
Active Hierarchical Metric Learning

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Abstract

Many learning problems require a well defined notion of distance between points in space. Constructing or finding such a measure falls into the field of metric learning. Applications where data is collected in an interactive or online fashion have become commonplace. A lot of downstream inference assumes an appropriate representation of this incoming data. To contribute to this problem, we attempt to formulate similarity learning in a bandits framework. We exploit LinUCB like methods, in both online as well as active settings to design and empirically investigate algorithms that try to learn with linear as well as more expressive non-linear similarity function classes.

1 Introduction

Contextual bandits are a framework that leverage the ability to act and potentially influence the incoming data distribution. In a traditional contextual bandits problem in each round t , the learner observes some context c , chooses some action a to perform, and receives some reward $r(c,a)$ based on the context and action. The learners goal is to maximize its total rewards over a fixed number of total rounds. A lot of interactive repeated decision problems can be modelled using contextual bandits. They serve as a simplified version of the reinforcement learning framework, while providing a toolset needed to analyse performance of the algorithm. This estimate is usually measured by regret, an expected difference between the sum of optimal rewards and collected rewards. Online learning algorithms are designed with the informal goal of minimizing prediction errors. These goals, if aligned can allow the construction of bandit algorithms that solve online learning problems.

Learning the notion of similarity between datapoints is important for lots of machine learning, information retrieval and pattern recognition tasks. For instance, clustering relies on being able to measure some distance between points, recommendation systems try to predict which unseen items are "closest" to the ones already viewed. Nearest neighbor classifiers assume that data are closer to points of the same class. There are lots of metric learning algorithms out there that use batch data and learn in a supervised fashion. A good example is large margin nearest neighbor, which uses the knowledge of local neighbors of points to formulate and solve a convex program. Metric learning has also been approached via the online framework, especially to tackle problems where the magnitude of the data is large enough that batch algorithms are less scalable. One such example is POLA [8], where the metric is parametrized by a positive semidefinite matrix. At each iteration, the algorithm works by projecting the current matrix into the obtained constraint set, and then back onto the PSD cone. Another algorithm, RDML [4] builds on top of POLA using more efficient update methods to speed up the projections.

In order to move to the bandits framework, we relax our requirement for searching for a distance function in the formal sense of satisfying metric axioms, and instead focus our attention on similarity functions of any function class such that for $2n$ dimensional objects, $\phi : \mathbb{R}^{2n} \rightarrow \mathbb{R}^2$. The key idea is

engineer the bandit reward to encourage actions that choose *similar* points, and coax the algorithm to model this reward in the hopes that it transitively captures this notion of similarity. In this paper we build intuition of this concept by first restricting our function class to linear similarities, and devising a method similar to the LinUCB contextual bandit algorithm. Then we move on to more expressive model classes. Although various non-linear methods for the estimation of the reward exist we chose to focus on neural based ones. Previous work examines the use of these methods in the context of bayesian optimization [7] or ucb based methods [11][10] we chose to focus on ucb based methods that make use of the full neural network to estimate its optimistic bound. We design an algorithm that encourages the creation of embeddings to behave well under cosine similarity. Our algorithm formulations are somewhat inspired by the methods discussed in [7]. Our exploration is broadly divided into two frameworks, the online framework that aims to minimize cumulative regret, and an active framework that prioritises efficient search of the optimum function. We looked at experimental methodologies for active metric learning in [6]. Our motivation for active learning comes from studying problems like active ranking by pairwise comparison [3] and interactive structure learning which presents a generalised framework for interactive learning problems [9].

2 Problem Statement

We focus our attention on two different problems. The first consists of making a series of sequential predictions while learning a similarity measure. We refer to this problem as Online Similarity Learning. The second problem consists of learning a similarity measure while actively querying points in space. We refer to this problem as Active Similarity Learning.

2.1 Online Similarity Learning

We consider an online similarity learning problem played over T rounds. At round t the environment samples K pairs of points $(x_{t,k}, y_{t,k}) \in \mathbb{R}^{2n}$. The agent then chooses pair $k_t \in [K]$ and is given a reward $r_{t,k_t} \in \{1, -1\}$. We assume that there exists some similarity function unknown to the agent $\phi : \mathbb{R}^{2n} \rightarrow \{1, -1\}$ and that the rewards are such that if at time $t \in [T]$ the agent chooses pair $(x_{t,k}, y_{t,k})$ then the reward is $\phi(x_{t,k}, y_{t,k})$.

As usual we define the regret as

$$R_T = \mathbb{E} \left[\sum_{t=1}^T \phi(x_{t,k_t^*}, y_{t,k_t^*}) - \phi(x_{t,k_t}, y_{t,k_t}) \right]$$

where $k_t^* = \operatorname{argmax}_{k \in [K]} \phi(x_{t,k}, y_{t,k})$

2.2 Active similarity learning

We assume that the learner has access to a dataset $D = \{x_i \in \mathbb{R}^n | i \in [N]\}$ of unlabeled points and that there exists some function $\phi : \mathbb{R}^{2n} \rightarrow \{-1, 1\}$ which the learner is trying to learn. The learner can query T pairs of points in this set D to obtain a dataset $D_T = \{(x_t, y_t, r_t) | t \in [T]\}$ where x_t and y_t are the points in space and r_t is their similarity. The learner maintains and estimate $\hat{\phi}_t \in \mathcal{F}$ of ϕ , where \mathcal{F} is its function class and we denote the loss between an estimate $\hat{\phi}$ a ϕ as

$$\mathcal{L}(\phi, \hat{\phi}) = \mathbb{E}_{(x,y) \sim \mathcal{D} \times \mathcal{D}}[(\hat{\phi}(x, y) - \phi(x, y))^2]$$

In this problem the goal is to find $\min_{\phi \in \mathcal{F}} \mathcal{L}(\hat{\phi}_T, \phi)$.

