Deep Neural Linear Bandits: 
Overcoming Catastrophic Forgetting through Likelihood Matching

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Abstract

We study the neural-linear bandit model for solving sequential decision-making problems with high dimensional side information. Neural-linear bandits leverage the representation power of deep neural networks and combine it with efficient exploration mechanisms, designed for linear contextual bandits, on top of the last hidden layer. Since the representation is being optimized during learning, information regarding exploration with "old" features is lost. Here, we propose the first limited memory neural-linear bandit that is resilient to this phenomenon, which we term catastrophic forgetting. We evaluate our method on a variety of real-world data sets, including regression, classification, and sentiment analysis, and observe that our algorithm is resilient to catastrophic forgetting and achieves superior performance.

1. Introduction

Deep reinforcement learning (DRL) methods such as the Deep Q-Network (DQN) have achieved state-of-the-art results in a variety of challenging, high-dimensional domains (Mnih et al., 2015; Silver et al., 2016). Using deep neural networks (DNNs) for function approximation in reinforcement learning (RL) enables the agent to generalize across states without domain-specific knowledge, and learn rich domain representations from raw, high-dimensional inputs (Mnih et al., 2015; Zahavy et al., 2016; Zrihem et al., 2016). For contextual bandits, generalized linear models were proposed to model nonlinear costs (Filippi et al., 2010). However, they lack representation power, and achieve inferior performance in practice when compared to DNNs (Riquelme et al., 2018).

Despite this great success, efficient exploration using DNNs is still an open problem. The $\epsilon$-greedy policy (Langford & Zhang, 2008) is simple to implement and widely used in practice (Mnih et al., 2015). However, it is statistically suboptimal. Alternatively, Optimism in the Face of Uncertainty (Abbasi-Yadkori et al., 2011; Auer, 2002, OFU), and Thompson Sampling (Thompson, 1933; Agrawal & Goyal, 2013, TS) use confidence sets to balance exploitation and exploration.

For DNNs, such confidence sets may not be accurate enough to allow efficient exploration. For example, using dropout as a posterior approximation for exploration does not concentrate with observed data (Osband et al., 2018) and was shown empirically to be insufficient (Riquelme et al., 2018). Alternatively, pseudo-counts, a generalization of the number of visits, were used as an exploration bonus (Bellemare et al., 2016; Pathak et al., 2017). Inspired by tabular RL, these ideas ignore the uncertainty in the value function approximation in each context. As a result, they may lead to inefficient confidence sets (Osband et al., 2018).

Linear models, on the other hand, are considered more stable and provide accurate uncertainty estimates but require substantial feature engineering to achieve good results. Additionally, they are known to work in practice only with "medium-sized" inputs (with around 1,000 features) due to numerical issues. A natural attempt at getting the best of both worlds is to learn a linear exploration policy on top of the last hidden layer of a DNN, which we term the neural-linear approach. In RL, this approach was shown to refine the performance of DQNs (Levine et al., 2017) and improve exploration when combined with TS (Azizzadenesheli et al., 2018) and OFU (O’Donoghue et al., 2018; Zahavy et al., 2018a). For contextual bandits, Riquelme et al. (2018) showed that neural-linear TS achieves superior performance on multiple data sets.

A practical challenge for neural-linear bandits is that the representation (the activations of the last hidden layer) change after every optimization step, while the features are assumed to be fixed over time when used by contextual bandits. Riquelme et al. (2018) tackled this problem by storing the entire data set in a memory buffer and computing new features for all the data after each DNN learning phase. This approach does not scale to large data sets; thus, the authors experimented with using a bounded memory buffer. They
observed a significant decrease in performance due to catastrophic forgetting (Kirkpatrick et al., 2017), i.e., due to the loss of information from previous experience.

Catastrophic forgetting was also observed in neural-linear DRL. Levine et al. (2017) proposed a DRL method that uses the experience replay (ER) of the DQN (a limited memory buffer) and computes new weights for the last layer of the DQN using Bayesian linear regression. Levine et al. observed that using the previous weights of the DQN as prior improved their results, and prevented forgetting of past experience that is not available in the ER buffer. Zahavy et al. (2018a) proposed the Action-Elimination DQN, that combines a DQN with a neural-linear bandit that eliminates sub-optimal actions with high probability. The bandit was trained to predict wrong actions, supervised by an external elimination signal. Whenever the representation changes, new uncertainty estimates were calculated using the ER. However, once the bandit has learned to eliminate an action, this action was not explored by the DQN and vanished from the ER. As a result, sub-optimal actions had to be re-explored.

In this work, we propose a neural-linear bandit that uses TS on top of the last layer of a DNN (Figure 1). Key to our approach is a novel method to compute priors whenever the DNN features change that makes our algorithm resilient to catastrophic forgetting. Specifically, we adjust the moments of the likelihood of the reward conditioned on new features to match the likelihood conditioned on old features. We achieve this by solving a semi-definite program (Vandenberghe & Boyd, 1996, SDP) to approximate the covariance and using the weights of the last layer as prior to the mean.

