Differentiable Bandit Exploration

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Abstract

We learn bandit policies that maximize the average reward over bandit instances drawn from an unknown distribution \( P \), from a sample from \( P \). Our approach is an instance of meta-learning and its appeal is that the properties of \( P \) can be exploited without restricting it. We parameterize our policies in a differentiable way and optimize them by policy gradients – an approach that is easy to implement and pleasantly general. Then the challenge is to design effective gradient estimators and good policy classes. To make policy gradients practical, we introduce novel variance reduction techniques. We experiment with various bandit policy classes, including neural networks and a novel soft-elimination policy. The latter has regret guarantees and is a natural starting point for our optimization. Our experiments highlight the versatility of our approach. We also observe that neural network policies can learn implicit biases, which are only expressed through sampled bandit instances during training.

1. Introduction

A stochastic bandit (Lai & Robbins, 1985; Auer et al., 2002; Lattimore & Szepesvari, 2019) is an online learning problem where the learning agent sequentially pulls arms to incur stochastic rewards. The goal of the agent is to maximize its expected cumulative reward. Since the agent does not know the mean rewards of the arms in advance, it must learn them by pulling the arms. This results in the so-called exploration-exploitation trade-off: explore, and learn more about an arm; or exploit, and pull the arm with the highest estimated reward thus far. One example of a bandit is a clinical trial, where the arm is a treatment and its reward is the outcome of that treatment on a patient.

Bandit algorithms are typically designed to have low regret, worst-case or instance-adaptive, for a problem class chosen by the designer (Lattimore & Szepesvari, 2019).

While such regret guarantees are reassuring, this approach is somewhat inflexible. In particular, it may result in algorithms that are overly conservative, since they do not exploit all properties of the actual problem class or objective. An alternative, which we explore in this work, is to learn a bandit algorithm. Specifically, we assume that the learner has access to sampled bandit instances from an unknown distribution \( P \) and the goal is to learn a bandit algorithm that achieves a high reward on average over the instances drawn from \( P \), the so-called Bayes reward. In essence, we automatize the learning of policies for Bayesian bandits (Berry & Fristedt, 1985). Our approach can be viewed as an instance of meta-learning (Thrun, 1996; 1998; Baxter, 1998; 2000) by gradient ascent (Finn et al., 2017).

A classic approach to Bayesian bandits is to design Bayes optimal policies (Gittins, 1979; Gittins et al., 2011), which take a simple form for specific priors \( P \). Our approach is more general, since it makes minimal assumptions about \( P \) and optimized policies. It is also more computationally efficient and easy to parallelize. However, we lose guarantees on Bayes optimality. Another line of work (Russo & Van Roy, 2014; Wen et al., 2015; Russo & Van Roy, 2016) bounds the Bayes regret of various classic bandit policies. These policies tend to be more conservative than our approach because we directly optimize the quantity of interest, the Bayes reward of the policy.

Overall, our aim is to make learning of bandit policies as seamless as applying gradient descent to supervised learning problems. This work makes the following progress towards this goal. First, we carefully formulate the problem of policy-gradient optimization of the Bayes reward of bandit policies. Second, we derive the reward gradient and propose subtracting specific novel baselines to reduce the variance of its empirical estimate. This is critical to making our approach practical. These baselines are available thanks to the specific form of our meta-learning problem. Third, we show how to differentiate several softmax bandit policies: Exp3, SoftElim, and neural networks with a softmax output layer. SoftElim is a new algorithm where the probability of pulling an arm is directly parameterized. We prove that the \( n \)-round regret of SoftElim is sublinear in \( n \) in any 2-armed bandit, as in UCB1 and TS. However, unlike UCB1 and TS, SoftElim can be easily differentiated and further optimized. Finally, we empirically evaluate our techniques on several tasks and compare them with existing baselines.

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methodology on a range of bandit problems. Our experiments highlight the versatility of our approach. We also show that neural network policies can automatically learn interesting biases encoded in the prior distribution $P$.

2. Setting

We start by introducing notation. The expectation operator is denoted by $\mathbb{E} [\cdot]$ and the corresponding probability measure is $P (\cdot)$. We define $[n] = \{1, \ldots, n\}$ and denote the $i$-th component of vector $x$ by $x_i$.

A Bayesian multi-armed bandit (Gittins, 1979; Berry & Fristedt, 1985) is an online learning problem where the learning agent interacts with problem instances that are drawn i.i.d. from a known prior distribution. We formally define the problem as follows. Let $K$ be the number of arms and $n$ be the number of rounds. Let $P$ be a prior distribution over problem instances. Each problem instance $P$ is a joint probability distribution of arm rewards with support $[0, 1]^K$. Let $Y_{i,t}$ be the reward of arm $i$ in round $t$ and $Y_t = (Y_{1,t}, \ldots, Y_{K,t})$ be a vector of all rewards in round $t$. Before the learning agent interacts with the environment, $P \sim P$ and $Y_t \sim P$ for all $t \in [n]$. Then, in round $t \in [n]$, the agent pulls arm $I_t \in [K]$ and observes its reward $Y_{I_t,t}$. The agent knows $P$ but not $P$, the problem instance that it interacts with.

We define $I_{i:t} = (I_1, \ldots, I_t)$ and $Y_{i:t} = (Y_{i,1}, \ldots, Y_{i,t})$, with the corresponding $n$-round quantities being $I = I_{1:n}$ and $Y = Y_{1:n}$. Let $H_t = (I_1, \ldots, I_t, Y_{I_{1:t},1}, \ldots, Y_{I_{1:t},t})$ be the history of the learning agent in the first $t$ rounds.

Our learning agent is parameterized by a parameter vector $\theta \in \Theta$, where $\Theta \subseteq \mathbb{R}^d$ is the space of feasible parameters. We refer to the agent as a policy. We denote by $p_\theta (i \mid I_{1:t-1}, Y_{1:t-1})$ the probability that policy $\theta$ pulls arm $i$ in round $t$, conditioned on all previously pulled arms $I_{1:t-1} \in [K]^{t-1}$ and their rewards $Y_{1:t-1} \in [0, 1]^{t-1}$. Thus $I_t \sim p_\theta (\cdot \mid H_{t-1})$. The $n$-round Bayes reward of $\theta$ is

$$r(n; \theta) = \mathbb{E} \left[ \sum_{t=1}^n Y_{I_t,t} \right],$$

where the expectation is over problem instances $P$, the random realizations of rewards $Y$, and the randomness in choosing $I_t$. We want to learn a policy that maximizes the $n$-round Bayes reward, $\theta_* = \arg \max_{\theta \in \Theta} r(n; \theta)$. This is equivalent to minimizing the $n$-round Bayes regret,

$$R(n; \theta) = \mathbb{E} \left[ \sum_{t=1}^n Y_{i_*(P),t} - \sum_{t=1}^n Y_{I_t,t} \right],$$

where $i_*(P) = \arg \max_{i \in [K]} \mathbb{E} [Y_{i,1} \mid P]$ is the best arm in problem instance $P$.

3. Policy Optimization

Our main idea is to maximize (2) approximately on sampled problem instances from the prior distribution $P$. This distribution is assumed to be known in Bayesian bandits. We solve the maximization problem iteratively by gradient ascent, using a simple and extremely general design.

We develop GradBand, an iterative algorithm for gradient-based optimization of bandit policies, and show it in Algorithm 1. GradBand is initialized with policy $\theta_0 \in \Theta$, from some policy class $\Theta$.

