An operator view of policy gradient methods

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Abstract

We cast policy gradient methods as the repeated application of two operators: a policy improvement operator $I$, which maps any policy $\pi$ to a better one $I\pi$, and a projection operator $P$, which finds the best approximation of $I\pi$ in the set of realizable policies. We use this framework to introduce operator-based versions of traditional policy gradient methods such as Reinforce and PPO, which leads to a better understanding of their original counterparts. We also use the understanding we develop of the role of $I$ and $P$ to propose a new global lower bound of the expected return. This new perspective allows us to further bridge the gap between policy-based and value-based methods, showing how Reinforce and the Bellman optimality operator, for example, can be seen as two sides of the same coin.

1 Introduction

Model-free reinforcement learning algorithms aim at learning a policy that maximizes the (discounted) sum of rewards directly from samples generated by the agent’s interactions with the environment. These techniques mainly fall in one of two categories: value-based methods, where the agent predicts the value of taking an action and then chooses the action with the largest predicted value; and policy-based methods, where the agent directly learns a good distribution over actions at each state. Although several past works created connections between the two views \cite[e.g.,][]{Nachum2017, Schulman2017}, such connections are often limited to the optimal policy and they do not capture training dynamics.

In particular, value-based methods are often cast as the iterative application of an improvement operator, the Bellman optimality operator, which transforms the value function into a “better” one (unless the value function is already the optimal one) \cite{Bellman1957}. When dealing with a restricted set of policies, we often use function approximation for the value function. In this case, the learning procedure interleaves the improvement operator with a projection operator, which finds the best approximation of this improved value function in the space of realizable value functions.

While this view is the basis for many intuitions around the convergence of value-based methods, no such view exists for policy-gradient (PG) methods, which are usually cast as doing gradient ascent on a parametric function representing the expected return of the policy \cite[e.g.,][]{Williams1992, Schulman2015}. Although this property can be used to show the convergence of such methods when following the expected gradient, it does little to our understanding of the relationship of these methods to value-based ones.

In this work, we show that PG methods can also be seen as repeatedly applying two operators akin to those encountered in value-based methods: (a) a policy improvement operator, which maps any policy to a policy achieving strictly larger return; and (b) a projection operator, which finds the best approximation of this new policy in the space of realizable policies. We then recast common PG methods under this framework, using their operator interpretations to shed light on their properties.

We also make the following additional contributions: (a) We present a lower bound on the performance of a policy using the state-action formulation, leading to an alternative to conservative policy improvement; (b) We provide a formal justification of $\alpha$-divergences in the imitation learning setting.
2 Background

We consider an infinite-horizon discounted Markov decision process (MDP) [Puterman, 1994] defined by the tuple \( \mathcal{M} = \langle S, A, p, r, d_0, \gamma \rangle \) where \( S \) is a finite set of states, \( A \) is a finite action set, \( p : S \times A \to S \) is the transition probability function, \( r : S \times A \to [0, R_{\text{max}}] \) is the reward function, \( d_0 \) is the initial distribution of states, and \( \gamma \in [0, 1) \) is the discount factor. Letting \( \Delta(\cdot) \) denote the probability simplex, the agent’s goal is to learn a policy \( \pi : S \times A \to \Delta(S) \) that maximizes the expected discounted return. Below we formalize these concepts and we discuss representative algorithms in the trajectory and value-based formulations.

In this paper, we are not interested in the stochastic gradient updates, but the updates on expectation. Thus, our presentation and analyses use the true gradient of the functions of interest.

2.1 Trajectory Formulation

The expected discounted return can be defined as

\[
E = \sum_{t=0}^{\infty} \gamma^t r(s_t, a_t),
\]

where \( s_0 \sim d_0, a_t \sim \pi(a_t|s_t), \) and \( s_{t+1} \sim p(s_{t+1}|s_t, a_t). \) Moreover, \( \tau \) denotes a specific trajectory, \( \tau = (s_0, a_0, s_1, \ldots) \), and \( R(\tau) \) denotes the return of that trajectory, that is, \( R(\tau) = \sum_{t=0}^{\infty} \gamma^t r(s_t, a_t). \)

PG methods seek the \( \pi^* \) maximizing \( J \), i.e., \( \pi^* = \arg \max_\pi J(\pi) = \arg \max_\pi \int \tau R(\tau) \pi(\tau) \, d\tau \). Policies often live in a restricted class \( \Pi \) parameterized by \( \theta \in \mathbb{R}^d \), and the problem becomes

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

where \( \pi_\theta(\tau) \) is the probability of \( \tau \) under the policy indexed by \( \theta \). Note that, although we write \( \pi_\theta(\tau) \), policies define distributions over actions given states and they only indirectly define distributions over trajectories.

REINFORCE [Williams, 1992] is one of the most traditional PG methods. It computes, at each step, the gradient of \( J(\pi_\theta) \) with respect to \( \theta \) and performs the following update:

\[
\theta_{t+1} = \theta_t + \epsilon_t \int \pi_{\theta_t}(\tau) R(\tau) \frac{\partial \log \pi_\theta(\tau)}{\partial \theta} \bigg|_{\theta=\theta_t} \, d\tau,
\]

where \( \epsilon_t \) is a stepsize. We shall replace \( \pi_{\theta_t} \) by \( \pi_t \) when the meaning is clear from context.

2.2 Value-Based Formulation

In the value-based formulation, we use the standard notions of state and state-action value function:

\[
V^\pi(s_t) = \mathbb{E}_{a_t, s_{t+1}, \ldots} \left[ \sum_{k=0}^{\infty} \gamma^k r(s_{t+k}, a_{t+k}) \right], \quad Q^\pi(s_t, a_t) = \mathbb{E}_{s_{t+1}, a_{t+1}, \ldots} \left[ \sum_{k=0}^{\infty} \gamma^k r(s_{t+k}, a_{t+k}) \right],
\]

where \( a_t \sim \pi(a_t|s_t), \) and \( s_{t+1} \sim p(s_{t+1}|s_t, a_t), \) for \( t \geq 0. \) The goal of the agent is to maximize \( \mathbb{E}_{s_0} V^\pi(s_0) \) and the policy gradient theorem [Sutton et al., 2000] gives an update for the state-action formulation that is equivalent to the REINFORCE update discussed above:

\[
\theta_{t+1} = \theta_t + \epsilon \sum_s d^\pi(s) \sum_a \pi_t(a|s) Q^\pi(s, a) \frac{\partial \log \pi_\theta(a|s)}{\partial \theta} \bigg|_{\theta=\theta_t},
\]

where \( d^\pi \) is the discounted stationary distribution induced by the policy \( \pi \).

