \log(1 - e^{\theta_0 - \alpha b})\right)$$
$$= (1 - e^{\theta_0 - \alpha b})^{\frac{1}{\alpha}}$$

Finally we have:

$$P(\text{left forever}) \geq (1 - e^{\theta_0})(1 - e^{\theta_0 - \alpha b})^{\frac{1}{\alpha}}$$
If $\theta_0 > 0$, then there is a positive probability of reaching $\theta < 0$ in a finite number of steps since choosing action 2 makes a step of size $ab$ in the left direction and we will reach $\theta_t < 0$ after $m = \frac{\theta_0}{0b}$ steps leftwards. The probability of making $m$ left steps in a row is positive. So, we can simply lower bound the probability of picking left forever by the product of that probability and the derived bound for $\theta_0 \leq 0$.

\[ \Pr(\text{left forever}) = T \times \Pr(\text{left forever}) \]

Corollary 1.1. The regret for the previously described two-armed bandit is linear.

Proof. Letting $R_t$ be the reward collected at time $t$,

\[
\text{Regret}(T) = \mathbb{E} \left[ \sum_{t=1}^{T} (1 - b - R_t) \right] \\
\geq \sum_{t=1}^{T} 1 \times \Pr(\text{left } T \text{ times}) \\
\geq \sum_{t=1}^{T} \Pr(\text{left forever}) \\
= T \times \Pr(\text{left forever}).
\]

The second line follows since choosing the left action at each step incurs a regret of 1 and this is one term in the entire expectation. The third line follows since choosing left $T$ times is a subset of the event of choosing left forever. The last line implies linear regret since we know $\Pr(\text{left forever}) > 0$ by the previous theorem.

B.2 Analysis of perturbed minimum-variance baseline

In this section, we look at perturbations of the minimum-variance baseline in the two-armed bandit, i.e. baselines of the form $b = 1 - p_t + \epsilon$. In summary:

- For $\epsilon < -1$, convergence to a suboptimal policy is possible with positive probability.
- For $\epsilon \in (-1, 1)$, we have convergence almost surely to the optimal policy.
- For $\epsilon \geq 1$, the supremum of the iterates goes to $\infty$ (but we do not have convergence to an optimal policy).

It is interesting to note that there is a subtle difference between the case of $\epsilon \in (-1, 0)$ and $\epsilon \in (0, 1)$, even though both lead to convergence. The main difference is that when $\theta_t$ is large, positive $\epsilon$ leads to both updates being positive and hence improvement is guaranteed at every step. But, when $\epsilon$ is negative, then only one of the actions leads to improvement, the other gives a large negative update. So, in some sense, for $\epsilon \in (-1, 0)$, convergence is less stable because a single bad update could be catastrophic.

Also, the case of $\epsilon = -1$ proved to be difficult. Empirically, we found that the agent would incur linear regret and it seemed like some learning curves also got stuck near $p = 0$, but we were unable to theoretically show convergence to a suboptimal policy.

Proposition 3. For the two-armed bandit with sigmoid parameterization, natural policy gradient and a perturbed minimum-variance baseline $b = 1 - p_t + \epsilon$, with $\epsilon < -1$, there is a positive probability of choosing the suboptimal arm forever and diverging.

Proof. We can reuse the result for the two-armed bandit with constant baseline $b < 0$. Recall that for the proof to work, we only need $\theta$ to move by at least a constant step $\delta > 0$ in the negative direction at every iteration.

In detail, the update after picking the worst arm is $\theta_{t+1} = \theta_t + \alpha (1 + \frac{\epsilon}{1 - p})$. So, if we choose $\epsilon < -1 - \delta$ for some $\delta > 0$, we get the update step magnitude is $\frac{\epsilon + \delta}{1 - p} > \delta$ and hence the previous result applies (replace $ab$ by $\delta$). \qed
Proposition 4. For the two-armed bandit with sigmoid parameterization, natural policy gradient and a perturbed minimum-variance baseline $b = 1 - p_t + \epsilon$, with $\epsilon \in (-1, 0)$, the policy converges to the optimal policy with probability 1.

Proof. Recall that the possible updates when the parameter is $\theta$ are:

- $\theta_{t+1} = \theta_t + \alpha (1 - \frac{\epsilon}{\sigma(\theta_t)})$ if we choose action 1, with probability $\sigma(\theta_t)$
- $\theta_{t+1} = \theta_t + \alpha (1 + \frac{\epsilon}{1 - \sigma(\theta_t)})$ if we choose action 2, with probability $1 - \sigma(\theta_t)$.

First, we will partition the real line into three regions ($A$, $B$, and $C$ with $a < b < c$ for $a \in A$, $b \in B$, $c \in C$), depending on the values of the updates. Then, each region will be analyzed separately.

We give an overview of the argument first. For region $A$ (very negative), both updates are positive so $\theta_t$ is guaranteed to increase until it reaches region $B$.

For region $C$ (very positive), sampling action 2 leads to the update $\alpha (1 + \frac{\epsilon}{1 - \sigma(\theta_t)})$, which has large magnitude and results in $\theta_{t+1}$ being back in region $A$. So, once $\theta_t$ is in $C$, the agent needs to sample action 1 forever to stay there and converge to the optimal policy. This will have positive probability (using the same argument as the divergence proof for the two-armed bandit with constant baseline).

For region $B$, the middle region, updates to $\theta_t$ can make it either increase or decrease and stay in $B$. For this region, we will show that $\theta_t$ will eventually leave $B$ with probability 1 in a finite number of steps, with some lower-bounded probability of reaching $A$.

Once we’ve established the behaviours in the three regions, we can argue that for any initial $\theta_0$ there is a positive probability that $\theta_t$ will eventually reach region $C$ and take action 1 forever to converge. In the event that does not occur, then $\theta_t$ will be sent back to $A$ and the agent gets another try at converging. Since we are looking at the behaviour when $t \rightarrow \infty$, the agent effectively gets infinite tries at converging. Since each attempt has some positive probability of succeeding, convergence will eventually happen.

We now give additional details for each region.