We present simulation results on several real-world and simulated data sets, including classification and regression, using Multi-Layered Perceptrons (MLPs). Our findings suggest that using our method to approximate priors improves performance when memory is limited. Finally, we demonstrate that our neural-linear bandit performs well in a sentiment analysis data set where the input is given in natural language (of size $\mathbb{R}^{8k}$) and we use a Convolution Neural Network (CNNs). In this regime, it is not feasible to use a linear method due to computational problems. To the best of our knowledge, this is the first neural-linear algorithm that is resilient to catastrophic forgetting due to limited memory.

2. Background

A contextual bandit algorithm observes a context, chooses an action (from a set of alternative actions), and observes the outcome (reward) of that action. The goal is to maximize the total cumulative reward. For example, contextual bandits are used to select which news article to show on the
main page of your website to optimize click-through rate (Li et al., 2010). Contextual bandits allow personalization, as they decide how to act using the context information. They are very similar to supervised learning (regression and classification) but with one key difference. The learner observes the reward (e.g., the label in classification) only for the chosen action (bandit feedback), thus, if the algorithm made a mistake, it does not get feedback on the right arm. For this reason, the algorithm decisions must balance exploration and exploitation. We now formalize the framework explicitly.

### 2.1. Problem setting

We consider the stochastic contextual multi-armed bandit problem with $N$ arms. At time $t$ a context vector $b(t) \in \mathbb{R}^d$, is revealed. These context vectors may be chosen by an adversary in an adaptive manner, after observing the arms played and their rewards up to time $t-1$. The history at time $t$ is defined to be

$$H_{t-1} = \{b(\tau), a(\tau), r_{a(\tau)}(\tau), \tau = 1, ..., t-1\},$$

where $a(\tau)$ denotes the arm played at time $\tau$. The contexts $b(t)$ are assumed to be realizable, i.e., the reward for arm $i$ at time $t$ is generated from an (unknown) distribution $s.t.$

$$E[r_t(i)|b(t), H_{t-1}] = b(t)^T\mu_i,$$

where $\{\mu_i \in \mathbb{R}^d\}_{i=1}^N$ are fixed but unknown parameters. Furthermore, we assume that $r_t(i) = b(t)^T\mu_i + \eta_t$, where $\eta_t, t$ is conditionally R-sub-Gaussian. An algorithm for this problem needs to choose at every time $t$ an arm $a(t)$ to play, with the knowledge of history $H_{t-1}$ and current context $b(t)$. Let $a^*(t)$ denote the optimal arm at time $t$, i.e. $a^*(t) = \arg\max\limits_i b(t)^T\mu_i$, and let $\Delta_t(i)$ the difference between the mean rewards of the optimal arm and of arm $i$ at time $t$, i.e.,

$$\Delta_t(i) = b(t)^T\mu_{a^*(t)} - b(t)^T\mu_i.$$ 

The objective is to minimize the total regret $R(T) = \sum_{t=1}^T \Delta_t(i)$, where the time horizon $T$ is finite but possibly unknown.

### 2.2. TS for linear contextual bandits

TS, a heuristic for choosing actions that addresses the exploration-exploitation dilemma in the multi-armed bandit problem. Empirically, TS enjoys superior performance (Lattimore & Szepesvári, 2018), in particular, when applied to problems with complex action spaces and costs (Gopalan et al., 2014). For linear contextual bandits, TS was introduced in (Agrawal & Goyal, 2013, Algorithm 1). Suppose that the likelihood of reward $r_t(i)$, given context $b(t)$ and parameter $\mu_i$, were given by the pdf of Gaussian distribution $N(b(t)^T\mu_i, \sigma^2)$, and let $B_t(i) = B_{0,i} + \sum_{\tau=1}^{t-1} b(\tau)r_{a(\tau)}(\tau)\mathbb{1}_{i=a(\tau)}, \hat{\mu}_i(t) = B_t^{-1}(t)\sum_{\tau=1}^{t-1} b(\tau)r_{a(\tau)}(\tau)\mathbb{1}_{i=a(\tau)},$ where $\mathbb{1}$ is the indicator function. For this case, it is known that using a Gaussian prior $\mu_0$ on the parameters of arm $i$ at time $t$, $\mu_{0,i}(t) \sim N(\hat{\mu}_i(t), \sigma^2B_t^{-1}(t))$, allows to compute the posterior distribution at time $t+1$ analytically as,

$$Pr(\hat{\mu}_i(t)|r_t(i)) \sim Pr(r_t(i)|\hat{\mu}_i(t))Pr(\hat{\mu}_i(t)) \sim N(\hat{\mu}_i(t+1), \sigma^2B_t^{-1}(t+1)).$$

At each time step $t$, the algorithm generates samples $\{\hat{\mu}_i(t)\}_{i=1}^N$ from the posterior distribution $N(\hat{\mu}_i(t), \sigma^2B_t^{-1}(t))$, plays the arm $i$ that maximizes $b(t)^T\hat{\mu}_i(t)$ and updates the posterior.