We start by introducing notation. The expectation operator is denoted by $\mathbb{E} [\cdot]$ and the corresponding probability measure is $P (\cdot)$. We define $[n] = \{1, \ldots, n\}$ and denote the $i$-th component of vector $x$ by $x_i$. 3.3. Other Objectives and Algorithm Designs

Before we proceed, we want to contrast our objective and algorithm design to other common choices. Our objective, the maximization of $\mathbb{E} \sum_{t=1}^n Y_{I_t,t}$, differs from the maximization of $\mathbb{E} \sum_{t=1}^n Y_{I_t,t} \mid P$ in any problem instance $P$, which is standard in stochastic multi-armed bandits (Lai & Robbins, 1985; Auer et al., 2002; Lattimore & Szepesvari, 2019). The latter objective is more demanding, as it requires optimizing equally for likely and unlikely problem instances $P \sim P$. Our objective is more appropriate when $P$ can be estimated from data and the average reward is preferred to guarding against worst-case failures.

Early works on Bayesian bandits (Gittins, 1979; Berry & Fristedt, 1985; Gittins et al., 2011) focused on deriving Bayes optimal policies. Such policies tend to require specific conjugate priors $P$ and are costly to compute. We do
Algorithm 1 Gradient-based optimization of bandit policies.

1: Inputs: Initial policy \( \theta_0 \in \Theta \), number of iterations \( L \), learning rate \( \alpha \), and batch size \( m \)

2: for \( \ell = 1, \ldots, L \) do
3:   for \( j = 1, \ldots, m \) do
4:     Sample \( P^j \sim \mathcal{P} \) and then \( Y^j \sim P^j \)
5:     Apply policy \( \theta_{\ell-1} \) to \( Y^j \) and obtain \( I^j \)
6:     Let \( \hat{g}(n; \theta_{\ell-1}) \) be an estimate of \( \nabla \log r(n; \theta_{\ell-1}) \)
7:       from \( (Y^j)^m_{j=1} \) and \( (P^j)^m_{j=1} \)
8:   \( \theta_\ell \leftarrow \theta_{\ell-1} + \alpha \hat{g}(n; \theta_{\ell-1}) \)

9: Output: Learned policy \( \theta_L \)

The key to our derivations is that the joint probability distribution over pulled arms in the first \( t \) rounds, conditioned on \( Y \), decomposes as

\[
P(I_{1:t} = i_{1:t} | Y) = \prod_{s=1}^{t} P(I_s = i_s | I_{1:s-1} = i_{1:s-1}, Y) \tag{4}
\]

by the chain rule of probabilities. Since the policy does not act based on future rewards, we have for any \( s \in [n] \) that

\[
P(I_s = i_s | I_{1:s-1} = i_{1:s-1}, Y) = p_\theta(i_s | i_{1:s-1}, (Y_{i_1,1}, \ldots, Y_{i_{s-1},s-1})) \tag{5}
\]

Finally, we use that \( \nabla \log f(\theta) = f(\theta) \nabla \log f(\theta) \) holds for any non-negative differentiable \( f \). This identity is known as the score-function identity (Aleksandrov et al., 1968) and is the basis of all policy-gradient methods. We apply it to \( \mathbb{E}[Y_{I_{t:t}} | Y] \) and obtain

\[
\nabla \theta \mathbb{E}[Y_{I_{t:t}} | Y] = \sum_{i_t} Y_{i_t,t} \nabla \theta P(I_{1:t} = i_{1:t} | Y) = \sum_{i_t} Y_{i_t,t} \mathbb{P}(I_{1:t} = i_{1:t} | Y) \nabla \theta \log P(I_{1:t} = i_{1:t} | Y) \]

\[
= \sum_{s=1}^{t} \mathbb{E}[Y_{I_{t:t}} \log p_\theta(I_s | H_{s-1}) | Y] ,
\]

where the last equality follows from (4) and (5). Now we chain all equalities to obtain the reward gradient

\[
\nabla \theta r(n; \theta) = \sum_{s=1}^{t} \sum_{l=1}^{n} \mathbb{E}[Y_{I_{l:t}} \nabla \theta \log p_\theta(I_s | H_{s-1})] \tag{6}
\]

\[
= \sum_{l=1}^{n} \mathbb{E} \left[ \nabla \theta \log p_\theta(I_l | H_{l-1}) \sum_{s=l}^{n} Y_{I_{l:s}} \right] .
\]

The empirical reward gradient given \( m \) samples is

\[
\hat{g}(n; \theta) = \frac{1}{m} \sum_{j=1}^{m} \sum_{l=1}^{n} \nabla \theta \log p_\theta(I_{l}^j | H_{l-1}^j) \sum_{s=l}^{n} Y_{I_{l,s}}^j ,
\]

where \( j \) indexes the \( j \)-th random experiment in \texttt{GradBand}.

4.2. Baseline Subtraction

The empirical gradient in (7) can have a very large variance, because a change in the policy in round \( t \) affects all future rewards. This is manifest in the \( \Omega(n^2) \) reward terms in (7). We now investigate baseline subtraction to reduce this variance. The baseline is chosen such that it does not change the reward gradient in (6). We compare to our design to other common approaches in Section 7.
Lemma 1. Let $b_t : [K]^{t-1} \times [0, 1]^{K \times n} \rightarrow \mathbb{R}$ be any function of $t - 1$ previously pulled arms and all reward realizations. Then

$$E[b_t(I_{1:t-1}, Y)\nabla \log p_{\theta}(I_t \mid H_{t-1})] = 0.$$ 

Proof. The lemma is proved in Appendix C. 

The proof of Lemma 1 relies on the observation that $b_t$ is independent of the future actions of policy $\theta$. Therefore, $b_t$ can be also a function of problem instance $P$ and $\theta$, although we do not make this dependence explicit.

We refer to the collection of functions $(b_t)_{t=1}^n$ as baseline $b$. The reward gradient with subtracted baseline $b$ is

$$\nabla \theta r(n; \theta) = \sum_{t=1}^n E \left[ \nabla \theta \log p_{\theta}(I_t \mid H_{t-1}) \times \left( \sum_{s=t}^n Y_{t,s} - b_t(I_{1:t-1}, Y) \right) \right].$$

(8)

The corresponding empirical gradient from $m$ samples is

$$\hat{g}(n; \theta) = \frac{1}{m} \sum_{j=1}^m \sum_{t=1}^n \nabla \theta \log p_{\theta}(I_t^j \mid H_{t-1}) \times \left( \sum_{s=t}^n Y_{t,s}^j - b_t(I_{1:t-1}, Y^j) \right),$$

(9)

where $j$ indexes the $j$-th random experiment in GradBand.

4.3. Baselines

We discuss several natural baselines below. The first is

$$b_t^{\text{NONE}}(I_{1:t-1}, Y) = 0.$$ 

In this case, (9) reduces to (7). This baseline is extremely poor and leads to slow learning of bandit policies even with short horizons (Section 6.2). The second baseline is

$$b_t^{\text{OPT}}(I_{1:t-1}, Y) = \sum_{s=t}^n Y_{t,s}^i(P),$$

where $i^*(P)$ is the best arm in problem instance $P$, as defined in (3). This baseline is suitable for tuning existing bandit policies that have theoretical guarantees. In particular, if a bandit policy has a high-probability guarantee on low regret, then $\sum_{s=t}^n Y_{t,s}^i(P) - Y_{t,t}^i$ is sublinear in $n$ with a high probability for any $P$. The limitation of $b_t^{\text{OPT}}$ is that the best arm may be unknown. This would be the case if GradBand was only given sampled realized rewards $Y^j$, but not sampled problem instances $P^j$.