To define region $A$, we check when both updates will be positive. The update from action 1 is always positive so we are only concerned with the second update.

\[
\begin{align*}
1 + \frac{\epsilon}{1 - p} &> 0 \\
1 - p + \epsilon &> 0 \\
1 + \epsilon &> p \\
\sigma^{-1}(1 + \epsilon) &> \theta
\end{align*}
\]

Hence, we set $A = (-\infty, \sigma^{-1}(1 + \epsilon))$. Since every update in this region increases $\theta_t$ by at least a constant at every iteration, $\theta_t$ will leave $A$ in a finite number of steps.

For region $C$, we want to define it so that an update in the negative direction from any $\theta \in C$ will land back in $A$. So $C = [c, \infty)$ for some $c \geq \sigma^{-1}(1 + \epsilon)$. By looking at the update from action 2, $\alpha (1 + \frac{\epsilon}{1 - \sigma(\theta_t)}) = \alpha (1 + \epsilon (1 + e^\theta))$, we see that it is equal to 0 at $\theta = \sigma^{-1}(1 + \epsilon)$ but it is a decreasing function of $\theta$ and it decreases at an exponential rate. So, eventually for $\theta_t$ sufficiently large, adding this update will make $\theta_{t+1} \in A$.

So let $c = \inf \{ \theta : \theta + \alpha \left(1 - \frac{\epsilon}{1 - \sigma(\theta)} \right), \theta \geq \sigma^{-1}(1 + \epsilon) \}$. Note that it is possible that $c = \sigma^{-1}(1 + \epsilon)$. If this is the case, then region $B$ does not exist.

When $\theta_t \in C$, we know that there is a positive probability of choosing action 1 forever and thus converging (using the same proof as the two-armed bandit with constant baseline).

Finally, for the middle region $B = [a, c)$ ($a = \sigma^{-1}(1 + \epsilon)$), we know that the updates for any $\theta \in B$ are uniformly bounded in magnitude by a constant $u$.

We define a stopping time $\tau = \inf \{ t ; \theta_t \leq a \text{ or } \theta_t \geq c \}$. This gives the first time $\theta_t$ exits the region $B$. Let "∧" denote the min operator.

Since the updates are bounded, we can apply Azuma’s inequality to the stopped martingale $\theta_{t\wedge \tau} - \alpha(t \wedge \tau)$,
for $\lambda \in \mathbb{R}$.

\[
P(\theta_{t \wedge \tau} - \alpha (t \wedge \tau) < \lambda) \leq \exp\left(-\frac{\lambda^2}{2tu}\right)
\]

\[
P(\theta_{t \wedge \tau} - \alpha (t - (t \wedge \tau)) < \lambda) \leq \exp\left(-\frac{(c + \alpha t)^2}{2tu}\right)
\]

The second line follows from substituting $\lambda = -\alpha t + c$. Note that the RHS goes to 0 as $t$ goes to $\infty$.

Next, we continue from the LHS. Let $\theta_i^* = \sup_{0 \leq n \leq t} \theta_n$

\[
P(\theta_{t \wedge \tau} - \alpha (t - (t \wedge \tau)) < c) \\
\geq P(\theta_{t \wedge \tau} - \alpha (t - (t \wedge \tau)) < c, t \leq \tau) \\
\quad + P(\theta_{t \wedge \tau} - \alpha (t - (t \wedge \tau)) < c, t > \tau), \text{ splitting over events} \\
\geq P(\theta_{t \wedge \tau} < c, t < \tau), \text{ dropping the second term} \\
\geq P(\theta_t < c, \sup \theta_t < c, \inf \theta_t < c), \text{ definition of } \tau \\
= P(\sup \theta_t < c, \inf \theta_t < c), \text{ this event is a subset of the other} \\
= P(\tau > t)
\]

Hence the probability the stopping time exceeds $t$ goes to 0 and it is guaranteed to be finite almost surely.

Now, if $\theta_t$ exits $B$, there is some positive probability that it reached $C$. We see this by considering that taking action 1 increases $\theta$ by at least a constant, so the sequence of only taking action 1 until $\theta_t$ reaches $C$ has positive probability. This is a lower bound on the probability of eventually reaching $C$ given that $\theta_t$ is in $B$.

Finally, we combine the results for all three regions to show that convergence happens with probability 1. Without loss of generality, suppose $\theta_0 \in A$. If that is not the case, then keep running the process until either $\theta_t$ is in $A$ or convergence occurs.

Let $E_i$ be the event that $\theta_t$ returns to $A$ after leaving it for the $i$-th time. Then $E_i^C$ is the event that $\theta_t \rightarrow \infty$ (convergence occurs). This is the case because, when $\theta_t \in C$, those are the only two options and, when $\theta_t \in B$ we had shown that the process must exit $B$ with probability 1, either landing in $A$ or $C$.

Next, we note that $P(E_i^C) > 0$ since, when $\theta_t$ is in $B$, the process has positive probability of reaching $C$. Finally, when $\theta_t \in C$, the process has positive probability of converging. Hence, $P(E_i^C) > 0$.

To complete the argument, whenever $E_i$ occurs, then $\theta_t$ is back in $A$ and will eventually leave it almost surely. Since the process is Markov and memoryless, $E_{i+1}$ is independent of $E_i$. Thus, by considering a geometric distribution with a success being $E_i^C$ occurring, $E_i^C$ will eventually occur with probability 1. In other words, $\theta_t$ goes to $+\infty$.

\[\square\]

**Proposition 5.** For the two-armed bandit with sigmoid parameterization, natural policy gradient and a perturbed minimum-variance baseline $b = 1 - p_t + \epsilon$, with $\epsilon \in (-1, 0)$, the policy converges to the optimal policy with probability 1.

**Proof.** The overall idea is to ensure that the updates are always positive for some region $A = \{\theta : \theta > \theta_A\}$ then show that we reach this region with probability 1.

Recall that the possible updates when the parameter is $\theta_t$ are:

- $\theta_{t+1} = \theta_t + \alpha (1 - \frac{\epsilon}{\sigma(\theta_t)})$ if we choose action 1, with probability $\sigma(\theta_t)$
- $\theta_{t+1} = \theta_t + \alpha (1 + \frac{\epsilon}{1 - \sigma(\theta_t)})$ if we choose action 2, with probability $1 - \sigma(\theta_t)$.