### Algorithm 1 TS for Contextual bandits

Set $B = I_d, \mu = 0_d, f = 0_d$

for $t = 1, 2, \ldots, do$

Sample $\tilde{\mu}(t)$ from distribution $N(\hat{\mu}, \sigma^2B^{-1})$

Play arm $a(t) := \arg\max\limits_i b(t)^T\tilde{\mu}(t)$

Observe reward $r_t$

Update: $B_{a(t)} = B_{a(t)} + b(t)b(t)^T$

$f_{a(t)} = f_{a(t)} + b(t)r_t, \quad \mu_{a(t)} = B_{a(t)}^{-1}f_{a(t)}$

end for

TS is guaranteed to have a total regret at time $T$ that is not larger than $O(d^{3/2}/\sqrt{T})$, which is within a factor of $\sqrt{d}$ of the information-theoretic lower bound for this problem. It is also known to achieve excellent empirical results.

### 2.3. Bayesian Linear Regression

Although that TS is a Bayesian approach, the description of the algorithm and its analysis are prior-free, i.e., the regret bounds hold irrespective of whether or not the actual reward distribution matches the Gaussian likelihood function used to derive this Bayesian heuristic (Agrawal & Goyal, 2013). Nevertheless, the prior distribution assumes that the sub-Gaussian parameter of the model noise is known (Agrawal & Goyal, 2013; Abeille et al., 2017) and as a result, it appears as a constant in the bound of the regret.

A different Bayesian mechanism, based on Bayesian Linear Regression, was proposed by Riquelme et al. (2018). Here, the sub-Gaussian parameter is replaced with a prior belief that is being updated over time. The prior is given by $Pr(\mu|\nu^2) = Pr(\nu^2)Pr(\mu_i|\nu^2)$, where $Pr(\nu^2)$ is an inverse-gamma distribution Inv-Gamma$(\alpha_0, \beta_0)$. Further the conditional prior density $Pr(\mu_i|\nu^2)$ is a normal distribution, $Pr(\mu_i|\nu^2) \propto N(\mu_{0,i}, \nu^2B_0^{-1})$. Under Gaussian likelihood, there exists an analytical conjugate posterior $Pr(\mu_i, \nu^2|H) \propto Pr(\mu_i|\nu^2, H_t)Pr(\nu^2|H_t)$, where the two factors correspond to the densities of $N(\hat{\mu}_i(t), \nu^2B_t^{-1}(t))$ and Inv-Gamma$(a_i(t), b_i(t))$ distributions, with $B_t(t) = \cdots$
\(B_{0,i} + \sum_{\tau=1}^{t-1} b(\tau)b(\tau)^T \mathbb{1}_{i=a(\tau)}, \text{ and}
\)

\[\hat{\mu}_i(t) = B_i(t)^{-1}\left(B_{0,i} \mu_{0,i} + \sum_{\tau=1}^{t-1} b(\tau)r_i(\tau)\mathbb{1}_{i=a(\tau)}\right),\]

\[a_i(t) = a_{0,i} + \frac{t}{2},\]

\[b_i(t) = b_{0,i} + \frac{1}{2} \left(\sum_{\tau=1}^{t-1} r_i^2(\tau)\mathbb{1}_{i=a(\tau)} + \mu_{0,i}^T B_{0,i} \mu_{0,i} - \hat{\mu}_i(t)^T B_i(t) \hat{\mu}_i(t)\right).\]

Unfortunately, the marginal distribution of \(\mu_i\) is the heavy tailed, multi-variate t-student distribution (see O’Hagan & Forster (2004), page 246, for derivation). Therefore, it does not satisfy the logarithmic concentration bounds in (Agrawal & Goyal, 2013; Abeille et al., 2017). Intuitively, since this distribution is heavy tailed, the algorithm explores “too much” to be efficient. Thus, in order to analyze the regret of this approach, new analysis has to be derived. Most likely, the updates in the posterior parameters \(b_i(t), a_i(t)\) compensate for the lack of shrinkage due to the heavy tail distribution. Heavy tailed bandits were investigated in (Bubeck et al., 2013), but this was in the multi armed bandit scenario (without context) and the heavy tail distribution was used to model the noise (and not the TS distribution). We leave the theoretical analysis of this case to future work, but still use it in our implementation as the updates were shown to convergence to the true posterior and demonstrated excellent empirical performance (Riquelme et al., 2018).

3. Method

3.1. TS with changing features

We now present our limited memory neural-linear TS algorithm (Algorithm 2). The algorithm uses a DNN, denoted by \(D\), to learn a nonlinear representation of the context, and explores using linear TS using on top of its last hidden layer. Given a context \(b(t)\), we denote the activations of the last hidden layer of \(D\) applied to this context as \(\phi(t) = \text{LastLayerActivations}(D(b(t)))\). The context \(b(t)\) represents raw measurements that can be high dimensional (e.g., image or text), where the size of \(\phi(t)\) is a design parameter that we choose to be smaller. This makes contextual bandit algorithms practical for such data sets. Moreover, \(\phi(t)\) can potentially be linearly realizable (even if \(b(t)\) is not) since a DNN is a global function approximator (Barron, 1993) and the last layer is linear.