The third baseline is the reward of an independent run of policy $\theta$. Let $(J_t)_{t=1}^n$ be the pulled arms in that run. Then the baseline is defined as

$$b_t^{\text{SELF}}(I_{1:t-1}, Y) = \sum_{s=t}^n Y_{J_t,s}.$$ 

Similar to $b_t^{\text{OPT}}$, this baseline is suitable for any bandit policy that concentrates on a single arm over time; but unlike $b_t^{\text{OPT}}$, $b_t^{\text{SELF}}$ does not need to know the best arm. In practice, $b_t^{\text{SELF}}$ is comparable to or better than $b_t^{\text{OPT}}$ (Section 6.2).

The last baseline is rewards of $n$ independent runs of policy $\theta$, one for each round $t$ that starts with history $H_{t-1}$. This baseline is generally superior to $b_t^{\text{SELF}}$. However, it is also computationally costly, so we do not evaluate it here. In Section 6, we empirically compare all other proposed baselines from this section.

5. Differentiable Algorithms

Most popular bandit algorithm designs, such as upper confidence bounds (UCBs) (Auer et al., 2002; Dani et al., 2008; Abbasi-Yadkori et al., 2011) and Thompson sampling (TS) (Thompson, 1933; Agrawal & Goyal, 2012; 2013), are not differentiable. To explain this more technically, let $p_\theta(i \mid H_{t-1})$ be the probability that an algorithm pulls arm $i$ given its history $H_{t-1}$ and parameters $\theta$, as defined in (1). In UCB algorithms, $p_\theta(i \mid H_{t-1}) \in [0, 1]$. The presence of the indicator means that it cannot be differentiated with respect to $\theta$. While TS methods are randomized, $p_\theta(i \mid H_{t-1})$ is induced by a hard maximization over random variables, and thus $p_\theta(i \mid H_{t-1})$ may not be differentiable at all $\theta$. Even if it was, $p_\theta(i \mid H_{t-1})$ is not known to have a closed form, and therefore its differentiation is computationally costly.

We introduce three softmax designs that can be differentiated analytically and derive a gradient for each of them. In Section 5.1, we discuss Exp3 (Auer et al., 1995), a popular algorithm for non-stochastic bandits. In Section 5.2, we propose a new stochastic algorithm where the probability of pulling an arm is proportional to the difference of its estimated mean from the highest estimated mean. This can be viewed as “soft” elimination of arms and is of independent interest. In Section 5.4, we propose a general neural network policy where the last layer is a softmax over arms.

All derived gradients in this section are conditioned on a fixed round $t$ and history $H_{t-1}$. To simplify notation, we define $p_{t,i} = p_\theta(i \mid H_{t-1})$. Although we do not study the $\varepsilon$-greedy (Sutton & Barto, 1998) or Boltzmann exploration (Sutton & Barto, 1998; Cesa-Bianchi et al., 2017), we note that they can be differentiated analogously.
5.1. Algorithm Exp3

Exp3 (Auer et al., 1995) is a popular algorithm for non-stochastic bandits, where the probability of pulling arm $i$ in round $t$ is

$$p_{i,t} = (1 - \theta) \frac{\exp[\eta S_{i,t}]}{\sum_{j=1}^{K} \exp[\eta S_{j,t}]} + \theta \frac{1}{K}, \quad (10)$$

where $S_{i,t}$ are sufficient statistics of arm $i$ in round $t$, $\eta$ is a learning rate, and $\theta$ is a parameter that guarantees sufficient exploration of all arms. In Exp3, $S_{i,t}$ is the estimated cumulative reward of arm $i$ in the first $t - 1$ rounds. It is updated in round $t$ as $S_{i,t+1} = S_{i,t} + 1\{I_t = i\} p_{i,t}^{-1} Y_{i,t}$ and initialized as $S_{i,0} = 0$.

When rewards are in $[0, 1]$, the regret bound of Auer et al. (1995) suggests setting

$$\eta = \theta / K, \quad \theta = \min \left\{ 1, \sqrt{K \log K / (e - 1)n} \right\}.$$

In this work, we optimize the choice of $\theta$ using policy gradients. When $\eta$ is set as above, the gradient can be written as follows.

**Lemma 2.** Let $p_{i,t}$ be defined as in (10). Let $\eta = \theta / K$, $V_{i,t} = \exp[\theta S_{i,t} / K]$, and $V_t = \sum_{j=1}^{K} V_{j,t}$. Then

$$\nabla_{\theta} \log p_{i,t} = \frac{1}{p_{i,t}} \left[ \frac{V_{i,t}}{V_t} \left( (1 - \theta) \left[ \frac{S_{i,t}}{K} - \sum_{j=1}^{K} \frac{V_{i,t} S_{j,t}}{V_{j,t} K} \right] - 1 \right) + \frac{1}{K} \right].$$

**Proof.** The lemma is proved in Appendix C. \qed

Although Exp3 is differentiable, it is too conservative in stochastic problems, even after we optimize $\theta$. Therefore, we propose a new algorithm SoftElim.

5.2. Algorithm SoftElim

Our bandit algorithm works as follows. Each arm is pulled once in the first $K$ rounds. Let $\hat{\mu}_{i,t}$ be the empirical mean of arm $i$ after $t$ rounds and $T_{i,t}$ be the number of pulls of arm $i$ after $t$ rounds. Then in round $t > K$, arm $i$ is pulled with probability

$$p_{i,t} = \frac{\exp[\theta S_{i,t}]}{\sum_{j=1}^{K} \exp[\theta S_{j,t}]}, \quad (11)$$

where $\theta > 0$ is a tunable parameter and

$$S_{i,t} = -2 \left( \max_{j \in [K]} \hat{\mu}_{j,t-1} - \hat{\mu}_{i,t-1} \right)^2 T_{i,t-1}. \quad (12)$$

Since $\exp[\theta S_{i,t}] \in [0, 1]$ and $p_{i,t}$ is defined as in (11), this algorithm can be viewed as “soft” elimination of arms with low empirical means. Therefore, we call it SoftElim.

This design has two important properties. First, an arm is unlikely to be pulled if it has been pulled “often” and its empirical mean is low relative to the highest mean. Second, when a suboptimal arm has been pulled “often” and has the highest empirical mean, the optimal arm is pulled proportionally to how much its empirical mean is likely to deviate from the actual mean. Because of this, $\exp[\theta S_{i,t}]$ resembles the upper bound in Hoeffding’s inequality. This latter property implies optimism.

Since $\log p_{i,t} = \theta S_{i,t} - \log \sum_{j=1}^{K} \exp[\theta S_{j,t}]$, we have

$$\nabla_{\theta} \log p_{i,t} = S_{i,t} - \frac{\sum_{j=1}^{K} S_{j,t} \exp[\theta S_{j,t}]}{\sum_{j=1}^{K} \exp[\theta S_{j,t}]}.$$

Therefore, SoftElim can be easily differentiated and used in our gradient estimators.