First, we observe that the update for action 2 is always positive. As for action 1, it is positive whenever $p \geq \epsilon$, equivalently $\theta \geq \theta_A$, where $\theta_A = \sigma^{-1}(\epsilon)$. Call this region $A = \{\theta : \theta > \theta_A = \sigma^{-1}(\epsilon)\}$.

If $\theta_t \in A$, then we can find a $\delta > 0$ such that the update is always greater than $\delta$ in the positive direction, no matter which action is sampled. So, using the same argument as for the $\epsilon = 0$ case with steps of $+\delta$, we get convergence to the optimal policy (with only constant regret).
In the next part, we show that the iterates will enter the good region $A$ with probability 1 to complete the proof. We may assume that $\theta_0 < \theta_A$ since if that is not the case, we are already done. The overall idea is to create a transformed process which stops once it reaches $A$ and then show that the stopping time is finite with probability 1. This is done using the fact that the expected step is positive ($+\alpha$) along with Markov’s inequality to bound the probability of going too far in the negative direction.

We start by considering a process equal to $\theta_t$ except it stops when it lands in $A$. Defining the stopping time $\tau = \inf \{ t : \theta_t > \theta_A \}$ and “∧” by $a \wedge b = \min(a, b)$ for $a, b \in \mathbb{R}$, the process $\theta_{t, \tau}$ has the desired property.

Due to the stopping condition, $\theta_{t, \tau}$ will be bounded above and hence we can shift it in the negative direction to ensure that the values are all nonpositive. So we define $\tilde{\theta}_t = \theta_{t, \tau} - C$ for all $t$, for some $C$ to be determined.

Since we only stop the process $\{\theta_{t, \tau}\}$ after reaching $A$, then we need to compute the largest value $\theta_{t, \tau}$ can take after making an update which brings us inside the good region. In other words, we need to compute $\sup_t \{ \theta + \alpha (1 + \frac{\epsilon}{1 - \sigma(\theta)}) : \theta \in A \}$. Fortunately, since the function to maximize is an increasing function of $\theta$, the supremum is easily obtained by choosing the largest possible $\theta$, that is $\theta = \sigma^{-1}(\epsilon)$. This gives us that

$$C = \theta_A + U_A,$$

where $U_A = \alpha (1 + \frac{\epsilon}{1 - \sigma(\theta)})$.

All together, we have $\tilde{\theta}_t = \theta_{t, \tau} - \theta_A - U_A$. By construction, $\tilde{\theta}_t \leq 0$ for all $t$ (note that by assumption, $\theta_0 < \theta_A$ which is equivalent to $\tilde{\theta}_0 < -U_A$ so the process starts at a negative value).

Next, we separate the expected update from the process. We form the nonpositive process $Y_t = \tilde{\theta}_t - \alpha (t \wedge \tau) = \theta_{t, \tau} - U_A - \theta_A - \alpha (t \wedge \tau)$. This is a martingale as it is a stopped version of the martingale $\{\theta_t - U_A - \theta_A - \alpha t\}$.

Applying Markov’s inequality, for $\lambda > 0$ we have:

$$P(\lambda \leq Y_t) \leq -\frac{\mathbb{E}[Y_t]}{\lambda},$$

$$P(Y_t \leq -\lambda) \leq \frac{\mathbb{E}[Y_t]}{\lambda},$$

since $\{Y_t\}$ is a martingale

$$P(\theta_{t, \tau} - \alpha (t \wedge t) - \theta_A - U_A \leq -\lambda) \leq \frac{\theta_A + U_A - \theta_0}{\lambda} \quad \text{for all } 0 \leq n \leq t.$$ 

Note the RHS goes to 0 as $t \to \infty$. We then manipulate the LHS to eventually get an upper bound on $P(t \leq \tau)$.

$$P(\theta_{t, \tau} \leq \alpha (\tau \wedge t - t) + \theta_A)$$

$$= P(\theta_{t, \tau} \leq \alpha (\tau \wedge t - t) + \theta_A, t \leq \tau) + P(\theta_{t, \tau} \leq \alpha (\tau \wedge t - t) + \theta_A, t > \tau),$$

splitting over disjoint events

$$\geq P(\theta_{t, \tau} \leq \alpha (\tau \wedge t - t), t \leq \tau),$$

second term is nonnegative

$$= P(\theta_t \leq \theta_A, t \leq \tau),$$

since $t \leq \tau$ in this event

$$= P(\theta_t \leq \theta_A, \sup_{0 \leq n \leq t} \theta_n \leq \theta_A),$$

by definition of $\tau$

$$\geq P(\text{sup}_{0 \leq n \leq t} \theta_n \leq \theta_A),$$

this event is a subset of the other

$$= P(t \leq \tau).$$

Since the first line goes to 0, the last line goes to 0 and hence we have that $\theta_t$ will enter the good region with probability 1.

$\square$

Note that there is no contradiction with the nonconvergence result for $\epsilon < -1$ as we cannot use Markov’s inequality to show that the probability that $\theta_t < c (c > 0)$ goes to 0. The argument for the $\epsilon \in (0, 1)$ case relies on being able to shift the iterates $\theta_t$ sufficiently left to construct a nonpositive process $\tilde{\theta}_t$. In the case of $\epsilon < 0$, for $\theta < c (c \in \mathbb{R})$, the right update $(1 - \frac{\sigma(\theta)}{\epsilon})$ is unbounded hence we cannot guarantee the process will be nonpositive. As a sidenote, if we were to additionally clip the right update so that it is $\max(B, 1 - \frac{\sigma(\theta)}{\epsilon})$ for some $B > 0$ to avoid this problem, this would still not allow this approach to be used because then we would no longer have a submartingale. The expected update would be negative for $\theta$ sufficiently negative.
Proposition 6. For the two-armed bandit with sigmoid parameterization, natural policy gradient and a perturbed minimum-variance baseline $b = 1 - p_i + \epsilon$, with $\epsilon \geq 1$, we have that $P(\sup_{0 \leq t \leq \tau} \theta_t > C) \to 1$ as $t \to \infty$ for any $C \in \mathbb{R}$.

Proof. We follow the same argument as in the $\epsilon \in (0, 1)$ case with a stopping time defined as $\tau = \inf \{ t : \theta_t > c \}$ and using $\theta_A = c$, to show that

$$P \left( \sup_{0 \leq t \leq \tau} \theta_t \leq c \right) \to 0$$

B.3 Convergence with vanilla policy gradient

In this section, we show that using vanilla PG on the two-armed bandit converges to the optimal policy in probability. The idea to show optimality of policy gradient will be to use Azuma’s inequality to prove that $\theta_t$ will concentrate around their mean $E[\theta_t]$, which itself converges to the right arm.