Every \(L\) iterations, we train a DNN to minimize the mean squared error (MSE), where the reward of the played arm is used as a label (similar to Riquelme et al. (2018)). After this learning phase, the weights (and activations) of the DNN have changed. We denote the new activations by \(\psi(t)\). For analysis purposes, we will assume that all the representations that are produced by the DNN are realizable\(^1\), i.e.,

\[\mathbb{E}[r_i(t)|\phi(t)] = \phi(t)^T \mu_i = \psi(t)^T \beta_i = \mathbb{E}[r_i(t)|\psi(t)].\]

Next, observe that under the realizability assumption, the likelihood of the reward is invariant to the choice of representation, i.e. \(N(\phi(t)^T \mu_i, \nu^2) \sim N(\psi(t)^T \beta_i, \nu^2)\). Thus, if we can guarantee that the estimation of the likelihood given the new features will be the same as with the old features, then the algorithm should be oblivious to the change of parametrization. Recall that the estimation of the reward at time \(t\), given by \(\phi(t)^T \hat{\mu}_{a(t)}(t)\) is a Gaussian random variable with mean \(\phi(t)^T \hat{\mu}_{a(t)}(t)\) and standard deviation \(\nu s_{i,t}\), where, \(s_{i,t} = \sqrt{\phi(t)^T \Phi_t(t)^{-1} \phi(t)}\) is the standard deviation of estimate \(b(t)^T \hat{\mu}_i(t)\) (Section 2.2). Thus, to approximate the likelihood, it is enough to estimate its moments.

The following lemma summarizes this intuition and highlights that our algorithm is well motivated by theory. In the supplementary material, we provide a proof sketch based on the analysis performed in (Agrawal & Goyal, 2013). In Section 3.2 we give an example of a simple scenario in which the assumptions of Lemma 1 hold.

**Lemma 1.** For the stochastic contextual bandit problem with linear payoff functions, given a set of realizable feature functions \(\{\phi_i\}_{i=1}^k\), performing TS with features \(\phi_i\) gives the same regret as performing TS with changing features \(\{\phi_i\}_{i=1}^k\) while matching the moments of the likelihood whenever the features change.

We highlight two main differences between our algorithm and the vanilla TS for linear contextual bandits (Algorithm 1, Agrawal & Goyal (2013)). First, we perform TS while updating the posterior both for \(\mu\), the mean of the estimate, and \(\nu\), its variance. This is done following Bayesian linear regression equations, as suggested in (Riquelme et al., 2018). Second, whenever the features change, we compute an approximation for the moments of the new features in the following manner.

**Approximation of the mean \(\hat{\mu}_{0,a}\):** Recall that the DNN is trained to minimize the MSE, (with the labels being reward samples). Thus, given the new last layer activations \(\psi(t)\), the weights of the last layer of the DNN make a good prior for \(\mu\). This approach was shown empirically to make a good approximation (Levine et al., 2017), as the DNN was optimized online by observing all the data.

**Approximation of the variance \(s_{i,t}\):** For each arm \(i\), we wish to find a solution \(\Psi_i\) such that \(s_{i,t}^2 \equiv \phi(t)^T (\Psi_t(t))^{-1} \phi(t) = \psi(t)^T (\Psi_t)^{-1} \psi(t)\). We are given a
set of samples of the old and new features \( \{\phi(t), \psi(t)\}_{t=1}^n \) from the memory buffer (of size \( n \)) \(^2\) and the inverse covariance matrix \( \Phi(t)^{-1} \) (which was estimated using "old" features \( \phi \) at previous iterations). The solution \( \Psi_t \) will act as a prior for arm \( i \) with the next set of features and is denoted in Algorithm 2 as \( \Psi_{0,i} \). Using the cyclic property of the trace, this is equivalent to finding \( \Psi_t \), s.t. \( \forall t \in [1..n], i \in [1..n] : \) \( s_{t,i} = \text{Trace}(\Psi_t^{-1}(\psi(t)\psi(t)^T)) \).

Algorithm 2 Limited Memory Neural-linear TS

Set \( \forall a : \Phi_{0,a} = I_d, \mu_{0,a} = 0_d, \phi_a = 0_{d	imes d}, f_a = 0_d, a_0 = a_{0,a}, b_0 = b_{0,a} \)

Initialize Replay Buffer \( E \) and DNN \( D \)

Define \( h(t) \leftarrow \text{LastLayerActivations}(D(b(t))) \)

for \( t = 1, 2, \ldots, \) do

Bayesian linear regression update:

\[
\hat{\mu}_a(t) = (\Phi_{0,a} + \mu_{0,a})^{-1}(\Phi_{0,a} \mu_{0,a} + f_a)
\]

\[
\hat{a}_a(t) = + \frac{1}{2}(\sum_{r=1}^{t-1} \hat{a}_0(r)\hat{a}_0(r)) - \hat{\mu}_0(a(t)) + \mu_{0,a}(t) \Phi_{a(t)}(t)\hat{\mu}_{a(t)}(t)
\]

Observe \( b(t), \) evaluate \( \hat{f}(t) \)

Posterior sampling: \( \forall a, \) sample:

\[
\hat{\mu}_a(t) \sim \text{Inv-Gamma}(a_0(t), b_0(t))
\]

\[
\hat{a}_a(t) \sim N(\hat{\mu}_a(t), (\Phi_{a(t)}(t) + \Phi_{a(t)}(t))^{-1})
\]

Play arm \( a(t) := \arg \max \phi(t)^T \hat{\mu}_a(t) \)

Observe reward \( r_t \)

Store \( \{b(t), a(t), r_t\} \) in \( E \). If \( E \) is full: first remove the first tuple in \( E \) with \( a = a(t) \) (round robin)