5.3. Analysis of SoftElim

We informally justify SoftElim with $\theta = 1$. Fix any 2-armed bandit where arm 1 is optimal, that is $\mu_1 > \mu_2$. Let $\Delta = \mu_1 - \mu_2$. Fix any round $t$ by which arm 2 has been pulled “often”, so that we get $T_{2,t-1} = \Omega(\Delta^{-2} \log n)$ and $\hat{\mu}_{2,t-1} \leq \mu_2 + \Delta/3$ with high probability. Let $\hat{\mu}_{\max,t} = \max \{ \hat{\mu}_{1,t}, \hat{\mu}_{2,t} \}$.

Now consider two cases. First, when $\hat{\mu}_{\max,t-1} = \hat{\mu}_{1,t-1}$, by definition of $p_{1,t}$, arm 1 is pulled with probability of at least 0.5. Second, when $\hat{\mu}_{\max,t-1} = \hat{\mu}_{2,t-1}$, we have

$$p_{1,t} = \exp[-2(\hat{\mu}_{2,t-1} - \hat{\mu}_{1,t-1})^2 T_{1,t-1}] p_{2,t} \geq \exp[-2(\mu_1 - \hat{\mu}_{1,t-1})^2 T_{1,t-1}] p_{2,t},$$

where the last inequality holds with high probability, and follows from $\hat{\mu}_{1,t-1} \leq \hat{\mu}_{2,t-1} \leq \mu_2 + \Delta/3 \leq \mu_1$. Thus, arm 1 is pulled “sufficiently often” relative to arm 2, proportionally to the deviation of $\hat{\mu}_{1,t-1}$ from $\mu_1$.

As a consequence, SoftElim eventually enters a regime in which arm 1 has been pulled “often”, so that $T_{1,t-1} = \Omega(\Delta^{-2} \log n)$ and $\hat{\mu}_{1,t-1} \geq \mu_1 - \Delta/3$ with high probability. Then $S_{1,t} = 0$ and $S_{2,t} = -\Omega(\log n)$ hold with high probability, and arm 2 is unlikely to be pulled.

This argument can be formalized to derive a regret bound. In particular, let the expected $n$-round regret of policy $\theta$ in problem instance $P$ be

$$R(n, P; \theta) = \mathbb{E} \left[ \sum_{t=1}^{n} Y_{i,(P),t} - Y_{i,t} \mid P \right], \quad (13)$$

where $i,(P)$ is defined as in (3). Then we have the following regret bound.
Theorem 3. Let \( P \) be any 2-armed bandit where arm 1 is optimal, that is \( \mu_1 > \mu_2 \). Let \( \Delta = \mu_1 - \mu_2 \) and \( \theta = 0.5 \). Then the \( n \)-round regret of SoftElim is bounded as

\[
R(n, P; \theta) \leq (e^2 + 2e + 3) \left( \frac{9}{\Delta} \log n + \Delta \right) + 5\Delta.
\]

Proof. The theorem is proved in Appendix B. \( \square \)

This upper bound has the standard dependence on the gap \( \Delta \) and \( \log n \), as in UCB1 (Auer et al., 2002).

5.4. Recurrent Neural Network

We can take designs (10) and (11) a step further. Both are softmaxes on hand-crafted features, which facilitate theoretical analysis. Now we attempt to learn the features using a recurrent neural network (RNN). The RNN works as follows. In round \( t \), it takes the pulled arm \( I_t \) and reward \( Y_{i,t} \) as inputs, updates its internal state \( s_t \), and outputs the probability \( p_{i,t+1} \) of pulling each arm \( i \) in the next round. More formally,

\[
\begin{align*}
    s_t &= \text{RNN}_\Phi(s_{t-1}, (I_t, Y_{i,t}, t)), \\
    p_{i,t+1} &= \frac{\exp[w_i^t s_t]}{\sum_{j=1}^{K} \exp[w_j^t s_t]}.
\end{align*}
\]

The optimized parameters \( \theta = (\Phi, \{w_i^t\}_{i=1}^{K}) \) are the RNN parameters \( \Phi \) and per-arm parameters \( w_i \). The aim for the RNN is to learn to track suitable sufficient statistics through its internal state \( s_t \). That state is initialized at \( s_0 = 0 \).

Our RNN is an LSTM (Hochreiter & Schmidhuber, 1997) with a \( d \)-dimensional latent state. We assume that the rewards are Bernoulli. The details of our implementation are in Appendix D.

6. Experiments

We conduct four experiments. In Section 6.1, we study the reward gradient and its variance in a simple problem. In Section 6.2, we optimize Exp3 and SoftElim policies on this problem. In Section 6.3, we study more complex problems. In Section 6.4, we discuss curriculum learning with policy gradients and then we apply it to RNN policies in Section 6.5. All policies are evaluated using the Bayes regret in (3), which offers a better indication of closeness to optimality than the Bayes reward; though optimizing either optimizes the other. We estimate the regret using 1 000 i.i.d. samples from \( P \), independent of the training instances in GradBand. Shaded areas in plots show standard errors.

6.1. Reward Gradient

Our first experiment is on a Bayesian bandit with \( K = 2 \) arms. The prior distribution \( P \) is over two problems, with means \( \mu = (0.6, 0.4) \) and \( \mu = (0.4, 0.6) \). Each problem is sampled from \( P \) with probability 0.5. The reward distributions are Bernoulli. The horizon is \( n = 200 \) rounds.

The Bayes regret of Exp3 and SoftElim, as a function of their parameter \( \theta \), is shown in Figure 1a. In both cases, it is unimodal in \( \theta \), and thus suitable for being optimized by GradBand. We observe that SoftElim has a lower regret than Exp3 for all \( \theta \). In fact, the lowest regret of Exp3 is higher than that of SoftElim without tuning, at \( \theta = 1 \).

The reward gradients of Exp3 and SoftElim are reported in Figures 1b and 1c, respectively. We observe that the gradients with baselines \( b^{\text{opt}} \) and \( b^{\text{SELF}} \) have orders of magnitude lower variance than those with \( b^{\text{NONE}} \). In SoftElim gradients, the variance due to \( b^{\text{opt}} \) and \( b^{\text{SELF}} \) is comparable. In Exp3 gradients, the variance due to \( b^{\text{SELF}} \) is two orders of magnitude lower for higher values of \( \theta \).

6.2. Policy Optimization

In the second experiment, we apply Exp3 and SoftElim to the problem in Section 6.1. The policies are optimized by GradBand; with \( \theta_0 = 1 \), \( L = 100 \) iterations, learning rate \( \alpha = c^{-1} L^{-\frac{1}{2}} \), and batch size \( m = 1000 \). The constant \( c \) is chosen automatically such that \( \| \hat{g}(n; \theta_0) \| \leq c \) holds with a high probability, and its purpose is to avoid manual tuning of the learning rate for each problem.

In Figure 2a, we optimize Exp3 with all baselines. For baseline \( b^{\text{SELF}} \), GradBand learns a near-optimal policy in less than 10 iterations. This is consistent with Figure 1b, where \( b^{\text{SELF}} \) has the lowest variance. In Figure 2b, we optimize SoftElim with all baselines. Both baselines \( b^{\text{opt}} \) and \( b^{\text{SELF}} \) perform comparably. This is consistent with Figure 1c, where the variances of \( b^{\text{opt}} \) and \( b^{\text{SELF}} \) are comparable. We conclude that \( b^{\text{SELF}} \) is the best baseline overall and use it in all remaining experiments.