We now proceed to prove the necessary requirements.

Lemma 2 (Bounded increments for vanilla PG). Assuming bounded rewards and a bounded baseline, the martingale $\{X_t\}$ associated with vanilla policy gradient has bounded increments

$$|X_t - X_{t-1}| \leq C\alpha_t$$

Proof. Then, the stochastic gradient estimate is

$$g_t = \begin{cases} (r_1 - b)(1 - p_t), & \text{with probability } p_t, r_1 \sim P_1 \\ -(r_0 - b)p_t, & \text{with probability } (1 - p_t), r_0 \sim P_0 \end{cases}$$

Furthermore, $E[g_t|\theta_t] = E[E[g_t|\theta_t]|\theta_0] = E[\Delta p_t(1 - p_t)|\theta_0]$. As the rewards are bounded, for $i = 0, 1$, $\exists R_i > 0$ so that $|r_i| \leq R_i$

$$|X_t - X_{t-1}| = \left| \sum_{i=1}^{t} \alpha_i (g_i - E[g_i]) - \sum_{i=1}^{t-1} \alpha_i (g_i - E[g_i]) \right|$$

$$\leq \alpha_t |\Delta p_t(1 - p_t)|$$

$$\leq \alpha_t (\max(|r_1 - b|, |r_0 - b|) + |E[\Delta p_t(1 - p_t)]|), \quad r_1 \sim P_1, r_0 \sim P_0$$

$$\leq \alpha_t \left( \max(|R_1| + |b|, |R_0| + |b|) + \frac{\Delta}{4} \right)$$

Thus $|X_t - X_{t-1}| \leq C\alpha_t$

Lemma 3 (Bounded increments with IS). Assuming bounded rewards and a bounded baseline, the martingale $\{X_t\}$ associated with policy gradient with importance sampling distribution $q$ such that $\min\{q, 1 - q\} \geq \epsilon > 0$ has bounded increments

$$|X_t - X_{t-1}| \leq C\alpha_t$$

Proof. Let us also call $\epsilon > 0$ the lowest probability of sampling an arm under $q$.

Then, the stochastic gradient estimate is

$$g_t = \begin{cases} (r_1 - b)p_t(1 - p_t), & \text{with probability } q_t, r_1 \sim P_1 \\ -(r_0 - b)p_t(1 - p_t), & \text{with probability } (1 - q_t), r_0 \sim P_0 \end{cases}$$
As the rewards are bounded, \( \exists R_t > 0 \) such that \( |r_i| \leq R_t \) for all \( i \)

\[
|X_t - X_{t-1}| = \left| \sum_{i=1}^{t} \alpha_i (g_i - E[g_i]) - \sum_{i=1}^{t-1} \alpha_i (g_i - E[g_i]) \right|
\]

\[
= \alpha_t |g_t - E[\Delta p_t(1-p_t)]| \leq \frac{\alpha_t (\max(|R_t| + |b|, |R_0| + |b|) + \Delta)}{4\epsilon}
\]
as \( q_t, 1 - q_t \geq \epsilon \)

Thus \( |X_t - X_{t-1}| \leq C \alpha_t \)

\[\square\]

Lemma 4. For vanilla policy gradient and policy gradient with non-singular importance sampling, the expected parameter \( \theta_t \) has infinite limit, i.e. if \( \mu_1 \neq \mu_0 \),

\[
\lim_{t \to +\infty} E[\theta_t - \theta_0] = +\infty
\]

In other words, the expected parameter value converges to the optimal arm.

Proof. We reason by contradiction. The contradiction stems from the fact that on one hand we know \( \theta_t \) will become arbitrarily large with \( t \) with high probability as this setting satisfies the convergence conditions of stochastic optimization. On the other hand, because of Azuma’s inequality, if the average \( \theta_t \) were finite, we can show that \( \theta_t \) cannot deviate arbitrarily far from its mean with probability 1. The contradiction will stem from the fact that the expected \( \theta_t \) cannot have a finite limit.

We have \( \theta_t - \theta_0 = \sum_{i=0}^{t} \alpha_i g_i \). Thus

\[
E[\theta_t - \theta_0] = E[\sum_{i=0}^{t} \alpha_i g_i | \theta_0]
\]

\[
= \sum_{i=0}^{t} \alpha_i E[g_i | \theta_0]
\]

\[
= \sum_{i=0}^{t} \alpha_i E[E[g_i | \theta_i] | \theta_0] \text{ using the law of total expectations}
\]

\[
= \sum_{i=0}^{t} \alpha_i E[\Delta p_i (1-p_i) | \theta_0]
\]

where \( \Delta = \mu_1 - \mu_0 > 0 \) the optimality gap between the value of the arms. As it is a sum of positive terms, its limit is either positive and finite or \(+\infty\).

1. Let us assume that \( \lim_{t \to +\infty} E[\sum_{i=0}^{t} \alpha_i g_i] = \beta > 0 \).

As \( \sum_{i=0}^{\infty} \alpha_i^2 = \gamma \), using Azuma-Hoeffing’s inequality

\[
\mathbb{P}(\theta_t \geq M) = \mathbb{P}(\theta_t - \theta_0 - E[\sum_{i=0}^{t} \alpha_i g_i] \geq M - E[\sum_{i=0}^{t} \alpha_i g_i] - \theta_0)
\]

\[
\leq \exp \left( - \frac{(M - E[\sum_{i=0}^{t} \alpha_i g_i] - \theta_0)^2}{2 \sum_{i=1}^{t} c_i^2} \right)
\]

where \( c_i = \alpha_i C \) like in the proposition above. And for \( M > |\theta_0| + \beta + 2C\sqrt{\gamma \log 2} \) we have

\[
\lim_{t \to +\infty} M - E[\sum_{i=0}^{t} \alpha_i g_i] - \theta_0 \geq |\theta_0| + \beta + 2C\sqrt{\gamma \log 2} - \beta - \theta_0
\]

\[
\geq 2C\sqrt{\gamma \log 2}
\]
As \(\sum_{i=0}^{\infty} c_i = \gamma C^2\), we have

\[
\lim_{t \to +\infty} \frac{(M - E[\sum_{i=0}^{t} \alpha_i g_i] - \theta_0)^2}{2\sum_{i=1}^{t} c_i^2} = \frac{4C^2\gamma \log 2}{2\gamma C^2} \geq 2\log 2 = \log 4
\]