3 An Operator View of REINFORCE

The parameter updates in Eq. 2 and Eq. 4 involve the current policy \( \pi_\theta \), twice: once in the sampling distribution (resp. the stationary distribution) and once inside the log. While the latter term is generally easy to deal with, the former is the source of many difficulties in the optimization process. One possibility to alleviate this issue is to maintain the sampling distribution fixed while only optimizing the parameters of the policy inside the log, an approach which finds its justification by devising a lower bound on \( J \) [Kober].
and Peters, 2009, Le Roux, 2016, Abdolmaleki et al., 2018] or a locally valid approximation [Kakade and Langford, 2002, Schulman et al., 2015].

All these approaches can be cast as minimizing a divergence measure between the current policy $\pi$ and a fixed policy $\mu$ which achieves higher return than $\pi$. Thus, moving from $\pi$ to $\mu$ can be seen as a policy improvement step and we have $\mu = I(\pi)$ with $I$ the improvement operator. Since the resulting $\mu$ might not be in the set of realizable policies, the divergence minimization acts as a projection step using a projection operator $\mathcal{P}$. In all these cases, when only performing one gradient step to minimize the divergence, we recover the original updates of Eq. 2 and Eq. 4.

This decomposition in improvement and projection steps allows us to see PG methods not simply as performing gradient ascent on a function representing a policy’s expected return, but as the successive application of a policy improvement and a projection operator. It highlights, for example, that because these operators are always coupled, it is not always beneficial to choose the best possible $\mu$ when using a generic projection instead of one tailored to $J$. In fact, this perspective makes us wonder which policies $\mu$ and which projections to use. In particular, we are interested in operators which satisfy the following two properties:

(a) The optimal policy $\pi(\theta^*)$ should be a stationary point of the composition $\mathcal{P} \circ I$, as iteratively applying $\mathcal{P} \circ I$ would otherwise lead to a suboptimal policy, and (b) Doing an approximate projection step of $I\pi$, using gradient ascent starting from $\pi$, should always lead to a better policy than $\pi$. In particular, if the combination leads to maximizing a function that is a lower bound of $J$ everywhere, we know the combination of the two steps, even when solved approximately, leads to an increase in $J$ and will converge to a locally optimal policy.

These tools allow us to explore several possibilities for these operators. In this section we present standard PG methods under the view of operators, in both trajectory and value-function formulations. Later we discuss some consequences and insights this perspective gives us about existing methods.

3.1 Trajectory Formulation

The proposition below formalizes, in the trajectory formulation, the idea of casting PG methods as the successive application of a policy improvement and a projection operator. It does so by presenting two operators that give rise to OP-Reinforce, an operator version of Reinforce [Williams, 1992].

**Proposition 1.** Assuming all returns $R(\tau)$ are positive, Eq. 2 can be seen as doing a gradient step to minimize $KL(R\pi|\pi)$ with respect to $\pi$, where $R\pi_t$ is the policy defined by

$$R\pi_t(\tau) = \frac{1}{J(\pi_t)} R(\tau)\pi_t(\tau).$$

Hence, the two operators associated with OP-Reinforce are:

$$I_{\tau}(\pi)(\tau) = R\pi(\tau), \quad \mathcal{P}_{\tau}(\mu) = \arg\min_{\pi \in \Pi} KL(\mu|\pi),$$

where $\Pi$ is the set of realizable policies.

We prove this proposition and the following in the appendix.

Even in the tabular case, $R\pi$ might not be achievable when the environment is stochastic and so the projection operator $\mathcal{P}_{\tau}$ is needed. Note that OP-Reinforce is different from the original Reinforce algorithm because it solves the projection exactly rather than doing just one step of gradient descent. Nevertheless, OP-Reinforce maintains the following important property:

**Proposition 2.** $\pi(\theta^*)$ is a fixed point of $\mathcal{P}_{\tau} \circ I_{\tau}$.

3.2 Value-Based Formulation

While a policy was defined as a distribution over trajectories in the trajectory formulation, it will be defined as a stationary distribution over state-action pairs in the value-based formulation. Similar to the trajectory formulation, the policy improvement step can lead to policies which are not realizable.

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1“Policy” is loosely defined here as a distribution over trajectories.
2OP-Reinforce was introduced by Le Roux [2016] under the name “Iterative PoWER”.

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We saw in section 3.1 that doing the full projection implied by the operators leads to Op-Reinforce, which is slightly different from Reinforce. Similarly, although the policy gradient theorem states that the updates of Eq. 2 and 4 are identical, the resulting operators will be different:

**Proposition 3.** If all $Q^\pi(s, a)$ are positive, Eq. 4 can be seen as doing a gradient step to minimize

$$D_{V^\pi} V^\pi_t (Q^\pi_t || \pi) = \sum_s d^\pi(s) V^\pi_t (s) KL(Q^\pi_t || \pi),$$

where $D_{V^\pi}$ and the distribution $Q^\pi$ over actions are defined as

$$D_z (\mu || \pi) = \sum_s z(s) KL(\mu(\cdot|s)||\pi(\cdot|s)),$$

$$Q^\pi(a|s) = \frac{1}{\sum_{a'} Q(s, a') \pi(a'|s)} Q(s, a) \pi(a|s) = \frac{1}{V^\pi(s)} Q(s, a) \pi(a|s).$$

Hence, the two operators associated with the state-action formulation are:

$$\mathcal{I}_V (\pi)(s, a) = \left( \frac{1}{E_{\pi}[V^\pi]} d^\pi(s) V^\pi(s) \right) Q^\pi(a|s),$$

$$\mathcal{P}_V (\mu) = \arg\min_{z \in \Pi} \sum_s \mu(s) KL(\mu(\cdot|s)||z(\cdot|s)).$$

The improvement operator $\mathcal{I}_V$ affects both the distribution over states, where it increases the probabilities of states $s$ with large values $V(s)$, and the conditional distribution over actions given states, where it increases the probabilities of actions $a$ with large values $Q(s, a)$.