Update:

\[
\Phi_{a(t)}(t) = (\phi(t)\phi(t)^T, f_a(t)) + (\phi(t)^T r_t
\]

if \( (t \mod L) = 0 \) then

\( \forall a \) set \( \{\phi_a\} = \{h(i), \forall i \in E, a(i) = a\} \)

Train DNN for \( P \) steps

Compute priors for new features:

for \( a \in A \) do

\( \{\psi_a, r_a\} = \{(h(i), r(i)), \forall i \in E, a(i) = a\} \)

Solve for \( \Phi_{0,a} \) using Eq. 3 with \( \{\psi_a\} , \{\phi_a\} , \Phi_a^{-1} \)

Set \( \mu_{0,a} \leftarrow \text{LastLayerWeights}(D)_a \)

\( \Phi_a = \sum_{\psi \in \{\psi_a\}} \psi \psi^T, f_a = \sum_{\psi \in \{\psi_a\}, r \in \{r_a\}} \psi^T r \)

end for

end if

Next, we define \( X_t \) to be a vector of size \( m \) in the vector space of \( d \times d \) symmetric matrices, with its \( t \)th element \( X_{t,i} \) to be the matrix \( \psi(t)\psi(t)^T \). We also define \( S_t \) to be a vector of dimension \( m \) with scalar elements \( s_{t,i} \). \( \Psi_t^{-1} \) is also constrained to be semi positive definite (being a correlation matrix), thus, the solution can be found by solving an SDP (Equation 3). Note that \( \text{Trace}(X_t^T \Psi_t^{-1}) \) is an inner product over the vector space of symmetric matrices, known as the Frobenius inner product. Therefore the optimization problem is very similar to linear regression in the vector space of symmetric matrices. In practice, we use cvxpy (Diamond & Boyd, 2016) to solve for all actions \( i \in [1..N] : \)

\[
\text{minimize } \|\text{Trace}(\sum_{t=1}^m X_t^T \Psi_t^{-1}) - S_i \|^2 \quad \text{subject to } \Psi_t^{-1} \succeq 0.
\]

3.2. Sanity check: the realizable case

We now show that under the realizability assumption, our approach performs optimally, i.e., its performance does not deteriorate due to limited memory. Recall that the realizability assumption implies a linear connection between \( \beta \) and \( \psi \) : \( \beta^T \psi = \mu^T \phi \). This implies that the features \( \phi \) and \( \psi \) are linear mappings of the raw context \( b \), i.e., \( \phi = A \phi b, \psi = A \phi b \).

In addition, we assume in this section that \( \Phi_m \) is full rank. The realizability assumption implies that we can solve a linear set of equations and get a linear mapping from \( \beta \) to \( \beta^T = \mu^T \phi \). Now, assume that we learned \( \hat{\mu} \) using observations \( \{\phi_i\}_{i=1}^n \) (denoted by \( \Phi_n \)) and we use the linear mapping to find an approximation for \( \beta \) using observations \( \{\phi_j, \psi_j\}_{j=1}^{m+n} \) (denoted by \( D_m, \Psi_m \)). Also, we denote by \( \Sigma_n, \Sigma_m \) the correlation matrix from measurements \( \Psi_n \) (and respectively for \( \Sigma_m, \Sigma_m \)), and by \( R_m \), the measurement vector. The realizability assumption gives us a method to compute a prior \( \beta_0 \) to use with measurement \( \Psi_m \) based on the measurement \( \Phi_n \):

\[
\beta_0 = \mu_n^T \Phi_n \Psi_n^{-1} = ((\Phi_n \Phi_n^T)^{-1} \Phi_n^T R_m) \Phi_n \Psi_m^{-1},
\]

and therefore \( \beta_0 = \Psi_m \Phi_m \Psi_m^{-1} \Phi_m \Psi_m^{-1} \Phi_m \Psi_m^{-1} \). Similarly, if we solve the SVP exactly, we get \( \psi_m(\Sigma_n)^{-1} \psi_m = \phi_m(\Sigma_m)^{-1} \phi_m \), which gives \( \Sigma_0, \Sigma_0 \Psi_0 = \psi_m(\Sigma_n)^{-1} \phi_m \), and \( \Sigma_0, \Sigma_0 \Psi_0 = \psi_m(\Sigma_n)^{-1} \phi_m \).

Then, after some basic algebra we get:

\[
\Sigma_0, \Sigma_0 \Psi_0 = \psi_m(\Sigma_n)^{-1} \phi_m \]

Plugging these estimates as priors in the Bayesian linear regression equation we get the following solution for \( \beta : \)

\[
\hat{\beta} = (\sum_{i=1}^{n+m} \psi_i \psi_i^T)^{-1} (\sum_{i=1}^{n+m} \psi_i \psi_i^T) \psi_t \}
\]

i.e., we got the linear regression solution for \( \beta \) as if all the data \( \{\psi_i\}_{i=1}^{n+m} \) was observed!

4. Experiments

Our experiments are divided into five subsections. In Section 4.1 we use synthetic data to test the ability of our algorithm to learn nonlinear representations during exploration.