Therefore

\[
\lim_{t \to +\infty} P(\theta_t \geq M) \leq \frac{1}{4}
\]

By a similar reasoning, we can show that

\[
\lim_{t \to +\infty} P(\theta_t \leq -M) \leq \frac{1}{4}
\]

Thus

\[
\lim_{t \to +\infty} P(|\theta_t| \leq M) \geq \frac{1}{2}
\]

i.e for any \(M\) large enough, the probability that \(\{\theta_t\}\) is bounded by \(M\) is bigger than a strictly positive constant.

2. Because policy gradient with diminishing stepsizes satisfies the convergence conditions defined by Bottou et al. [2018], we have that

\[
\forall \epsilon > 0, P(\|\nabla J(\theta_t)\| \geq \epsilon) \leq \frac{E[\|\nabla J(\theta_t)\|^2]}{\epsilon^2} \quad \text{as} \quad t \to \infty 
\]

(see proof of Corollary 4.11 by Bottou et al. [2018]). We also have \(\|\nabla J(\theta_t)\| = \|\Delta \sigma(\theta_t)(1 - \sigma(\theta_t))\| = \Delta \sigma(\theta_t)(1 - \sigma(\theta_t))\) for \(\Delta = \mu_1 - \mu_0 > 0\) for \(\mu_1\) (resp. \(\mu_0\)) the expected value of the optimal (res. suboptimal arm). Furthermore, \(f: \theta_t \mapsto \Delta \sigma(\theta_t)(1 - \sigma(\theta_t))\) is symmetric, monotonically decreasing on \(\mathbb{R}^+\) and takes values in \([0, \Delta/4]\). Let’s call \(f^{-1}\) its inverse on \(\mathbb{R}^+\).

We have that

\[
\forall \epsilon \in [0, \Delta/4], \quad \Delta \sigma(\theta)(1 - \sigma(\theta)) \geq \epsilon \iff |\theta| \leq f^{-1}(\epsilon)
\]

Thus \(\forall M > 0,\)

\[
P(|\theta_t| \leq M) = P(\|\nabla J(\theta_t)\| \geq f(M)) \leq \frac{E[\|\nabla J(\theta_t)\|^2]}{(\Delta \sigma(M)(1 - \sigma(M)))^2} \quad \text{as} \quad t \to \infty 
\]

Here we show that \(\theta_t\) cannot be bounded by any constant with non-zero probability at \(t \to \infty\). This contradicts the previous conclusion.

Therefore \(\lim_{t \to +\infty} E[\theta_t - \theta_0] = +\infty\)

\[\Box\]

**Proposition 7** (Optimality of stochastic policy gradient on the 2-arm bandit). **Policy gradient with stepsizes satisfying the Robbins-Monro conditions (\(\sum \alpha_t = \infty, \sum \alpha_t^2 < \infty\)) converges to the optimal arm.**

Note that this convergence result addresses the stochastic version of policy gradient, which is not covered by standard results for stochastic gradient algorithms due to the nonconvexity of the objective.

**Proof.** We prove the statement using Azuma’s inequality again. We can choose \(\epsilon = (1 - \beta)E[\sum_{i=0}^{t} \alpha_i g_i] \geq 0\) for \(\beta \in [0, 1]\).
\[ P\bigg(\theta_t > \theta_0 + \beta \mathbb{E}\left[ \sum_{i=0}^{t} \alpha_i g_i \right] \bigg) = P\bigg(\theta_t - \mathbb{E}\left[ \sum_{i=0}^{t} \alpha_i g_i \right] - \theta_0 > \beta \mathbb{E}\left[ \sum_{i=0}^{t} \alpha_i g_i \right] - \mathbb{E}\left[ \sum_{i=0}^{t} \alpha_i g_i \right] \bigg) \]
\[ = 1 - P\left(\theta_t - \theta_0 - \mathbb{E}\left[ \sum_{i=0}^{t} \alpha_i g_i \right] \leq -\epsilon \right) \]
\[ = 1 - P\left(\theta_0 + \mathbb{E}\left[ \sum_{i=0}^{t} \alpha_i g_i \right] - \theta_t \geq \epsilon \right) \]
\[ \geq 1 - \exp\left(-\frac{(1 - \beta)^2}{2} \mathbb{E}[\sum_{i=0}^{t} \alpha_i g_i]^2 \right) \]

Thus \( \lim_{t \to \infty} P\left(\theta_t > \theta_0 + \beta \mathbb{E}[\sum_{i=0}^{t} \alpha_i g_i] \right) = 1 \), as \( \lim_{t \to \infty} \mathbb{E}[\sum_{i=0}^{t} \alpha_i g_i] = +\infty \) and \( \sum_{i=0}^{\infty} \alpha_i^2 < +\infty \). Therefore \( \lim_{t \to \infty} \theta_t = +\infty \) almost surely.

C Three-armed bandit theory

**Theorem 1.** There exists an MDP where using the stochastic natural gradient, on a softmax-parameterized policy, with the minimum-variance baseline, can lead to convergence to a suboptimal policy with probability \( \rho > 0 \); but there is a different baseline (with larger variance) which results in convergence to the optimal policy with probability 1.

**Proof.** The example of convergence to a suboptimal policy for the minimum-variance baseline and convergence to the optimal policy for a gap baseline are outlined in the next two subsections.

C.1 Convergence issues with the minimum-variance baseline

**Proposition 8.** Consider a three-armed bandit with rewards of 1, 0.7 and 0. Let the policy be parameterized by a softmax (\( \pi_i \propto e^{x_i} \)) and optimized using natural policy gradient paired with the minimum-variance baseline. If the policy is initialized to be uniform random, there is a nonzero probability of choosing a suboptimal action forever and converging to a suboptimal policy.