The projection operator is not the KL-divergence over the full distribution over state-action pairs. Rather, it treats each state independently, weighting them using the distribution over states of its first argument. In the tabular case, the optimum may be found immediately and is independent of the distribution over states, i.e. $\mathcal{P}_V (\mu)(a|s) = \mu(a|s)$.

**Proposition 4.** $\pi(\theta^*)$ is a fixed point of $\mathcal{P}_V \circ \mathcal{I}_V$.

Now that we derived operator versions of classical PG methods, further bridging the gap between policy-based and value-based methods, we study their properties.

### 3.3 $\mathcal{I}_\gamma (\pi)$ can be arbitrarily close to $\pi$

The Bellman optimality operator is a $\gamma$-contraction where $\gamma$ is the discount factor, leading to a linear convergence rate of the value function in the tabular case. By contrast, in the trajectory formulation, the improvement obtained by $\mathcal{I}_\gamma$ can be arbitrarily small, as formalized in the proposition below.

**Proposition 5.**

$$J(\mathcal{I}_\gamma(\pi)) = J(\pi) \left( 1 + \frac{\text{Var}_\pi(R)}{(E_\pi[R])^2} \right) \geq J(\pi).$$

If $\pi$ is almost deterministic and the environment is deterministic, then we have $\text{Var}_\pi(R) \approx 0$ and $J(\mathcal{I}_\gamma(\pi)) \approx J(\pi)$. This result justifies the general intuition that deterministic policies can be dangerous for PG methods; not because they may perform poorly, but because they stall the learning process. In that sense, entropy regularization can be seen as helping the algorithm make consistent progress. Moreover, note that the improvement operator $\mathcal{I}_\gamma$ is weaker than the equivalent operator for value-based methods, which can be seen as a consequence of the smoothness of change in the policies of PG methods when compared to the abrupt changes that can occur in value-based methods.
3.4 A lower bound on the overall improvement

Although we established that the improvement operator leads to a policy achieving higher return, it could still be the case that the projection operator $P$ annihilates all these gains, leading $P \circ I(\pi)$ to having a smaller expected return than $\pi$. The proposition below derives a lower bound for the difference in expected returns, proving this cannot be the case, even when the projection is not computed exactly.

**Proposition 6.** For any two policies $\pi$ and $\mu$ such that the support of $\mu$ covers that of $\pi$, we have

$$J(\pi) \geq J(\mu) + \mathbb{E}_\pi[V(\mu)](D_\mu(I_V|\mu) - D_\mu(I_V|\pi)).$$

Hence, any policy $\pi$ such that $D_{\pi_t}(I_V(\pi_t)||\pi) < D_{\pi_t}(I_V(\pi_t)||\pi_t)$ implies $J(\pi) > J(\pi_t)$.

Fig. 1 compares our lower bound to the surrogate approximation used by conservative policy iteration (CPI) [Kakade and Langford 2002], which provides the theoretical motivation for TRPO [Schulman et al. 2015] and PPO [Schulman et al. 2017b]. Although both are equivalent to first-order terms, matching the value and first derivative of $J$ for $\pi = \pi_t$, the CPI approximation is not a bound on the true objective and only guarantees improvement of the original objective for small stepsizes unlike our global lower bound.

3.5 Optimal off-policy sampling distribution

The operator view is inherently linked to off-policy sampling since applying $P \circ I$ is equivalent to minimizing the divergence between a fixed policy $I\pi_t$ and the current policy $\pi$. When using off-policy data without importance weights, this is a biased estimate of the gradient. [Schaul et al. 2019] partially explored this biased gradient, and report that off-policy sampling sometimes works better than on-policy sampling.

Importantly, when $\pi_\theta$ is in the exponential family, the surrogate loss is strictly convex and minimizing $KL(I_\mu||\pi)$ over $\pi$ converges to the same solution regardless of the initial point. Since $\pi(\theta^*)$ is a fixed point of $P \circ I$, it is the minimum of $KL(I\pi(\theta^*)||\pi)$ and gradient descent will converge to a solution with the optimal return $J^*$.

Although this result is of no practical interest since it requires knowing $\pi(\theta^*)$ in advance, it proves that there are better sampling distributions than the current policy and that, in some sense, off-policy learning without importance correction is “optimal” when sampling from the optimal policy.

4 Other policy gradient methods under the operators perspective

Now that we have shown that REINFORCE can be cast as iteratively applying two operators, we might wonder whether other operators could be used instead. In this section, we explore the use of other policy improvement and projection operators. We shall see that there are two main categories of transformation: the first one performs a nonlinear transformation of the rewards in the hope of reaching faster convergence; the second
changes the distribution over state-action pairs and possibly the ordering of the KL divergence. With this perspective, we recover operators that give rise to PPO [Schulman et al., 2017b] and MPO [Abdolmaleki et al., 2018] to shed some light on what these methods truly accomplish.

4.1 Moving beyond rewards

While REINFORCE improves the policy by weighting the policy by the rewards, one might wonder if we can potentially substitute in other non-linear transformations of the reward to speed up the learning process. Intuitively, policies at the beginning of training are usually of such poor quality, asking them to focus solely on the highest-reward trajectories may lead to larger improvement steps. As such, one might wonder if policy improvement operators that transform the rewards can lead to faster convergence and, if so, whether the policy at convergence remains optimal. We discuss two such transformations that place increased emphasis on the highest-reward trajectories.

4.1.1 Polynomial rewards

Since, in the trajectory formulation, the improvement step consists in multiplying the probability of each trajectory by its associated return, one might wonder what would happen if we instead used the return raised to the \( k \)-th power, i.e. replacing \( \mathcal{I} \) by \( \mathcal{I}_k^\alpha : \pi \rightarrow R^k \pi \). Larger values of \( k \) place higher emphasis on high-return trajectories and, as \( k \) grows to infinity, \( R^k \pi \) becomes the deterministic distribution that assigns probability 1 to the trajectory achieving the highest return. However, for any \( k \neq 1 \), \( \pi(\theta^*) \) may not be a fixed point of \( \mathcal{P}_\tau \circ \mathcal{I}_k^\alpha \), since projecting a policy that achieves a higher expected return can still lead to a worse policy. Thankfully, the following proposition allows us to address the issue by changing the projection operator accordingly:

**Proposition 7.** Let \( \alpha \in (0, 1) \). Then \( \pi(\theta^*) \) is a fixed point of \( \mathcal{P}_\tau \circ \mathcal{I}_\alpha^\frac{1}{\alpha} \) with \( \mathcal{P}_\tau^\alpha \) defined by

\[
\mathcal{P}_\tau^\alpha(\mu) = \arg\min_{\pi \in \Pi} D^\alpha(\mu||\pi),
\]

where \( D^\alpha \) is the \( \alpha \)-divergence or Rényi divergence of order \( \alpha \).