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\(^2\)In our experiments the contexts are drawn stochastically from the empirical data distribution, and not adversarially. Therefore, the random sample \( \{\phi(t), \psi(t)\}_{t=1}^n \) is used to learn the prior.
In Section 4.2 we test the resilience of our method to catastrophic forgetting. We present an ablative analysis of our approach and show that the prior on the covariance is crucial. In Section 4.3 we present simulation results using MLPs on ten real world data sets. Finally, in Section 4.4 we demonstrate that our model works well with high dimensional natural language data on a task of sentiment analysis.

In all the experiments we used the default hyperparameters of the model and network architecture. In Sections 4.1 - 4.3, we used the hyperparameters from (Riquelme et al., 2018). The network architecture is an MLP with a single hidden layer of size 50. In Section 4.4 we use a text CNN (details below). The size of the memory buffer is set to be 100 per action.

### 4.1. Representation learning

**Setup:** we adapted a synthetic data set, known as the “wheel bandit” (Riquelme et al., 2018), to investigate the exploration properties of bandit algorithms when the reward is a nonlinear function of the context. Specifically, contexts $x \in \mathbb{R}^2$ are sampled uniformly at random in the unit circle, and there are $k = 5$ possible actions.

One action, $a_5$, always offers reward $r_5 \sim N(\mu_5, \sigma)$, independently of the context. The reward of the other actions depend on the context and a parameter $\delta$, that defines a $\delta$-circle $\|x\| \leq \delta$.

For contexts that are outside the circle, actions $a_1, ..., a_4$ are equally distributed and sub-optimal, with $r_i \sim N(\mu, \sigma)$ for $\mu < \mu_5, i \in [1..4]$.

For contexts that are inside a circle, the reward of each action depends on the respective quadrant. Each action achieves $r_i \sim N(\mu_i, \sigma)$, where $\mu_5 < \mu_i = \mu$ in exactly one quadrant, and $\mu_i = \mu < \mu_5$ in all the other quadrants. For example, $\mu_1 = \mu$ in the first quadrant $\{x : \|x\| \leq \delta, x_1, x_2 > 0\}$ and $\mu_1 = \mu$ elsewhere. We set $\mu = 0.1, \mu_5 = 0.2, \mu = 0.4, \sigma = 0.1$. Note that the probability of a context randomly falling in the high-reward region is proportional to $\delta$. For lower values of $\delta$, observing high rewards for arms $a_1, ..., a_4$ becomes more scarce, and the role of the nonlinear representation is less significant.

We train our model on $n = 4000$ contexts, where we optimize the network every $L = 200$ steps for $P = 400$ mini batches. The results can be seen in Table 1.

Not surprisingly, the neural-linear approaches, even with limited memory, achieved better reward than the linear method (Table 1).

Figure 3.2 presents the reward of each arm as a function of the context. In the top row, we can see empirical samples from the reward distribution. In the middle row, we...
see the predictions of the linear bandit. Since it is limited to linear predictions, the predictions become a function of the distance from the learned hyper-plane. This representation is not able to separate the data well, and also makes mistakes due to the distance from the hyperplane. For the neural linear method (bottom row), we can see that the DNN was able to learn good predictions successfully. Each of the first four arms learns to make high predictions in the relevant quadrant of the inner circle, while arm 5 makes higher predictions in the outer circle.

|       | Linear          | Neural-Linear Limited Memory |
|-------|-----------------|------------------------------|
| δ=0.5 | 737.44 ± 3.04   | 899.72 ± 12.79              |
| δ=0.3 | 735.37 ± 2.58   | 781.09 ± 11.34              |
| δ=0.1 | 735.51 ± 2.59   | 751.75 ± 3.6               |

*Table 1. Cumulative reward on the wheel bandit*

### 4.2. Catastrophic forgetting

We now show that the prior on the covariance is necessary to avoid catastrophic forgetting due to limited memory.

**Setup:** we use the Shuttle Statlog data set (Newman et al., 2008), a real world, nonlinear data set. Each context is composed of 9 features of a space shuttle flight, and the goal is to predict the state of the radiator subsystem of the shuttle (the reward). There are \( k = 7 \) possible actions, and if the agent selects the right action, then reward \( 1 \) is generated. Otherwise, the agent obtains no reward \( (r = 0) \).

We experimented with the following algorithms: (1) Linear TS (Agrawal & Goyal, 2013, Algorithm 1) using the raw context as a feature, with an additional uncertainty in the variance (Riquelme et al., 2018). (2) Neural-Linear TS (Riquelme et al., 2018). (3) Neural-Linear TS with limited memory, a version of Algorithm 2 that does not use prior calculations when changing the feature representation. (4) Neural-linear with limited memory and calculation of a prior only for the mean, similar to (Levine et al., 2017). (5) Neural-linear with limited memory, with both priors computed according to Algorithm 2.

Algorithms 3-5 make an ablative analysis for the limited memory neural-linear approach. As we will see, adding each one of the priors improves learning and exploration.

Figure 3 shows the performance of each of the algorithms in this setup. We let each algorithm run for 4000 steps (contexts) and average each algorithm over 10 runs. The x-axis corresponds to the number of contexts seen so far, while the y-axis measures the instantaneous regret. All the neural-linear methods retrain the DNN every \( L = 400 \) steps for \( P = 800 \) mini-batches.