**Proof.** The policy probabilities are given by \( \pi_i = \frac{e^{x_i}}{\sum_{j=1}^{3} e^{x_j}} \) for \( i = 1, 2, 3 \). Note that this parameterization is invariant to shifting all \( \theta_i \) by a constant.

The gradient for sampling arm \( i \) is given by \( g_i = e_i - \pi \), where \( e_i \) is the vector of zeros except for a 1 in entry \( i \). The Fisher information matrix can be computed to be \( F = \text{diag}(\pi) - \pi \pi^T \).

Since \( F \) is not invertible, then we can instead find the solutions to \( Fx = g_i \) to obtain our updates. Solving this system gives us \( x = \lambda e + \frac{1}{\lambda} e_i \), where \( e \) is a vector of ones and \( \lambda \in \mathbb{R} \) is a free parameter.

Next, we compute the minimum-variance baseline. Here, we have two main options. We can find the baseline that minimizes the variance of the sampled gradients \( g_i \), the “standard” choice, or we can instead minimize the variance of the sampled natural gradients, \( F^{-1}g_i \). We analyze both cases separately.

The minimum-variance baseline for gradients is given by \( b^* = \frac{\mathbb{E}[R(x)]}{\mathbb{E}[\nabla \log \pi(x) ||^2]}. \) In this case, \( \nabla \log \pi_i = e_i - \pi \), where \( e_i \) is the \( i \)-th standard basis vector and \( \pi \) is a vector of policy probabilities. Then, \( ||\nabla \log \pi_i|| = (1 - \pi_i)^2 + \pi_j^2 + \pi_k^2 \), where \( \pi_j \) and \( \pi_k \) are the probabilities for the other two arms. This gives us

\[ b^* = \frac{\sum_{i=1}^{3} r_i w_i}{\sum_{i=1}^{3} w_i} \]

where \( w_i = ((1 - \pi_i)^2 + \pi_j^2 + \pi_k^2) \pi_i. \)
The proof idea is similar to that of the two-armed bandit. Recall that the rewards for the three actions are 1, 0.7 and 0. We will show that this it is possible to choose action 2 (which is suboptimal) forever.

To do so, it is enough to show that we make updates that increase \( \theta_2 \) by at least \( \delta \) at every step (and leave \( \theta_1 \) and \( \theta_3 \) the same). In this way, the probability of choosing action 2 increases sufficiently fast, that we can use the proof for the two-armed bandit to show that the probability of choosing action 2 forever is nonzero.

In more detail, suppose that we have established that, at each step, \( \theta_2 \) increases by at least \( \delta \). The policy starts as the uniform distribution so we can choose any initial \( \theta \) as long as three components are the same (\( \theta_1 = \theta_2 = \theta_3 \)). Choosing the initialization \( \theta_i = -\log(1/2) \) for all \( i \), we see that \( \pi_2 = \frac{\theta_2}{1 + e^{\theta_2}} = \sigma(\theta_2) \) where \( \sigma(\cdot) \) is the sigmoid function. Since at the \( n \)-th step, \( \theta_2 > \theta_0 + n\delta \), we can reuse the proof for the two-armed bandit to show \( Pr(\text{action 2 forever} > 0) \).

To complete the proof, we need to show that the updates are indeed lower bounded by a constant. Every time we sample action 2, the update is \( \theta \leftarrow \theta + \alpha(r_2 - b^*)(\lambda e + \frac{1}{\pi} e_2) \). We can choose any value of \( \lambda \) since they produce the same policy after an update due to the policy’s invariance to a constant shift of all the parameters. We thus choose \( \lambda = 0 \) for simplicity. In summary, an update does \( \theta_2 \leftarrow \theta_2 + \alpha(r_2 - b^*) \frac{1}{\pi^2} \) and leaves the other parameters unchanged.

In the next part, we use induction to show the updates are lower bounded at every step. For the base case, we need \( r_2 - b^* > \delta \) for some \( \delta > 0 \). Since we initialize the policy to be uniform, we can directly compute the value of \( b^* \approx 0.57 \), so the condition is satisfied for, say, \( \delta = 0.1 \).

For the inductive case, we assume that \( r_2 - b^* > \delta \) for \( \delta > 0 \) and we will show that \( r_2 - b^*_+ > \delta \) also, where \( b^*_+ \) is the baseline after an update. It suffices to show that \( b^*_+ \leq b^* \).

To do so, we examine the ratio \( \frac{w_2}{w_1} \) in \( b^* \) and show that this decreases. Let \( \left( \frac{w_2}{w_1} \right)_+ \) be the ratio after an update and let \( c = r_2 - b^* \).

\[
\left( \frac{w_2}{w_1} \right) = \frac{2(\pi_2^2 + \pi_3^2 + \pi_1 \pi_3) \pi_2}{2(\pi_1^2 + \pi_2^2 + \pi_3) \pi_1} \approx \frac{(e^{2\theta_1} + e^{2\theta_3} + e^{\theta_1 + \theta_3}) e^{\theta_2}}{(e^{2\theta_2} + e^{2\theta_3} + e^{\theta_2 + \theta_3}) e^{\theta_1}}
\]

\[
\left( \frac{w_2}{w_1} \right)_+ = \frac{(e^{2\theta_1} + e^{2\theta_3} + e^{\theta_1 + \theta_3}) e^{\theta_2 + \frac{c}{\pi_2}}}{(e^{2\theta_2} + e^{2\theta_3} + e^{\theta_2 + \theta_3}) e^{\theta_1}}
\]

We compare the ratio of these:

\[
\left( \frac{w_2}{w_1} \right)_+ = \frac{e^{\theta_2 + \frac{c}{\pi_2}}}{e^{\theta_2} e^{2\theta_2 + \frac{c}{\pi_2}} + e^{2\theta_3} + e^{\theta_2 + \theta_3 + \frac{c}{\pi_2}}} = \frac{e^{2\theta_2} + e^{2\theta_3} + e^{\theta_2 + \theta_3}}{e^{2\theta_2} + e^{2\theta_3} + e^{\theta_2 + \theta_3}} \approx \frac{e^{2\theta_2} + e^{2\theta_3} + e^{\theta_2 + \theta_3}}{e^{2\theta_2} + e^{2\theta_3} + e^{\theta_2 + \theta_3}} < \frac{e^{2\theta_2} + e^{2\theta_3} + e^{\theta_2 + \theta_3}}{e^{2\theta_2} + e^{2\theta_3} + e^{\theta_2 + \theta_3}}
\]

The last line follows by considering the function \( f(z) = e^{x-y} + e^{y-z} \) for a fixed \( x \leq y \). \( f'(z) = -e^{x-z} + e^{y+z} > 0 \) for all \( z \), so \( f(z) \) is an increasing function. By taking \( x = 2\theta_2 \) and \( y = 2\theta_3 \) (\( \theta_2 \geq \theta_3 \)), along with the fact that \( \frac{c}{\pi_2} > \delta \) (considering these as \( z \) values), then we see that the denominator has increased in the last line and the inequality holds.