To assess the quality of our policies, we compare them to three bandit baselines: UCB1 (Auer et al., 2002), Bernoulli TS (Agrawal & Goyal, 2012) with Beta(1, 1) prior, and the Gittins index (Gittins, 1979). We use the randomized Bernoulli rounding of Agrawal & Goyal (2012) to apply TS to \([0, 1]\) rewards. The Gittins index is computed up to 200 Bernoulli pulls, as described in Section 35 in Lattimore & Szepesvari (2019). This computation takes almost 2 days and requires about 200^8 elementary operations.

The regret of the baselines in 200 rounds is 10.00 ± 0.03 (UCB1), 5.46 ± 0.05 (TS), and 3.89 ± 0.07 (Gittins index). The regret of tuned SoftElim is about 4.75, which falls between that of TS and the Gittins index. We conclude that tuned SoftElim outperforms a strong baseline, TS; and performs almost as well as the Gittins index. The optimization of SoftElim by GradBand takes about 20 seconds. This is nearly four orders of magnitude faster than
the computation of the Gittins index.

6.3. More Complex Problems

In the third experiment, we apply GradBand to two more complex problems. In both, the number of arms is $K = 10$ and the mean reward of arm $i$ is $\mu_i \sim \text{Beta}(1, 1)$. In the first bandit, the reward distribution of arm $i$ is $\text{Ber}(\mu_i)$. In the second bandit, the reward distribution of arm $i$ is $\text{Beta}(\nu\mu_i, \nu(1 - \mu_i))$, where $\nu = 4$ controls the variance of rewards. The horizon is $n = 1000$ rounds.

The regret of our learned policies is reported in Figure 2c. In the Bernoulli problem, the regret of tuned SoftElim is less than 25. By comparison, the regret of TS is 28.57 ± 0.45. In the beta problem, the regret of tuned SoftElim is close to 10. The regret of TS remains the same and is roughly three times that of SoftElim. The poor performance of TS is due to the Bernoulli rounding, which does not allow TS to distinguish between the Bernoulli and beta problems.

6.4. Curriculum Learning

Our initial experiments showed that learning of RNN policies (Section 5.4) for longer horizons, such as $n = 200$, is challenging if we use our variance reduction baselines (Section 4.3) alone. Thus, we propose an additional variance reduction technique, which is motivated by curriculum learning (Bengio et al., 2009).

The key idea is to apply GradBand successively to problems with increasing horizons. Let $M$ be the number of stages and $n_1 < \cdots < n_M$ be $M$ increasing horizons such that $n_M = n$. Let $\theta_i$ denote the output of GradBand at stage $i$. At stage $i \in [M]$, we run GradBand with initial policy $\theta_{i-1}$ and horizon $n_i$, and output policy $\theta_i$.

The reduction in variance arises as follows. Suppose that GradBand outputs policy $\theta_i$ that minimizes the empirical gradient at stage $i$, that is $\hat{g}(n_i; \theta_i) = 0$. By definition (9), $\hat{g}(n_i; \theta_i)$ is the sum of $\hat{g}(n_i; \theta_i)$ and additional $(n_i + 1 - n_i) n_{i+1}$ terms. Since $\hat{g}(n_i; \theta_i) = 0$, the variance at $\theta_i$ can arise only due to the extra terms.

6.5. RNN Policies

In the last experiment, we showcase RNN policies, which are learned by curriculum learning (Section 6.4). We use horizon $n = 200$; $M = 2$ curriculum stages with $n_1 = 20$ and $n_2 = n = 200$ (we did not optimize these values); and $L = 1000$ GradBand iterations. Results from the last stage of curriculum learning are reported in Figure 3.

We learn an RNN policy for the problem in Section 6.1 in Figure 3a. We observe that the policy outperforms both TS and the Gittins index. This does not contradict theory, as the Gittins index is not Bayes optimal in this problem. In Figure 3b, we consider the same problem, except that the mean reward of arm $i$ is $\mu_i \sim \text{Beta}(1, 1)$. We know that the Gittins index is Bayes optimal in this problem and we
do not outperform it. Nevertheless, our policy has a lower regret than TS.

In the last experiment, we have a $K$-armed Bayesian bandit with Bernoulli rewards. The prior distribution $\mathcal{P}$ is over two problem instances, $\mu = (0.6, 0.9, 0.7, 0.7, \ldots, 0.7)$ and $\mu = (0.2, 0.7, 0.9, 0.7, \ldots, 0.7)$, which are equally likely. This problem has an interesting structure. The problem instance, and thus the optimal arm, can be identified by pulling arm 1. Arms 4 and beyond are distractors. Our RNN policies do not learn this exact structure; but they do learn another strategy specialized to this problem. The strategy pulls only arms 2 or 3, as these are the only arms that can be optimal. Thus, the RNN successfully learns to ignore the distractors. As a result, the Bayes regret of our policies (Figure 3c) does not increase with $K$. This would not happen with classic bandit algorithms.

### 7. Related Work

Offline tuning of bandit algorithms often reduces their empirical regret (Vermorel & Mohri, 2005; Kuleshov & Precup, 2014). Maes et al. (2012) tuned existing algorithms and also learned linear policies of historical features. Hsu et al. (2019) proposed, analyzed, and evaluated a best-arm identification algorithm for bandit algorithm tuning. None of these papers used policy gradients, neural network policies, or even leveraged the sequential character of $n$-round rewards (Section 4).

Our approach is a variant of meta-learning (Thrun, 1996; 1998), where a learning algorithm is learned on a sample of tasks, to perform well on tasks that are drawn from the same distribution (Baxter, 1998; 2000). These approaches have been very successful recently in deep reinforcement learning (RL) (Finn et al., 2017; 2018; Mishra et al., 2018). Sequential multitask learning (Caruana, 1997) was studied in multi-armed bandits by Azar et al. (2013) and in contextual bandits by Deshmukh et al. (2017). In comparison, our setting is offline. A general template for sequential meta-learning was presented in Ortega et al. (2019). This work is conceptual and does not study policy gradients.

The score-function identity in Section 4.1 is due to Aleksandrov et al. (1968). Policy gradients in RL were proposed by Williams (1992), including the idea of baseline subtraction. Other earlier works on this topic are Sutton et al. (2000) and Baxter & Bartlett (2001). Policy gradients are plagued with a high variance. Therefore, the design of variance minimizing baselines was subject to numerous works (Greensmith et al., 2004; Zhao et al., 2011; Dick, 2015). Among these, Munos (2006) attained geometric variance reduction using sequential control variates and Liu et al. (2018) proposed control variates that also depend on the action. Our baselines differ from those in RL. Since the space of histories grows exponentially with round $t$, we use a Monte-Carlo estimate of future rewards, and do not estimate the $Q$ or value functions.

Both Yu et al. (2018) and Duan et al. (2016) applied policy gradients to multi-armed bandits. The policy of Yu et al. (2018) does not seem sound and is not compared to any bandit baseline. Their derived gradient also seem incorrect, since it neglects the cumulative effect of past actions on rewards. In Duan et al. (2016), a similar policy to our RNN policy (Section 5.4) was optimized using an existing optimizer. None of these papers formalizes the objective clearly, relates it to Bayesian bandits, or studies policies that are provably sound (Section 5.2 and Appendix A). We go beyond these works in both depth and breadth. Silver et al. (2014) applied policy gradients to a continuous bandit problem with a quadratic cost function. Since the cost is convex in arms, this exploration problem is easier than with discrete arms.