Proposition 7 is especially interesting in the context of imitation learning where the teacher distribution over trajectories is concentrated around few high performing trajectories. This distribution can be seen as \( R^k \pi \) for an arbitrary \( \pi \), say uniform, and a large value of \( k \). We should then use an \( \alpha \)-divergence, not the KL, to recover a good policy. Ke et al. [2019] pointed out the usefulness of \( \alpha \)-divergences in this context but we are not aware of previous connections with the fixed point property.

We can use a similar approach for the value-based formulation, leading to the following proposition:

**Proposition 8.** Let \( \alpha \in (0, 1) \). Then \( \pi(\theta^*) \) is a fixed point of \( \mathcal{P}_\tau^\alpha \circ \mathcal{I}_\alpha^\frac{1}{\alpha} \) with

\[
\mathcal{I}_\alpha^\alpha(\pi) = (Q^\pi)^{\frac{1}{\alpha}} \pi, \quad \mathcal{P}_\tau^\alpha(\mu|\pi) = \arg\min_{\pi \in \Pi} \sum_s d^\pi(s) Z^\pi\alpha(s) D^\alpha(\mu||z),
\]

where \( Z^\alpha\alpha(s) = \sum_a \pi(a|s) Q^\pi(s, a) \frac{1}{\alpha} \) is a normalization constant.

Note that, in the tabular case, because we are in the state-action formulation, we can ignore the projection operator and we get \( \pi_t(a|s) \propto \pi_0(a|s) \left( \prod_{i=1}^{t-1} Q^\pi(s, a) \right)^{\frac{1}{\alpha}} \), and the policy becomes more deterministic as \( \alpha \) goes to 0. In fact, at the limit \( \alpha = 0 \), \( \mathcal{I}_\alpha^\alpha(\cdot|\pi) \) is the policy which assigns probability 1 to the action \( a^*(s) = \arg\max_a Q^\pi(s, a) \), and \( I_\alpha \) becomes the greedy policy improvement operator. The operator view can then be seen as offering us an interpolation between REINFORCE and value-based methods: we recover REINFORCE with \( \alpha = 1 \) and the Bellman optimality operator at the limit \( \alpha = 0 \). From this perspective, one may say that the main difference between REINFORCE and value-based methods is how aggressively they use value estimates to define their policy. REINFORCE generates smooth policies that choose actions proportionally to their estimated value, value-based methods choose the action with higher value.

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3If there are multiple such trajectories, this is a uniform distribution over all of them.
Empirical analysis Although using an $\alpha$-divergence is necessary to maintain $\pi(\theta^*)$ as stationary point, it is possible that using the KL will still lead to faster convergence early in training. We studied the effect of this family of improvement operators $I^\alpha$ for different choices of $\alpha$ in the four-room domain [Sutton et al., 1999] (Figure 2). The agent starts in the lower-left corner and seeks to reach the upper-right corner; episode terminates with a reward of +1 upon entering the goal state. The policy is parameterized by a softmax and all states share the same parameters, i.e. we use function approximation.

When $I_\alpha^\alpha$ is paired with a KL projection step, the return increases faster than when using OP-REINFORCE’s improvement operator early in the process. However, such a combination converges to a suboptimal policy and incurs linear regret (Figure 2). In contrast, combining the improvement operator with a projection that uses the corresponding $\alpha$-divergence not only speeds up learning but also converges to the optimal policy. One can use $I^\alpha$ with the KL projection step heuristically, by selecting an aggressive improvement operator $I^\alpha$ (low $\alpha$) early in optimization, and annealing $\alpha$ to 1 to recover OP-REINFORCE updates asymptotically. We present results of using line search to dynamically anneal the value of $\alpha$ as the policy converges (details in Appendix F.1).

4.1.2 Exponential rewards

So far, all of our analysis assumed the returns were nonnegative. If the returns are lower bounded, this can be addressed by shifting them upward until they are all nonnegative. However, Le Roux [2016] showed this is equivalent to adding a KL term that might slow down convergence. Another possibility is to transform these returns using a strictly increasing function with nonnegative outputs. The most common such transformation is the exponential function, used by PPO and MPO, leading to the operator $T^{\exp,T}(\pi) = \exp\left(\frac{R}{T}\right)\pi$, with $T > 0$. Although that transformation solves the nonnegativity issue and makes the algorithm invariant to a shift in the rewards, similar to the original REINFORCE, we are not aware of any result guaranteeing that $\pi(\theta^*)$ remains a fixed point. However, the following proposition shows that $T^{\exp,T}$, as well as any transformation using a strictly increasing function with nonnegative outputs, achieves higher expected return than $\pi$ for all $T$.

**Proposition 9.** Let $f$ be an increasing function such that $f(x) > 0$ for all $x$. Then

$$J(f(R)\pi) = J(\pi) + \frac{\text{Cov}_\pi(R, f(R))}{E_\pi[f(R)]} \geq J(\pi).$$

(16)
4.2 An operator view of PPO

PPO [Schulman et al., 2017b] is one of the most widely used policy gradient methods. It maximizes a surrogate objective where the distribution over states and Q values is kept fixed, while the algorithm tries to maximize $\sum_{s,a} \pi(a|s)Q^\pi(s,a)$ at each state. Moreover, PPO uses an entropy bonus to its objective and, to avoid excessively large policy updates, PPO also performs some form of clipping. The operators that allow us to recover PPO are presented below.

$$I_V(\pi)(s, a) = d^\pi(s) \frac{\exp (\beta Q^\pi(s, a))}{\sum_{a'} \exp (\beta Q^\pi(s, a'))}$$

(17)

$$P_V(\mu) = \arg \min_{z \in \Pi} \sum_{s} \mu(s) KL(\text{clip}(z(\cdot|s))||\mu(\cdot|s)),$$