By the same argument, recalling that \( \delta > 0 \), we have that the last ratio is less than 1. Hence, \( \left( \frac{w_2}{w_1} \right)_+ < \left( \frac{w_2}{w_1} \right) \).

Returning to the baseline, \( b^* = \frac{w_1 r_1 + w_2 r_2 + w_3 r_3}{w_1 + w_2 + w_3} \). We see that this is a convex combination of the rewards.
Focusing on the (normalized) weight of \( r_2 \):

\[
\frac{w_2}{w_1 + w_2 + w_3} = \frac{w_2}{2w_1 + w_2} = \frac{w_2/\pi_1}{2 + w_2/\pi_1}
\]

The first line follows since \( w_1 = w_3 \) and the second by dividing the numerator and denominator by \( w_1 \). This is an increasing function of \( w_2/\pi_1 \) so decreasing the ratio will decrease the normalized weight given to \( r_2 \). This, in turn, increases the weight on the other two rewards equally. As such, since the value of the baseline is under \( r_2 = 0.7 \) (recall it started at \( b^* \approx 0.57 \)) and the average of \( r_1 \) and \( r_3 \) is 0.5, the baseline must decrease towards 0.5.

Thus, we have shown that the gap between \( r_2 \) and \( b^* \) remains at least \( \delta \) and this completes the proof for the minimum-variance baseline of the gradients.

Next, we tackle the minimum-variance baseline for the updates. Recall that the natural gradient updates are of the form \( x_i = \lambda e + \frac{1}{\pi} \epsilon_i \) for action \( i \) where \( e \) is a vector of ones and \( \epsilon_i \) is the \( i \)-th standard basis vector.

The minimum-variance baseline for updates is given by

\[
b^* = \frac{E[R_i ||x_i||^2]}{E[||x_i||^2]}
\]

We have that

\[
||x_i||^2 = 2\lambda^2 = (\lambda + \frac{1}{\pi})^2.
\]

At this point, we have to choose which value of \( \lambda \) to use since it will affect the baseline. The minimum-norm solution is a common choice (corresponding to use of the Moore-Penrose pseudoinverse of the Fisher information instead of the inverse). We also take a look at fixed values of \( \lambda \), but we find that this requires an additional assumption \( 3\lambda^2 < 1/\pi_i^2 \).

First, we consider the minimum-norm solution. We find that the minimum-norm solution gives \( \frac{2}{3\pi_i} \) for \( \lambda = \frac{-1}{3\pi_i} \).

We will reuse exactly the same argument as for the minimum-variance baseline for the gradients. The only difference is the formula for the baseline, so all we need to check is that the ratio of the weights of the rewards decreases after one update, which implies that the baseline decreases after an update.

The baseline can be written as:

\[
b^* = \frac{\sum_{i=1}^{3} \pi_i r_i \frac{2}{3\pi_i}}{\sum_{i=1}^{3} \frac{2}{3\pi_i}} = \frac{\sum_{i=1}^{3} \pi_i r_i \frac{1}{\pi_i}}{\sum_{i=1}^{3} \frac{1}{\pi_i}}
\]

So we have the weights \( w_i = \frac{1}{\pi_i} \) and the ratio is

\[
\left( \frac{w_2}{w_1} \right) = \frac{\pi_1}{\pi_2} = e^{\theta_1 - \theta_2}
\]

So, after an update, we get

\[
\left( \frac{w_2}{w_1} \right) = e^{\theta_1 - \theta_2 - \frac{c}{\pi_i}}
\]

for \( c = \alpha(r_2 - b^*) \), which is less than the initial ratio. This completes the case where we use the minimum-norm update.

Finally, we deal with the case where \( \lambda \in \mathbb{R} \) is a fixed constant. We don’t expect this case to be very important as the minimum-norm solution is almost always chosen (the previous case). Again, we only need to check the ratio of the weights.
The weights are given by \( w_i = (2\lambda^2 + (\lambda + \frac{1}{\pi_i})^2)\pi_i \)

\[
\begin{align*}
\left( \frac{w_2}{w_1} \right) &= \frac{(2\lambda^2 + (\lambda + \frac{1}{\pi_i})^2)\pi_2}{(2\lambda^2 + (\lambda + \frac{1}{\pi_i})^2)\pi_1} \\
&= \frac{2\lambda^2\pi_2 + (\lambda + \frac{1}{\pi_i})^2\pi_2}{2\lambda^2\pi_1 + (\lambda + \frac{1}{\pi_i})^2\pi_1}
\end{align*}
\]

We know that after an update \( \pi_2 \) will increase and \( \pi_1 \) will decrease. So, we check the partial derivative of the ratio to assess its behaviour after an update.

\[
d\frac{d}{d\pi_1} \left( \frac{w_2}{w_1} \right) = -\frac{2\lambda^2\pi_2 + (\lambda + \frac{1}{\pi_i})^2\pi_2}{(2\lambda^2\pi_1 + (\lambda + \frac{1}{\pi_i})^2\pi_1)} (3\lambda^2 - \frac{1}{\pi_i^2})
\]

We need this to be an increasing function in \( \pi_1 \) so that a decrease in \( \pi_1 \) implies a decrease in the ratio. This is true when \( 3\lambda^2 < \frac{1}{\pi_1^2} \). So, to ensure the ratio decreases after a step, we need an additional assumption on \( \lambda \) and \( \pi_1 \), which is that \( 3\lambda^2 < \frac{1}{\pi_1^2} \). This is notably always satisfied for \( \lambda = 0 \).

\[\square\]

C.2 Convergence with gap baselines

**Proposition 9.** For a three-arm bandit with deterministic rewards, choosing the baseline \( b \) so that \( r_1 > b > r_2 \) where \( r_1 \) (resp. \( r_2 \)) is the value of the optimal (resp. second best) arm, natural policy gradient converges to the best arm almost surely.