The design of SoftElim in (11) resembles Boltzmann exploration (Sutton & Barto, 1998; Cesa-Bianchi et al., 2017) and Exp3 (Section 5.1). The key difference is in how $S_{i,t}$ in (12) is chosen. In Exp3 and Boltzmann exploration, $S_{i,t}$ only depends on the history of arm $i$. In SoftElim, $S_{i,t}$ depends on all arms and makes SoftElim sufficiently optimistic. SoftElim can be also viewed as a form of elimination (Auer & Ortner, 2010), where suboptimal arms are
never eliminated, just pulled less often. Unlike traditional elimination algorithms, it is not conservative and outperforms Thompson sampling after tuning.

8. Conclusions

We take first steps towards understanding policy-gradient optimization of bandit policies. Our work addresses two main challenges of this problem. First, we derive the reward gradient of optimized policies and show how to estimate it efficiently from an empirical sample. Second, we propose novel differentiable bandit policies that can outperform state-of-the-art baselines after optimization. Our experiments highlight the simplicity and generality of our approach. We also show that neural network policies can learn interesting biases.

We leave open many questions of interest. First, we believe that our ideas can be generalized to structured problems, such as linear bandits. It is not obvious though, especially in RNN policies, how to restrict the policy class to learn such biases. Second, we find that the variance of empirical reward gradients can be overwhelmingly high, especially in RNN policies. Therefore, any progress in variance reduction would be of major importance. Finally, except for the explore-then-commit policy (Appendix A), we are unaware of any other policy class where the Bayes regret is provably unimodal in optimized parameters, and thus policy gradients lead to optimal solutions. Our experimental results (Figure 1a) suggest that other such classes may exist. We plan to investigate this more in future work.

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A. Concavity of the Bayes Reward

Let \( \mathcal{P} \) be any prior distribution over 2-armed bandits, where the reward distribution of arm \( i \) is \( \mathcal{N}(\mu_i, 1) \). The horizon is \( n \) rounds. We analyze the \( n \)-round Bayes reward of the explore-then-commit policy (Langford & Zhang, 2008). The policy is parameterized by \( \theta \in [[n/2]] \) and works as follows. In the first \( 2\theta \) rounds, it explores and pulls each arm \( \theta \) times. Let \( \hat{\mu}_{i,\theta} \) be the average reward of arm \( i \) after \( \theta \) pulls. Then, if \( \hat{\mu}_{i,\theta} > \hat{\mu}_{2,\theta} \), arm 1 is pulled for the remaining \( n - 2\theta \) rounds. Otherwise arm 2 is pulled.

Fix any problem instance \( P \sim \mathcal{P} \). Without loss of generality, let arm 1 be optimal, that is \( \mu_1 > \mu_2 \). Let \( \Delta = \mu_1 - \mu_2 \). The key observation is that the expected \( n \)-round reward in problem instance \( P \) has a closed form

\[
r(n, P; \theta) = \mu_1 n - \Delta [\theta + f(\theta)(n - 2\theta)] ,
\]

where

\[
f(\theta) = \mathbb{P}(\hat{u}_{1,\theta} < \hat{u}_{2,\theta}) = \mathbb{P}(\hat{u}_{1,\theta} - \hat{u}_{2,\theta} < 0) = \frac{1}{\sqrt{2\pi}} \int_{x=-\infty}^{-\Delta} \exp \left(-\frac{x^2\theta}{4}\right) dx .
\]

The last equality follows from the fact that \( \hat{u}_{1,\theta} - \hat{u}_{2,\theta} \sim \mathcal{N}(\Delta, 2/\theta) \).

Now we argue that \( f(\theta) \) is concave and decreasing in \( \theta \). As \( f(\theta) \) is an integral of \( \exp[-x^2\theta/4] \) with respect to \( x \), it suffices to show this for all \( \exp[-x^2\theta/4] \), where \( x \in [-\infty, -\Delta] \). This follows from elementary algebra,

\[
\left( \exp \left[-\frac{x^2\theta}{4}\right] \right)' = -\frac{x^2}{4} \exp \left[-\frac{x^2\theta}{4}\right] , \quad \left( \exp \left[-\frac{x^2\theta}{4}\right] \right)'' = \frac{x^4}{16} \exp \left[-\frac{x^2\theta}{4}\right].
\]

Based on the above, we conclude that \( f(\theta) \geq 0, f'(\theta) \leq 0, \) and \( f''(\theta) \geq 0 \).

Let \( g(\theta) = n - 2\theta \) and \( \theta \in [0, n/2] \). Then trivially \( g(\theta) \geq 0, g'(\theta) \leq 0, \) and \( g''(\theta) = 0 \). Now we combine all facts about \( f, g, \) and their derivatives; and get that \( f(\theta)g(\theta) \) is convex in \( \theta \),

\[
(f(\theta)g(\theta))'' = (f'(\theta)g(\theta) + f(\theta)g'(\theta))' = f''(\theta)g(\theta) + 2f'(\theta)g'(\theta) + f(\theta)g''(\theta) \geq 0.
\]

It follows that \( \theta + f(\theta)g(\theta) \) is convex in \( \theta \), and thus (14) is concave in \( \theta \) for any problem instance \( P \sim \mathcal{P} \). Finally, note that the Bayes reward \( r(n; \theta) \) is just a weighted sum of (14), and thus is concave in \( \theta \). This concludes the proof.

The last remaining issue is that parameter \( \theta \) in the explore-then-commit policy cannot be optimized by GradBand, as it is discrete. To allow for optimization, we extend the explore-then-commit policy to continuous \( \theta \) by randomized rounding.

The randomized explore-then-commit policy is parameterized by continuous \( \theta \in [1, [n/2]] \). The discrete \( \hat{\theta} \) is chosen as \( \hat{\theta} = \lfloor \theta \rfloor + 1 \{X = 1\} \), where \( X \sim \text{Ber}(\theta - \lfloor \theta \rfloor) \). Then we execute the original policy with \( \hat{\theta} \). The key property of the randomized policy is that its \( n \)-round Bayes reward is a piecewise linear interpolation of that of the original policy,

\[
([\theta] - \theta) r(n; \lfloor \theta \rfloor) + (\theta - [\theta]) r(n; \lfloor \theta \rfloor)
\]

By definition, the above function is continuous for \( \theta \in [1, [n/2] - 1 \) and concave. Therefore, GradBand has the same guarantees for maximizing it as stochastic gradient descent on convex functions.
B. Proof of Theorem 3

We bound the $n$-round regret of SoftElim below. We focus on $K = 2$ arms and assume without loss of generality that $\mu_1 > \mu_2$. Let $\Delta = \mu_1 - \mu_2$. The regret bound is stated below.

**Theorem 3.** Let $P$ be any 2-armed bandit where arm 1 is optimal, that is $\mu_1 > \mu_2$. Let $\Delta = \mu_1 - \mu_2$ and $\theta = 0.5$. Then the $n$-round regret of SoftElim is bounded as

$$R(n, P; \theta) \leq (e^2 + 2e + 3) \left( \frac{9}{\Delta} \log n + \Delta \right) + 5\Delta.$$  

**Proof.** Each arm is initially pulled once. Thus, $R(n, P; \theta) \leq \Delta + \Delta \sum_{t=3}^{n} \mathbb{P}(I_t = 2)$. Now we decompose the sum as

$$\sum_{t=3}^{n} \mathbb{P}(I_t = 2, T_{2,t-1} \leq m) + \sum_{t=3}^{n} \mathbb{P}(I_t = 2, T_{2,t-1} > m, T_{1,t-1} \leq m) + \sum_{t=3}^{n} \mathbb{P}(I_t = 2, T_{2,t-1} > m, T_{1,t-1} > m).$$

In the rest of the proof, we bound each above term separately.