(18)

leading to $$\pi_{t+1} = \arg \min \sum_{s} d^{\pi_t}(s) \left( \sum_{a} z(a|s)Q^\pi_t(s, a) - \frac{1}{\beta} \sum_{a} z(a|s) \log z(a|s) \right),$$

(19)

where we omitted the clipping on the last line for readability. There are three main differences between the operators that recover PPO and the operators of OP-REINFORCE (Eq. 10 and 11): (1) The policy improvement operator does not increase the probability of good states because, different from OP-REINFORCE, $V(s)$ is not part of $I_V$; (2) the policy improvement operator only uses the Q-values in its distribution over actions given states, instead of also using $\pi$; (3) the KL in the projection operator is reversed. The last point is particularly important as this reversed KL is mode seeking, so the resulting distribution $\pi_{t+1}$ will focus its mass on the mode of $I_V(\pi_t)$, which is the action with the largest Q-value. This can quickly lead to deterministic policies, especially when $\beta$ is large, justifying the necessity of the clipping in the KL. By comparison, the projection operator of Eq. 11 uses a KL that is covering, naturally preventing $\pi_{t+1}$ from becoming too deterministic. While our analysis fits current PG methods into the operator view, they can also be framed in the language of optimization, for example as performing approximate mirror descent in an MDP [Neu et al., 2017].

4.3 An operator view of control-as-inference and MPO

The operator view can be used to provide insight on control-as-inference, a line of work that casts RL as performing inference in a graphical model [Deisenroth et al., 2013, Levine, 2018]. We focus our discussion through MPO [Abdolmaleki et al., 2018], a state-of-the-art algorithm derived through this framework. The policy improvement operator that recovers MPO is:

$$I_V(\pi)(s, a) = d^\pi(s) \frac{\pi(a|s) \exp (\beta Q^\pi(s, a))}{\sum_{a'} \pi(a'|s) \exp (\beta Q^\pi(s, a'))} ,$$

(20)

with the projection operator being the same as OP-REINFORCE’s. Note that the improvement operator interpolates between those of OP-REINFORCE and PPO: it does not upweight good states and it uses an exponential transformation of the rewards, like PPO, but it still uses the policy $\pi(a|s)$ and not just the rewards. In this case, clipping is not necessary because the KL is in the “covering” direction.

MPO uses control-as-inference to interpret the return of a trajectory as an unnormalized log probability in a graphical model, and RL as discovering the maximum likelihood estimate. EM algorithms in this graphical model are analogous to OP-REINFORCE, where the expectation step corresponds to policy improvement, and the maximization step corresponds to projection. Similarly, incomplete projection steps by partially maximizing the lower bound in Proposition 6 is equivalent to doing incremental EM [Neal and Hinton, 1998]. Unlike the operator view, the control-as-inference formulation is limited because rewards often cannot easily be interpreted as probabilities, making it also difficult to establish connections with RL algorithms outside the formulation like PPO.

5 Conclusion

We cast PG methods as the repeated application of two operators: a policy improvement operator and a projection operator. Starting with a modification of REINFORCE, we introduced the operators that recover
traditional algorithms such as PPO and MPO. This operator perspective also allowed us to further bridge the gap between policy-based and value-based methods, showing how REINFORCE and the Bellman optimality operator can be seen as the same method with only one parameter changing.

Importantly, this perspective helps us improve our understanding behind decisions often made in the field. We showed how entropy regularization helps by increasing the variance of the returns, guaranteeing bigger improvements for PG methods; we showed how even single gradient steps towards the full projection operator are guaranteed to lead to an improvement; and how practices such as exponentiating rewards to make them non-negative, as done by MPO, still lead to a meaningful policy improvement operator. Finally, by introducing new operators based on the $\alpha$-divergence we were able to show that there are other operators that can still lead to faster learning, shedding some light into how to better use, for example, expert trajectories in reinforcement learning algorithms, as often done in high-profile success stories [Silver et al., 2016, Vinyals et al., 2019].

Finally, we hope the results we presented in this paper will empower researchers to design new policy gradient methods, either through the introduction of new operators, or by leveraging the intuitions we presented here. This operator perspective opens up a new avenue of research in analyzing policy gradient methods and it can also provide a different perspective on traditional problems in the field, such as how to choose appropriate basis functions to better represent policies, and how to do better exploration by design sampling policies different than the agent’s current policy.

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In the entirety of the appendix, we shall use $\pi^*$ instead of $\pi(\theta^*)$ for increased readability.

A Definition of the operators

Proposition 1. Assuming all returns $R(\tau)$ are positive, Eq. 3 can be seen as doing a gradient step to minimize $KL(R\pi_t||\pi)$ with respect to $\pi$, where $R\pi_t$ is the policy defined by

$$R\pi_t(\tau) = \frac{1}{J(\pi_t)} R(\tau)\pi_t(\tau).$$ (5)

Hence, the two operators associated with the state-action formulation are:

$$\mathcal{I}_\pi(\tau)(\pi) = R\pi_t(\tau), \quad \mathcal{P}_\pi(\mu) = \arg\min_{\pi \in \Pi} KL(\mu||\pi),$$ (6)

where $\Pi$ is the set of realizable policies.

Proof. Denoting $\mu$ the distribution over trajectories such that $\mu(\tau) \propto R(\tau)\pi(\tau)$, we have

$$KL(\mu||\pi) = \int \mu(\tau) \log \frac{\mu(\tau)}{\pi(\tau)} d\tau$$ (21)

$$\frac{\partial KL(\mu||\pi)}{\partial \theta} = -\int \mu(\tau) \nabla_\theta \log \pi(\tau) d\tau$$ (22)

$$\propto -\int R(\tau)\pi(\tau) \nabla_\theta \log \pi(\tau) d\tau$$ (23)

by definition of $\mu(\tau)$. \(\square\)

Proposition 3. If all $Q^\pi(s, a)$ are positive, Eq. 4 can be seen as doing a gradient step to minimize

$$D_{\mathcal{V}^\pi}(Q^\pi, \pi_t||\pi) = \sum_s d^\pi_t(s)V^\pi_t(s)KL(Q^\pi_t||\pi),$$ (7)

where $D_{\mathcal{V}^\pi}$, and the distribution $Q^\pi$ over actions are defined as

$$D_z(\mu||\pi) = \sum_s z(s)KL(\mu(|s)||\pi(|s)),$$ (8)

$$Q^\pi(a|s) = \frac{1}{\sum_{a'} Q(s, a'^\pi|a'|s)} Q(s, a)\pi(a|s) = \frac{1}{V^\pi(s)} Q(s, a)\pi(a|s).$$ (9)