**Proof.** Let us define \( \Delta_i = r_i - b \) which is strictly positive for \( i = 1 \), strictly negative otherwise. Then the gradient on the parameter \( \theta^i \) of arm \( i \)

\[
g^i_t = 1_{\{A_t = i\}} \frac{\Delta_i}{\pi_t(i)}, \quad i \sim \pi_t(\cdot)
\]

Its expectation is therefore

\[
E[\theta^i_t] = \alpha t \Delta_i + \theta^i_0
\]

Also note that there is a nonzero probability of sampling each arm at \( t = 0 \): \( \theta_0 \in \mathbb{R}^3, \pi_0(i) > 0 \). Furthermore, \( \pi_i(1) \geq \pi_0(1) \) as \( \theta_1 \) is increasing and \( \theta_i, i > 1 \) decreasing because of the choice of our baseline. Indeed, the updates for arm 1 are always positive and negative for other arms.

For the martingale \( X_t = \alpha \Delta_1 t + \theta^1_0 - \theta^1_t \), we have

\[
|X_t - X_{t-1}| \leq \alpha \frac{\Delta_1}{\pi_0(1)}
\]

thus satisfying the bounded increments assumption of Azuma’s inequality. We can therefore show

\[
\begin{align*}
P(\theta^i_t > \frac{\alpha \Delta_1}{2} t + \theta^i_0) &= P(\theta^i_t - \alpha \Delta_1 t - \theta^i_0 > -\frac{\alpha \Delta_1}{2} t) \\
&= P(X_t < \frac{\alpha \Delta_1}{2} t) \\
&= 1 - P(X_t \geq \frac{\alpha \Delta_1}{2} t) \\
&\geq 1 - \exp \left( -\frac{(\frac{\alpha \Delta_1}{2} t)^2 \pi_0(1)^2}{2t \alpha^2 \Delta_1^2} \right) \\
&\geq 1 - \exp \left( -\frac{\pi_0(1)^2}{8} t \right)
\end{align*}
\]
This shows that $\theta_i^t$ converges to $+\infty$ almost surely while the $\theta_i^t, i > 1$ remain bounded by $\theta_0^t$, hence we converge to the optimal policy almost surely.

\[\square\]

### C.3 Convergence with off-policy sampling

For natural policy gradient, the stochastic estimator of the gradient is

\[g_t = \begin{cases} \frac{(r_{1,b} - b)}{p_t}, & \text{with probability } p_t, r_1 \sim P_1 \\ -\frac{(r_0 - b)}{1-p_t}, & \text{with probability } (1-p_t), r_0 \sim P_0 \end{cases}\]

We therefore have $E[g_t] = E[r_1 - r_0] = \mu_1 - \mu_0 = \Delta$.

We define the martingale $X_t = \theta_t - \theta_0 - \alpha \Delta t$ which is valid as $E[g_t] = \Delta$.

**Lemma 5** (Bounded increments). Assuming bounded rewards and a bounded baseline, the martingale $\{X_t\}$ associated with natural policy gradient has bounded increments

\[|X_t - X_{t-1}| \leq \frac{C\alpha}{\epsilon_t}\]

**Proof.** Let us call $P_1$ the distribution over rewards of the optimal arm, and $P_0$ the distribution over rewards of the suboptimal arm. Then, the stochastic gradient estimate is

\[g_t = \begin{cases} \frac{(r_{1,b} - b)}{q_t}, & \text{with probability } q_t, r_1 \sim P_1 \\ -\frac{(r_0 - b)}{1-q_t}, & \text{with probability } (1-q_t), r_0 \sim P_0 \end{cases}\]

Furthermore $E[g_t|\theta_0] = E[E[g_t|\theta_t]|\theta_0] = \Delta$. As the rewards are bounded, for $i = 0, 1, \exists R_i > 0$ so that $|r_i| \leq R_i$

\[|X_t - X_{t-1}| = \left| \sum_{i=1}^{t} \alpha_i (g_i - E[g_i]) - \sum_{i=1}^{t-1} \alpha_i (g_i - E[g_i]) \right| = \alpha |g_t - \Delta| \leq \alpha (|g_t| + \Delta) \leq \frac{\alpha \max(|r_1 - b|, |r_0 - b|)}{\epsilon_t} + \Delta, \quad r_1 \sim P_1, r_0 \sim P_0 \leq \frac{\alpha \max(|R_1| + |b|, |R_0| + |b|) + \Delta}{\epsilon_t} \quad \text{as } \epsilon_t \leq 1\]

Thus $|X_t - X_{t-1}| \leq \frac{C\alpha}{\epsilon_t}$.

\[\square\]

**Proposition 2.** Let us consider a two-armed bandit with stochastic rewards with bounded support. We define $q_t$ to be the behavior policy, where $q_t$ is the probability of sampling the optimal arm at time $t$. Then, for $\epsilon_t = \min\{q_t, 1-q_t\}$, and for any finite baseline, if $\lim_{t \to \infty} \epsilon_t^2 = +\infty$, then the target policy $p_t$ converges to the optimal policy almost surely when using natural policy gradient.

**Proof.** We prove the statement using Azuma’s inequality again. $\epsilon = \frac{\alpha \Delta}{2} t \geq 0$

\[P(\theta_t \geq \theta_0 + \frac{\alpha \Delta}{2} t) = P(\theta_t - \theta_0 - \alpha \Delta t \geq -\frac{\alpha \Delta}{2} t) \geq 1 - \exp\left(-\frac{(\frac{\alpha \Delta}{2} t)^2 \epsilon_t^2}{2t \alpha^2 \Delta^2 C^2}\right) \geq 1 - \exp\left(-\frac{t \epsilon_t^2}{8 C^2}\right)\]

Thus $\lim_{t \to \infty} P(\theta_t \geq \theta_0 + \frac{\alpha \Delta}{2} t) = 1$ if $\lim_{t \to \infty} t \epsilon_t^2 = +\infty$ therefore $\lim_{t \to \infty} \theta_t = +\infty$ almost surely.

\[\square\]