**B.1. Upper Bound on Term 1**

This bound is trivial. In particular, since $T_{2,t} = T_{2,t-1} + 1$ on event $I_t = 2$, we have

$$\sum_{t=3}^{n} \mathbb{P}(I_t = 2, T_{2,t-1} \leq m) \leq m. \quad (15)$$

**B.2. Upper Bound on Term 3**

Fix round $t$. Let

$$E_{1,t} = \left\{ \hat{\mu}_{1,t-1} > \mu_1 - \frac{\Delta}{3} \right\}, \quad E_{2,t} = \left\{ \hat{\mu}_{2,t-1} < \mu_2 + \frac{\Delta}{3} \right\},$$

be the events that the empirical means of arms 1 and 2, respectively, are “close” to their means. Then

$$\mathbb{P}(I_t = 2, T_{2,t-1} > m, T_{1,t-1} > m) \leq \mathbb{P}(I_t = 2, T_{2,t-1} > m, E_{1,t}) + \mathbb{P}(\bar{E}_{1,t}, T_{1,t-1} > m)$$

$$\leq \mathbb{P}(I_t = 2, T_{2,t-1} > m, E_{1,t}, E_{2,t}) + \mathbb{P}(\bar{E}_{1,t}, T_{1,t-1} > m) + \mathbb{P}(\bar{E}_{2,t}, T_{2,t-1} > m).$$

By Hoeffding’s inequality, we get that

$$\mathbb{P}(\bar{E}_{1,t} | T_{1,t-1} > m) = \mathbb{P} \left( \mu_1 - \hat{\mu}_{1,t-1} \geq \frac{\Delta}{3} | T_{1,t-1} > m \right) < \exp \left[ -\frac{2\Delta^2}{9m} \right] = n^{-2},$$

$$\mathbb{P}(\bar{E}_{2,t} | T_{2,t-1} > m) = \mathbb{P} \left( \hat{\mu}_{2,t-1} - \mu_2 \geq \frac{\Delta}{3} | T_{2,t-1} > m \right) < \exp \left[ -\frac{2\Delta^2}{9m} \right] = n^{-2},$$

for $m = \lceil 9\Delta^{-2} \log n \rceil$, which we assume below. It follows that

$$\mathbb{P}(I_t = 2, T_{2,t-1} > m, T_{1,t-1} > m) \leq \mathbb{P}(I_t = 2, T_{2,t-1} > m, E_{1,t}, E_{2,t}) + 2n^{-2}.$$  

Now note that events $E_{1,t}$ and $E_{2,t}$ imply that $\hat{\mu}_{1,t-1} - \hat{\mu}_{2,t-1} \geq \Delta/3$. So, on events $E_{1,t}, E_{2,t}$, and $T_{2,t-1} > m$, we have

$$p_{2,t} = \frac{\exp[-2\theta(\hat{\mu}_{1,t-1} - \hat{\mu}_{2,t-1})^2T_{2,t-1}]}{\exp[-2\theta(\mu_1 - \mu_2)^2T_{2,t-1}]} + 1 \leq \exp \left[ -\frac{2\theta\Delta^2}{9m} \right] = n^{-2\theta}.$$  

Finally, we chain all inequalities over all rounds and get that term 3 is bounded as

$$\sum_{t=3}^{n} \mathbb{P}(I_t = 2, T_{2,t-1} > m, T_{1,t-1} > m) \leq 2n^{-1} + n^{1-2\theta}. \quad (16)$$
B.3. Upper Bound on Term 2

Fix round \( t \). First, we apply the same trick as in term 3 and get
\[
P(I_t = 2, T_{2,t-1} > m, T_{1,t-1} \leq m) \leq P(I_t = 2, T_{1,t-1} \leq m, E_{2,t}) + n^{-2}.
\]

Let \( \hat{\mu}_{\max,t} = \max \{ \hat{\mu}_{1,t}, \hat{\mu}_{2,t} \} \). Now we substitute \( I_t = 1 \) for \( I_t = 2 \) based on two observations. First,
\[
p_{2,t} = \frac{\exp[-2\theta(\hat{\mu}_{\max,t-1} - \hat{\mu}_{2,t-1})^2 T_{2,t-1}]}{\exp[-2\theta(\hat{\mu}_{\max,t-1} - \hat{\mu}_{1,t-1})^2 T_{1,t-1}]} p_{1,t} \leq \exp[2\theta(\hat{\mu}_{\max,t-1} - \hat{\mu}_{1,t-1})^2 T_{1,t-1}] p_{1,t}.
\]

Second, on event \( E_{2,t} \), we have
\[
(\hat{\mu}_{\max,t-1} - \hat{\mu}_{1,t-1})^2 \leq (\mu_1 - \hat{\mu}_{1,t-1})^2 I \{ \hat{\mu}_{1,t-1} \leq \mu_1 \} .
\]

We prove this claim as follows. When \( \hat{\mu}_{\max,t-1} = \hat{\mu}_{1,t-1} \), the claim holds trivially because the left-hand side is zero. On the other hand, when \( \hat{\mu}_{\max,t-1} > \hat{\mu}_{1,t-1} \), we have on event \( E_{2,t} \) that
\[
\hat{\mu}_{1,t-1} < \hat{\mu}_{\max,t-1} = \hat{\mu}_{2,t-1} < \mu_2 + \frac{\Delta}{3} \leq \mu_1 .
\]

Now apply (17) and (18), and get
\[
P(I_t = 2, T_{1,t-1} \leq m, E_{2,t}) \leq E[p_{2,t} I \{ T_{1,t-1} \leq m, E_{2,t} \}]
\[
\leq E[\exp[2\theta(\mu_1 - \hat{\mu}_{1,t-1})^2 I \{ \hat{\mu}_{1,t-1} \leq \mu_1 \} T_{1,t-1}] p_{1,t} I \{ T_{1,t-1} \leq m \}]
\[
= E[\exp[2\theta(\mu_1 - \hat{\mu}_{1,t-1})^2 I \{ \hat{\mu}_{1,t-1} \leq \mu_1 \} T_{1,t-1}] I \{ I_t = 1, T_{1,t-1} \leq m \}].
\]

With a slight abuse of notation, let \( \hat{\mu}_{1,s} \) denote the average reward of arm 1 after \( s \) pulls. Then, since \( T_{1,t} = T_{1,t-1} + 1 \) on event \( I_t = 1 \), we have
\[
\sum_{t=1}^{T_{1,t}} E[\exp[2\theta(\mu_1 - \hat{\mu}_{1,t-1})^2 I \{ \hat{\mu}_{1,t-1} \leq \mu_1 \} T_{1,t-1}] I \{ I_t = 1, T_{1,t-1} \leq m \}]
\[
\leq \sum_{s=1}^{m} E[\exp[2\theta(\mu_1 - \hat{\mu}_{1,s})^2 I \{ \hat{\mu}_{1,s} \leq \mu_1 \} s]] .
\]

Now fix the number of pulls \( s \) and note that
\[
E[\exp[2\theta(\mu_1 - \hat{\mu}_{1,s})^2 I \{ \hat{\mu}_{1,s} \leq \mu_1 \} s]] \leq P(\hat{\mu}_{1,s} > \mu_1) + \sum_{\ell=0}^{\infty} P \left( \frac{\ell}{\sqrt{s}} \leq \mu_1 - \hat{\mu}_{1,s} < \frac{\ell + 1}{\sqrt{s}} \right) \exp[2\theta(\ell + 1)^2]
\[
\leq 1 + \sum_{\ell=0}^{\infty} P(\mu_1 - \hat{\mu}_{1,s} \geq \frac{\ell}{\sqrt{s}}) \exp[2\theta(\ell + 1)^2]
\[
\leq 1 + \sum_{\ell=0}^{\infty} \exp[2\theta(\ell + 1)^2 - 2\ell^2] .
\]

where the last step is by Hoeffding’s inequality.