Hence, the two operators associated with the state-action formulation are:

$$\mathcal{I}_\mathcal{V}(\pi)(s, a) = \left(\frac{1}{E_{\pi}[V^\pi]} d^\pi(s)V^\pi(s)\right)Q^\pi(a|s)$$ (10)

$$\mathcal{P}_\mathcal{V}(\mu) = \arg\min_{z \in \Pi} \sum_s \mu(s)KL(\mu(||s)||z(|s))).$$ (11)

Proof.

$$\sum_s d^\pi_t(s)V^\pi(s) \frac{\partial KL(Q^\pi_t||\pi)}{\partial \theta} = -\sum_s d^\pi_t(s)V^\pi(s) \sum_a Q^\pi(\pi_t(a|s)\nabla_\theta \log \pi(a|s)

= -\sum_s d^\pi_t(s) \sum_a Q(s, a)\pi_t(a|s)\nabla_\theta \log \pi(a|s),$$ (24)

and we recover the update of Eq. 4. \(\square\)
\section*{B \textit{π} is a stationary point when using the KL}

\textbf{Proposition 2.} \(\pi(\theta^*)\) is a fixed point of \(\mathcal{P}_r \circ \mathcal{I}_r\).

\textit{Proof.} We have

\[
\begin{align*}
\nabla_{\theta} KL(R\pi^*||\pi) \bigg|_{\pi=\pi^*} &= \int R(\tau)\pi^*(\tau) \frac{\partial \log \pi(\theta|s)}{\partial \theta} d\tau \\
&= 0 \text{ by definition of } \pi^*. 
\end{align*}
\]

\textbf{Proposition 4.} \(\pi(\theta^*)\) is a fixed point of \(\mathcal{P}_V \circ \mathcal{I}_V\).

\textit{Proof.} We have

\[
\begin{align*}
\nabla_{\theta} \sum_s d\pi^*(s)V\pi^*(s)KL(Q\pi^*||\pi) \bigg|_{\pi=\pi^*} &= \sum_s d\pi^*(s) \sum_a \pi^*(a|s)Q\pi^*(s,a) \frac{\partial \log \pi(\theta|s)}{\partial \theta} \bigg|_{\theta=\theta^*} \\
&= 0 \text{ by definition of } \pi^*. 
\end{align*}
\]

\section*{C Expected return of the improved policy}

We use the same proof for the following two propositions:

\textbf{Proposition 5.}

\[
J(\mathcal{I}_r(\pi)) = J(\pi) \left(1 + \frac{\text{Var}_\pi(R)}{\mathbb{E}_\pi(R)^2}\right) \geq J(\pi). 
\]

\textbf{Proposition 9.} Let \(f\) be an increasing function such that \(f(x) > 0\) for all \(x\). Then

\[
J(f(R)\pi) = J(\pi) + \frac{\text{Cov}_\pi(R, f(R))}{\mathbb{E}_\pi[f(R)]} \geq J(\pi). 
\]

\textit{Proof.} We now show the expected return of the policy \(z\pi\), defined as

\[
\begin{align*}
z\pi(\tau) &= \frac{1}{\int \tau \, z(\tau')\pi(\tau') \, d\tau} z(\tau)\pi(\tau), 
\end{align*}
\]

for any function \(z\) over trajectories. In particular, we show that choosing \(z = R\) leads to an improvement in the expected return.

\[
\begin{align*}
J(z\pi) &= \int \tau R(\tau)z(\tau)\pi(\tau) \, d\tau \\
&= \int \tau \int \tau' z(\tau')\pi(\tau') \, d\tau' \, d\tau \\
&= \left(\int \tau R(\tau)\pi(\tau) \, d\tau\right) \frac{\int \tau R(\tau)z(\tau)\pi(\tau) \, d\tau}{\int \tau' z(\tau')\pi(\tau') \, d\tau'} \\
&= J(\pi) \frac{\mathbb{E}_\pi[Rz]}{\mathbb{E}_\pi[R][\mathbb{E}_\pi[z]]} \\
&= J(\pi) \left(1 + \frac{\text{Cov}_\pi(R, z)}{\mathbb{E}_\pi[R][\mathbb{E}_\pi[z]]}\right), 
\end{align*}
\]
where \( \text{Cov}_z(R, z) = \mathbb{E}_\pi[Rz] - \mathbb{E}_\pi[R]\mathbb{E}_\pi[z] \).

When \( z = R \), the expected return becomes
\[
J(R\pi) = J(\pi) \left(1 + \frac{\text{Var}_\pi(R)}{(\mathbb{E}_\pi[R])^2}\right)
\geq J(\pi).
\] (35)  (36)

\[\square\]

**D \ \ \pi^* \text{ is a stationary point when using } \alpha\text{-divergence}**

**Proposition 7.** Let \( \alpha \in (0, 1) \). Then \( \pi(\theta^*) \) is a fixed point of \( \mathcal{P}_\pi^\alpha \circ \mathcal{I}_V^{1/\alpha} \) with \( \mathcal{P}_\pi^\alpha \) defined by
\[
\mathcal{P}_\pi^\alpha(\mu) = \arg \min_{\pi \in \Pi} D^\alpha(\mu||\pi),
\] (14)
where \( D^\alpha \) is the \( \alpha \)-divergence or Rényi divergence of order \( \alpha \).