First, we can see that the neural linear method (2nd row) outperforms the linear one (1st row), suggesting that this data set is nonlinear. We can also see that our approach to computing the priors allows the limited memory algorithm (3rd row) to perform almost as good as the neural linear algorithm without memory constraints (2nd row).

In the last two rows we can see a version of the limited memory neural linear algorithm that does not calculate the prior for the covariance matrix (4th row), and a version that does not compute priors at all (5th row). Both of these algorithms suffer from "catastrophic forgetting" due to limited memory. Intuitively, the covariance matrix holds information regarding the number of contexts that were seen by the agent and are used by the algorithm for exploration. When no such prior is available, the agent explores sub-optimal arms from scratch every time the features are modified (every \( L = 400 \) steps, marked by the x-ticks on the graph). Indeed, we can observe “peaks” in the regret curve for these algorithms (rows 4&5). This phenomenon is significantly reduced when we compute the prior on the covariance matrix (3rd row) making our limited memory neural-linear bandit resilient to catastrophic forgetting.

### 4.3. Real world data

**Setup:** we evaluate our approach on a several (10) real-world data sets that are publicly available at the UC Irvine Machine Learning Repository ⁵; for each data set, we present the cumulative reward achieved by the algorithms, detailed in the previous subsection, averaged over 50 runs. Each run was performed for 5000 steps.

**Linear vs. nonlinear data sets:** The results are divided into two groups, linear and nonlinear data sets. The separation was performed post hoc, based on the results achieved by the full memory methods, i.e., the first group consists of five data sets on which Linear TS (Algorithm 1) outperformed Neural-Linear TS (Algorithm 2), and vice versa. We

⁵link
observed that most of the linear datasets consisted of a small number of features that were mostly categorical (e.g., the mushroom dataset has 22 categorical features that become 117 binary features). The DNN based methods performed better when the features were dense and high dimensional.

**Linear data sets:** Since there is no apriori reason to believe that real-world data sets should be linear, we were surprised that the linear method made a competitive baseline to DNNs. To investigate this further, we experimented with the best reported MLP architecture for the covertype data set (taken from Kaggle). Linear methods were reported to achieve around 60% test accuracy. This number is consistent with our reported cumulative reward (3000 out of 5000). Similarly, DNNs achieved around 60% accuracy, which indicates that the Covertype data set is indeed relatively linear. However, when we measure the cumulative reward, the deep methods take initial time to learn, which can explain the slightly worse score. One particular architecture (MLP with layers 54-500-800-7) was reported to achieve 68%; however, we didn’t find this architecture to yield better cumulative reward. Similarly, for the Adult data set, linear and deep classifiers were reported to achieve similar results (around 84%), which is again equivalent to our cumulative reward of 4000 out of 5000. A specific DNN was reported to achieve 90% test accuracy but did not yield improvement in cumulative reward. These observations can be explained by the different loss function that we optimize or by the partial observability of the bandit problem (bandit feedback). Alternatively, competitions tend to suffer from overfitting in model selection (see the "reusable holdout" paper for more details (Dwork et al., 2015)). Regret, on the other hand, is less prone to model overfitting, because the model is evaluated at each iteration, and because we shuffle the data at each run.

**Limited memory:** Looking at Table 2 we can see that on eight out of ten data sets, using the prior computations (Algorithm 5), significantly improved the performance of the limited memory Neural-Linear algorithms. On four out of ten data sets (Mushroom, Financial, Statlog, Epileptic), Algorithm 5 even outperformed the unlimited Neural-Linear algorithm (Algorithm 2).

**Limited memory neural linear vs. linear:** as linear TS is an online algorithm it can store all the information on past experience using limited memory. Nevertheless, in four (out of five) of the nonlinear data sets the limited memory TS (Algorithm 5) outperformed Linear TS (Algorithm 1). Our findings suggest that when the data is indeed not linear, than neural-linear bandits beat the linear method, even if they must perform with limited memory. In this case, computing priors improve the performance and make the algorithm resilient to catastrophic forgetting.

### 4.4. Sentiment analysis from text using CNNs

**Setup:** we use the ”Amazon Reviews: Unlocked Mobile Phones” data set, which contains reviews of unlocked mobile phones sold on ”Amazon.com”. The goal is to find out the rating (1 to 5 stars) of each review using only the text itself. We use our model with a Convolutional Neural Network (CNN) that is suited to NLP tasks (Kim, 2014; Zahavy et al., 2018b). Specifically, the architecture is a shallow word-level CNN that was demonstrated to provide state-of-the-art results on a variety of classification tasks by using word embeddings, while not being sensitive to hyperparameters. We use the architecture with its default

| Name          | Full memory | Limited memory, Neural-Linear |
|---------------|-------------|-------------------------------|
|               | d | A  | Linear | Neural-Linear | No Prior | μ Prior | Both Priors |
| Mushrooms     | 117 | 2 | 1302 ± 744 | 1080 ± 853 | 7631 ± 1670 | 9442 ± 1351 | 10923 ± 839 |
| Financial     | 21 | 8 | 4388 ± 587 | 4339 ± 584 | 4225 ± 594 | 4311 ± 598 | 4597 ± 597 |
| Jester        | 32 | 8 | 14800 ± 2240 | 12819 ± 2135 | 11114 ± 2050 | 10996 ± 2013 | 9624 ± 2186 |
| Adult         | 88 | 2 | 4086.1 ± 11.03 | 4010.0 ± 22.19 | 5608.2 ± 34.94 | 3839.5 ± 17.63 | 3934.0 ± 54.29 |
| Covertype     | 54 | 7 | 3054 ± 557 | 2808 ± 545 | 2334 ± 603 | 2347 ± 615 | 2828 ± 593 |