The above sum can be easily bounded for any \( \theta < 1 \). In particular, for \( \theta = 0.5 \), the bound is \( e^2 + 2e + 1 \) because
\[
\sum_{\ell=0}^{\infty} \exp[(\ell + 1)^2 - 2\ell^2] \leq e^{1-0} + e^{4-2} + e^{9-8} + \sum_{\ell=1}^{\infty} 2^{-\ell} ,
\]

Now we combine all above inequalities and get that term 2 is bounded as
\[
\sum_{t=3}^{n} P(I_t = 2, T_{2,t-1} > m, T_{1,t-1} \leq m) \leq (e^2 + 2e + 1)m + 1.
\]

Finally, we chain (15), (16), and (19); and use that \( m \leq 9\Delta^{-2} \log n + 1 \).
C. Technical Lemmas

Lemma 1. Let \( b_t : [K]^{t-1} \times [0,1]^{K \times n} \to \mathbb{R} \) be any function of \( t-1 \) previously pulled arms and all reward realizations. Then

\[
E [ b_t(I_{1:t-1}, Y) \nabla_\theta \log p_\theta(I_t | H_{t-1}) ] = 0 .
\]

Proof. Since \( b_t \) depends only on \( I_{1:t-1} \) and \( Y \),

\[
E [ b_t(I_{1:t-1}, Y) \nabla_\theta \log p_\theta(I_t | H_{t-1}) ] = E [ b_t(I_{1:t-1}, Y) E [ \nabla_\theta \log p_\theta(I_t | H_{t-1}) | I_{1:t-1}, Y ] ] .
\]

Now note that

\[
E [ \nabla_\theta \log p_\theta(I_t | H_{t-1}) | I_{1:t-1}, Y ] = \sum_{i=1}^K P(I_t = i | I_{1:t-1}, Y) \nabla_\theta \log p_\theta(i | H_{t-1})
\]

\[
= \sum_{i=1}^K p_\theta(i | H_{t-1}) \nabla_\theta \log p_\theta(i | H_{t-1})
\]

\[
= \nabla_\theta \sum_{i=1}^K p_\theta(i | H_{t-1}) = 0 .
\]

The last equality follows from \( \sum_{i=1}^K p_\theta(i | H_{t-1}) = 1 \), which is a constant independent of \( \theta \).

Lemma 2. Let \( p_{i,t} \) be defined as in (10). Let \( \eta = \theta / K \), \( V_{i,t} = \exp[\theta S_{i,t} / K] \), and \( V_t = \sum_{j=1}^K V_{j,t} \). Then

\[
\nabla_\theta \log p_{i,t} = \frac{1}{p_{i,t}} \left[ \frac{V_{i,t}}{V_t} \left( 1 - \theta \right) \left[ \frac{S_{i,t}}{K} - \sum_{j=1}^K \frac{V_{j,t} S_{j,t}}{V_t} \right] - 1 \right] + \frac{1}{K} .
\]

Proof. First, we express the derivative of \( \log p_{i,t} \) with respect to \( \theta \) as

\[
\nabla_\theta \log p_{i,t} = \frac{1}{p_{i,t}} \nabla_\theta p_{i,t} = \frac{1}{p_{i,t}} \left[ (1 - \theta) \nabla_\theta \frac{V_{i,t}}{V_t} - \frac{V_{i,t}}{V_t} + \frac{1}{K} \right] .
\]

Now note that

\[
\nabla_\theta \frac{V_{i,t}}{V_t} = \frac{1}{V_t} \nabla_\theta V_{i,t} + V_{i,t} \nabla_\theta \frac{1}{V_t} = \frac{V_{i,t} S_{i,t}}{V_t K} - \frac{V_{i,t}}{V_t} \sum_{j=1}^K \frac{V_{j,t} S_{j,t}}{V_t} \frac{S_{i,t}}{K} = \frac{V_{i,t} S_{i,t}}{V_t K} - \sum_{j=1}^K \frac{V_{j,t} S_{j,t}}{V_t K} .
\]

This concludes the proof.
D. RNN Implementation

We carry out the RNN experiments using PyTorch framework. In this paper, we restrict ourselves to binary 0/1 rewards. For all experiments, our policy network is a single layer LSTM followed by LeakyRELU non-linearity and a fully connected layer. We use the fixed LSTM latent state dimension of 50, irrespective of numbers of arms. The implementation of the policy network is provided in the code snippet below:

```python
class RecurrentPolicyNet(nn.Module):
    def __init__(self, K=2, d=50):
        super(RecurrentPolicyNet, self).__init__()
        self.action_size = K  # Number of arms
        self.hidden_size = d
        self.input_size = 2*d

        self.arm_emb = nn.Embedding(K, self.hidden_size)  # Number of arms
        self.reward_emb = nn.Embedding(2, self.hidden_size)  # For 0 reward or 1 reward
        self.rnn = nn.LSTMCell(input_size=self.input_size, hidden_size=self.hidden_size)
        self.relu = nn.LeakyReLU()
        self.linear = nn.Linear(self.hidden_size, self.action_size)

        self.hprev = None

    def reset(self):
        self.hprev = None

    def forward(self, action, reward):
        arm = self.arm_emb(action)
        rew = self.reward_emb(reward)

        inp = torch.cat((arm, rew), 1)
        h = self.rnn(inp, self.hprev)
        self.hprev = h

        h = self.relu(h[0])
        y = self.linear(h)

        return y
```

Listing 1. Policy Network

To train the policy we use the proposed GradBand algorithm as presented in Alg. 1. We used a batch-size \(m = 500\) for all experiments. Along with theoretically motivated steps, we had to apply a few practical tricks:

- Instead of SGD, we used adaptive optimizers like Adam or Yogi (Zaheer et al., 2018).
- We used an exponential decaying learning rate schedule. We start with a learning rate of 0.001 and decay every step by a factor of 0.999.
- We used annealing over the probability to play an arm. This encourages exploration in early phase of training. In particular we used temperature \(= 1/(1 - \exp(-5i/L))\), where \(i\) is current training iteration and \(L\) is the total number of training iterations.
- We applied curriculum learning as described in Section 6.4.

Our training procedure is highlighted in the code snippet below.

```python
optimizer = torch.optim.Adam(policy.parameters(), lr=0.001)
scheduler = torch.optim.lr_scheduler.ExponentialLR(optimizer, 0.999)
...
probs = rnn_policy_network(previous_action, previous_reward)
```
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```python
m = Categorical(probs/temperature)  # probability over K arms with temperature
action = m.sample()  # select one arm
reward = bandit.play(action)  # receive reward

...  

loss = -m.log_prob(action) * (cumulative_reward - baseline)  # Eq (3)
loss.backward()  # Eq (9)
optimizer.step()
scheduler.step()

...  

Listing 2. Training overview