**Proof.** We now show that \( \pi^* \) is the fixed point of \( \mathcal{P}_\pi^\alpha \circ \mathcal{I}_V^{1/\alpha} \). The minimizer of \( d^\alpha \) with respect to its second argument can be computed through iterative minimization of \( D^\alpha \) for any other nonzero \( \alpha' \) [Minka et al., 2005].

\[
z_{t+1} = \arg \min_z D_{\alpha'}(\pi_{\alpha}/\alpha' z_{t-\alpha/\alpha'}||z).
\] (37)

In the remainder of this proof, we shall use \( \alpha' = 1 \), leading to
\[
z_{t+1} = \arg \min_z KL(\pi_{\alpha} z_{t-\alpha}||z).
\] (38)

We know that \( \pi^* \) is a stationary point of \( \mathcal{P}_\pi^1 \circ \mathcal{I}_V^1 \), i.e.
\[
\pi^* = \arg \min_z KL(R\pi^*||z).
\] (39)

Hence, we see that, if \( \pi^*(\pi^*)^{1-\alpha} = R\pi^* \), the iterative process described in Eq. 38 initialized with \( z_0 = \pi^* \) will be stationary with \( z_i = \pi^* \) for all \( i \). This gives us the form we need for \( \pi = \mathcal{I}_V^{1/\alpha} \). Indeed, we must have
\[
\pi^*(\pi^*)^{1-\alpha} = R\pi^*
\] (40)
\[
(\mathcal{I}_V^{1/\alpha} \pi^*)(\pi^*)^{1-\alpha} = R\pi^*
\] (41)
\[
\mathcal{I}_V^{1/\alpha} \pi^* = [R(\pi^*)^\alpha]^{1/\alpha} = R^{1/\alpha} \pi^*
\] (42)
\[
\mathcal{I}_V^\alpha = (\pi \rightarrow R^{1/\alpha} \pi).
\] (43)

\[\square\]

**Proposition 8.** Let \( \alpha \in (0, 1) \). Then \( \pi(\theta^*) \) is a fixed point of \( \mathcal{P}_\pi^\alpha \circ \mathcal{I}_V^{1/\alpha} \) with
\[
\mathcal{I}_V^\alpha(\pi) = (Q_\pi)^{1/\alpha} \pi, \quad \mathcal{P}_\pi^\alpha(\mu) = \arg \min_{\pi \in \Pi} \sum_s d^\alpha(s) Z_\mu^\pi(s) D^\alpha(\mu||z),
\] (15)
where \( Z_\mu^\pi(s) = \sum_a \pi(a|s) Q_\pi(s, a)^{1/\alpha} \) is a normalization constant.

**Proof.** The proof is very similar to that of proposition [4]. We know that \( \pi^* \) is a stationary point of \( \mathcal{P}_\pi^\alpha \circ \mathcal{I}_V^1 \), i.e.
\[
0 = \sum_s d^\alpha(s) \sum_a \pi^*(a|s) Q_\pi^*(s, a) \frac{\partial \log \pi_\theta(a|s)}{\partial \theta} \bigg|_{\theta = \theta^*}
\] (45)
\[
= \sum_s d^\alpha(s) \sum_a \pi^*(a|s) ^{1-\alpha} \left( \pi^*(a|s) Q_\pi^*(s, a)^{1/\alpha} \right)^\alpha \frac{\partial \log \pi_\theta(a|s)}{\partial \theta} \bigg|_{\theta = \theta^*}
\] (46)
\[
= \sum_s d^\alpha(s) Z_\alpha(s) \nabla_\theta KL \left( \left( \pi^*(s) Q_\pi^*(s, a)^{1/\alpha} \right)^\alpha \pi^*(a|s) ^{1-\alpha} || \pi \right) \bigg|_{\pi = \pi^*},
\] (47)
where \( Z_\alpha(s) = \sum_a \pi^* (|s)Q^*(s, a)^{\frac{1}{\alpha}} \) is the normalization constant. Hence, each iteration of Eq. 38 will leave \( \pi^* \) unchanged.

Hence, we see that, if \( \pi^*(\pi^*)^{1-\alpha} = R\pi^* \), the iterative process described in Eq. 38 initialized with \( z_0 = \pi^* \) will be stationary with \( z_i = \pi^* \) for all \( i \). This gives us the form we need for \( \pi = \mathcal{I}^{\alpha} \pi^* \). Indeed, we must have

\[
\pi^*(\pi^*)^{1-\alpha} = Q\pi^* \\
(\mathcal{I}^{\alpha} \pi^*)^{\alpha}(\pi^*)^{1-\alpha} = Q\pi^* \\
\mathcal{I}^{\alpha} \pi^* = [Q(\pi^*)^\alpha]^{1/\alpha} \\
= Q^{1/\alpha} \pi^* \\
\mathcal{I}^{\alpha} = (\pi \rightarrow Q^{1/\alpha}) \tag{52}
\]

\[ \square \]

E Lower bounds

E.1 Trajectory formulation

We state here the proposition for the trajectory formulation

**Proposition 10** (Trajectory formulation). For any two distributions \( \pi \) and \( \mu \), we have

\[
J(\pi) \geq J(\mu) \left( 1 - KL(\mathcal{I}_\alpha \mu || \pi) + KL(\mathcal{I}_\alpha \mu || \mu) \right) \tag{53}
\]

Hence, any policy \( \pi \) such that \( KL(\mathcal{I}_\alpha (\pi_t) || \pi) < KL(\mathcal{I}_\alpha (\pi_t) || \pi_t) \) implies \( J(\pi) > J(\pi_t) \).

**Proof.** Let \( \pi \) and \( \mu \) be two arbitrary distributions over trajectories such that the support of \( \pi \) is included in that of \( \mu \). Then

\[
J(\pi) = \int_{\tau} R(\tau)\pi(\tau) \, d\tau \\
= \int_{\tau} R(\tau)\frac{\pi(\tau)}{\mu(\tau)} \mu(\tau) \, d\tau \\
\geq \int_{\tau} R(\tau) \left( 1 + \log \frac{\pi(\tau)}{\mu(\tau)} \right) \mu(\tau) \, d\tau \\
= \int_{\tau} R(\tau)\mu(\tau) \, d\tau + \int_{\tau} R(\tau)\mu(\tau) \log \pi(\tau) \, d\tau - \int_{\tau} R(\tau)\mu(\tau) \log \mu(\tau) \, d\tau \\
= J(\mu) - J(\mu)KL(R\mu || \pi) + J(\mu)KL(R\mu || \mu) \\
J(\pi) \geq J(\mu) \left( 1 - KL(R\mu || \pi) + KL(R\mu || \mu) \right) \tag{59}
\]

\[ \square \]

E.2 State-action formulation

To prove that minimizing Eq. 4 is equivalent to maximizing a lower bound on the expected return \( J \), we shall show that this function has the same gradient as a lower bound \( J_\mu \) on \( J \) and thus only differs by a constant.