Table 2. Cumulative reward of TS algorithms on 10 real world data sets. The context dim d and the size of the action space A are reported for each data set. The mean result and standard deviation of each algorithm is reported for 50 runs.
hyper-parameters\(^8\) and standard pre-processing (e.g., we use random embeddings of size 128, and we trim and pad each sentence to a length of 60). The only modification we made was to add a linear layer of size 50 to make the size of the last hidden layer consistent with our previous experiments.

Since the input is in \(\mathbb{R}^{7k} (60 \times 128)\), we did not include a linear baseline in these experiments as it is impractical to do linear algebra (e.g., calculate an inverse) in this dimension. Instead, we compared our method with the full memory neural linear TS, and add an \(\epsilon\)-greedy baseline. Looking at Table 3 we can see that the limited memory version performs almost as good as the full memory, and significantly better than the \(\epsilon\)-greedy baseline.

| \(\epsilon\)-greedy | Neural-Linear | Neural-Linear Limited Memory |
|---------------------|---------------|-----------------------------|
| 2963.9 ± 68.5       | 3155.6 ± 34.9 | 3143.9 ± 33.5               |

*Table 3. Cumulative reward on Amazon review’s*
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5. Supplementary material

5.1. Proof of Lemma 1

**Lemma.** For the stochastic contextual bandit problem with linear payoff functions, given a set of realizable feature functions \( \{\phi^i\}_{i=1}^n \), performing TS with features \( \phi \), gives the same regret as performing TS with changing features \( \{\phi^i\}_{i=1}^n \) while matching the moments of the likelihood whenever the features change.

**Proof sketch.** We follow the proof of (Agrawal & Goyal, 2013). When the features change, we will denote the features before the change by \( \phi(t) \) and after it by \( \psi(t) \). By definition of \( \hat{\mu}(t) \), the marginal distribution of the estimate \( \theta_i(t) = \phi(t)^T \hat{\mu}(t) \) is Gaussian with mean \( \phi(t)^T \mu(t) \) and standard deviation \( \nu \sqrt{\phi(t)^T \Phi(t)^{-1} \phi(t)} \). Since we match the moments of this estimate, then estimate given the new features \( \psi(t) \) have exactly the same moments and distribution. Since the distribution of the estimate did not change, its concentration and anti-concentration bounds do not change which implies that lemma’s 1&2 from (Agrawal & Goyal, 2013) still holds. Similarly, since the variance of the estimate did not change, saturated (unsaturated) arms remain saturated (unsaturated) by definition, thus, lemma 3 holds as well. We define the filtration \( F_{t-1} \), as the union of the history until time \( t-1 \), and the context at time \( t \), i.e., \( F_{t-1} = \{H_{t-1}, \phi^i(t) \} \). The history at time \( t \) is defined to be \( H_t = \{a(\tau), r_{a(\tau)}, \phi^{\mu(\tau)}(\tau), i = 1, ..., N, \tau = 1, ..., t \} \), i.e., the sequence of actions rewards and (time dependent) features. As a consequence, lemma 4 and the theorem hold as well.

5.2. Derivation of auxiliary results for Section 3.2

\[
\Sigma^\psi_0 \beta_0 = (A_\psi b_m)(A_\psi b_m)^{-1}A_\psi b_n R_n \\
= A_\psi b_m b_m^{-1}A_\psi^{-1}A_\psi b_n R_n \\
= A_\psi b_n R_n = \Psi_n R_n
\]

\[
\Sigma^\psi_0 = \Psi_m \Phi_m^{-1} \Sigma_\phi (\Phi_m^{-1})^T \Psi_m^T \\
= (A_\psi b_m)(A_\psi b_m)^{-1} \Sigma_\phi (b_m^{-1} A_\phi)^T (A_\psi b_m)^T \\
= A_\psi A_\phi^{-1} A_\phi \sum_{i=1}^n b_i b_i^T A_\phi^T (A_\phi^T)^{-1} A_\phi^T \\
= A_\psi \sum_{i=1}^n b_i b_i^T A_\phi^T = \Sigma^\psi_n
\]

Plugging these estimates as priors in the Bayesian linear regression equation we get the following solution for \( \beta \):

\[
\hat{\beta} = (\Sigma_m^\psi + \hat{\Sigma})^{-1}(\hat{\Sigma} \beta + \psi^T m R_n) \\
= (\Sigma_m^\psi + \Sigma_n^\psi)^{-1}(\Psi_m R_n + \psi^T m y_m) \\
= \left( \sum_{i=1}^{n+m} \psi_i \psi_i^T \right)^{-1} \left( \sum_{i=1}^{n+m} \psi_i y_i \right),
\]
i.e., we got the linear regression solution for \( \beta \) as if all the data \( \{\psi_i\}_{i=1}^{n+m} \) was observed!