**Proposition 11.** The function \( J_\mu \) defined as

\[
J_\mu(\pi) = \sum_{h=0}^{H} \gamma^h \int_{\tau_h} R_{-1}(\tau_h) \left( 1 + \log \frac{\pi_h(\tau_h)}{\mu_h(\tau_h)} \right) \mu_h(\tau_h) \, d\tau_h , \tag{60}
\]

where \( \tau_h \) is a trajectory of length \( h \) that is a prefix of a full trajectory \( \tau \), \( H \) is the horizon (which can be infinite), \( \pi_h \) is the policy restricted to trajectories of length \( h \), and \( R_{-1}(\tau_h) \) is the reward observed at the last state of the trajectory, satisfies \( J_\mu(\pi) \leq J(\pi) \) for any \( \mu \) and any \( \pi \) such that the support of \( \mu \) covers that of \( \pi \).
Proof. We can rewrite
\[
J(\pi) = \int_{\tau} R(\tau) \pi(\tau) \, d\tau
\]
\[
= \int_{\tau} \left( \sum_{h=1}^{H} R(a_h, s_h) \right) \pi(\tau) \, d\tau
\]
\[
= \sum_{h=0}^{H} \gamma^h \int_{\tau_h} R_{-1}(\tau_h) \pi_h(\tau_h) \, d\tau_h
\]

Then, using the same technique as for the trajectory formulation, we have
\[
J(\pi) = \sum_{h=0}^{H} \gamma^h \int_{\tau_h} R_{-1}(\tau_h) \frac{\pi_h(\tau_h)}{\mu_h(\tau_h)} \mu_h(\tau_h) \, d\tau_h
\]
\[
\geq \sum_{h=0}^{H} \gamma^h \int_{\tau_h} R_{-1}(\tau_h) \left( 1 + \log \frac{\pi_h(\tau_h)}{\mu_h(\tau_h)} \right) \mu_h(\tau_h) \, d\tau_h
\]
\[
= J_\mu(\pi).
\]

Then we can prove the following proposition:

**Proposition 6.** For any two policies \( \pi \) and \( \mu \) such that the support of \( \mu \) covers that of \( \pi \), we have
\[
J(\pi) \geq J(\mu) + \mathbb{E}_\mu[V^\mu(s)](D_\mu(\mathcal{I}_V || \mu) - D_\mu(\mathcal{I}_V || \mu)).
\]

Hence, any policy \( \pi \) such that \( D_\pi(\mathcal{I}_V || \pi) < D_\pi(\mathcal{I}_V || \pi) \) implies \( J(\pi) > J(\pi) \).

**Proof.** Since \( J_\mu \) is a lower bound on \( J \), by proposition 1 we prove that its gradient is the same as that of

\[
\nabla_\theta J_\mu(\pi) = \nabla_\theta \left( \sum_{h=0}^{H} \gamma^h \int_{\tau_h} R_{-1}(\tau_h) \left( 1 + \log \frac{\pi_h(\tau_h)}{\mu_h(\tau_h)} \right) \mu_h(\tau_h) \, d\tau_h \right)
\]
\[
= \nabla_\theta \left( \sum_{h=0}^{H} \gamma^h \int_{\tau_h} R_{-1}(\tau_h) \log \pi_h(\tau_h) \mu_h(\tau_h) \, d\tau_h \right)
\]
\[
= \sum_{h=0}^{H} \gamma^h \int_{\tau_h} R_{-1}(\tau_h) \nabla_\theta \log \pi_h(\tau_h) \mu_h(\tau_h) \, d\tau_h
\]
\[
= \sum_{h=0}^{H} \gamma^h \int_{\tau_h} r(s_h, a_h) \left( \sum_{h'=0}^{H} \nabla_\theta \log \pi(a_h' | s_h') \right) \mu_h(\tau_h) \, d\tau_h
\]
\[
= \int_{\tau} \sum_{h'=0}^{H} \nabla_\theta \log \pi(a_h' | s_h') \left( \sum_{h=0}^{H} \gamma^h r(s_h, a_h) \right) \mu(\tau) \, d\tau
\]
\[
= \sum_{h=0}^{H} \sum_s \sum_a \nabla_\theta \log \pi(a | s) d^h(\mu)(s) \mu(a | s) \gamma^h Q^\mu(s, a)
\]
\[
= \sum_{h'=0}^{H} \sum_s d^h(\mu)(s) \sum_a \nabla_\theta \log \pi(a | s) \mu(a | s) \gamma^h Q^\mu(s, a)
\]
\[
= \sum_s d^\mu(s) \sum_a Q^\mu(s, a) \mu(a | s) \nabla_\theta \log \pi(a | s)
\]
\[
= \nabla_\theta \left( -\sum_s d^\mu(s) V^\mu(s) KL(Q^\mu || \pi) \right)
\]
Hence these two functions only differ by a constant. Using $J_{\pi}(\pi) = \pi$, we identify the constant as being $J(\mu) + E_{\mu}[V^\mu(s)]D_{\mu}(\mu)$.

F Experimental Details

We reiterate the details of our didactic empirical study in the four-room domain [Sutton et al., 1999]. An agent starts in the lower-left corner and seeks to reach the upper-right corner; upon entering the goal state, the agent receives a reward of +1 and terminates the episode. The policy is parameterized by softmax probabilities, $\pi_{\theta}(a|s) = \frac{\exp(\theta_{a})}{\sum_{a \in A} \exp(\theta_{a})}$ for $\theta \in \mathbb{R}^{|A|}$, where all states share the same parameters. As with our analysis, these experiments compute gradients and operators exactly; in practice, stochasticity from sampling and approximate value estimation can affect the resultant performance. In Figure 1, we plot policies in the sub-segment $\{(0.1, 0.8t, 0.8(1 - t), 0.1) : t \in [0, 1]\}$, denoting the probability of taking the down, left, up, and right actions respectively.

F.1 Multi-step operators with line search

Proposition 6 implies that the single-step improvement operator converges to a desired solution by demonstrating that it fully minimizes a lower bound on the expected return. As partial minimization of this lower-bound also implies convergence, we propose a line-search approach that chooses the minimum $\alpha$ under which the lower-bound is optimized. Specifically, letting $L_{\mu}(\pi)$ be the lower bound in Proposition 6, we choose the lowest alpha such that

$$L_{\mu}(\mu) - L_{\mu}(\mathcal{P}_{\alpha}^1 \mu) \geq \frac{1}{2}(L_{\mu}(\mu) - L_{\mu}(\mathcal{P}_{1} \mu))$$

(76)