3 Description of the algorithms

We provide 4 algorithms which can be grouped into neural and linear bandit version. We refer to our algorithms as OnSim-LinUCB, ActSim-LinUCB, OnSim-NeuralUCB, ActSim-NeuralUCB, depending on whether the bandit algorithm they are based on and the problem they are trying to solve. The algorithms are all very similar but we provide them in full for completeness.

3.1 Online similarity learning

3.1.1 OnSim-LinUCB

By assuming a linear structure in the similarity function, our first algorithm performs a straightforward reduction of the online learning problem to that of regular contextual linear bandits as described in

[1]. Mathematically, we model the similarity of two points as $\phi(x, y) = x^\top A y$. This is reasonable if we consider that

$$\phi(x, y) = x^\top A y = \sum_{i=1}^n \sum_{j=1}^n x_i y_j A_{i,j}$$

which we is linear in A and thus allows us to use the framework of LinUCB for our problem. The algorithm can be found in the appendix in 4. We omit it from the main text due to its similarity with the first algorithm in [1].

3.1.2 OnSim-NeuralUCB

The expressive power of the above framework is quite limited because of the fact that Algorithm 4 assumes that similarity is the result of a dot product in which both points are independently mapped to a new representation via a linear transformation. This will obviously not be true for many datasets. To overcome these limitations we adapt NeuralUCB [11] to our circumstances.

Formally, we assume that

$$\phi(x, y) = \cos(f(x; \theta), f(y; \theta)) = \frac{\langle f(x; \theta), f(y; \theta) \rangle}{\|f(x; \theta)\|_2 \|f(y; \theta)\|_2}$$

¹ Here $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$ is a simple neural network of the form

$$f(x; \theta) = b_L + W_L \sigma(b_{L-1} + W_{L-1} \sigma(\dots \sigma(b_1 + W_1 x)))$$

for some $L \in \mathbb{N}_{\geq 2}$, $W_1 \in \mathbb{R}^{d \times n}$, $W_L \in \mathbb{R}^{m \times d}$, $W_l \in \mathbb{R}^{d \times d}$ if $l \in [2, L-1]$, $b_L \in \mathbb{R}^m$, $b_l \in \mathbb{R}^d$ for $l \neq L$, and where $\sigma(x) = \max\{0, x\}$ applied component wise. We use θ to denote the flattened vector of $(W_L, b_L, \dots, W_1, b_1)$. Using this notation OnSim-NeuralUCB is described below in Algorithm 1. We use p to denote the total number of trainable parameters in the neural network.

Algorithm 1: OnSim-NeuralUCB

Input : Rounds T , exploration parameter α , τ_r frequency of resets, τ_T frequency of training, E epochs for training, b_s batch size for training, ϵ learning rate.

```

1  $A \leftarrow I_p$ ;
2 for  $t \in [T]$  do
3   Observe  $K$  pairs of vectors  $x_t^k \in \mathbb{R}^n$ ,  $y_t^k \in \mathbb{R}^m$ ;
4   for  $k \in [K]$  do
5      $| p_{t,k} \leftarrow \phi(x_t^k, y_t^k) + \alpha \sqrt{(\nabla_\theta \phi(x_t^k, y_t^k))^\top A^{-1} \nabla_\theta \phi(x_t^k, y_t^k)}$ ;
6   end
7   Choose pair  $k_t = \text{argmax}_k p_{t,k}$  with ties broken arbitrarily;
8   Observe payoff  $r_t \in \{-1, 1\}$ ;
9   if  $t \bmod \tau_r = 0$  then
10     $| \theta \leftarrow \text{Train}(\epsilon, E, \{(x_i^{k_i}, y_i^{k_i}, r_i)\}_{i=1}^t, b_s)$ ;
11   end
12   if  $t \bmod \tau_T = 0$  then
13     $| A \leftarrow I_p$ 
14   end
15    $| A \leftarrow A + \nabla_\theta \phi(x_t^k, y_t^k) (\nabla_\theta \phi(x_t^k, y_t^k))^\top$ ;
16 end
```

Intuitively, this algorithm acts optimally with the current set of parameters with a bonus for exploration, and every so often it stops back to train the network. “Train” can be found in the appendix as 3 but it simply describes the normal process of training a neural network with MSE loss.

Our algorithm is very similar to that proposed in [11] but it differs in the following aspects: 1. We adopt a siamese neural network architecture unlike the paper. 2. We add bias 3. We use cosine similarity

¹ It is also possible to assume that we don't normalize the last inner product, we refer to this version and unnormalized NeuralUCB. We provide some comparisons of this version also below.

function in our last layer 4. We restart the the matrix A after every $t \bmod \tau_T = 0$ iterations 5. We use a constant exploration parameter. We propose these changes because we believe they are more sensible for our particular application (and do provide better empirical performance) but they destroy any theoretical guarantees. In [11] these assumptions alongside arguments related to the neural tangent kernel matrix [2] are used to provide a $\tilde{O}(\sqrt{T})$, bound on the regret of algorithm.

3.2 Active Similarity Learning

Despite the differences with online similarity learning, for the active version of the problem we modify the above algorithms only slightly. The idea is to use the optimism bonus as a measure of uncertainty and ignore completely the reward.

Algorithm 2: Active-LinUCB

```

Input : Rounds  $T$  and exploration parameter  $\alpha$ 
1  $A \leftarrow I_{n^2}$ ;
2  $b \leftarrow 0_{n^2}$ ;
3 for  $t \in [T]$  do
4    $\theta_t \leftarrow A^{-1}b$  Observe  $K$  pairs of vectors  $x^k \in R^n$ ,  $y^k \in R^n$ ;
5   Create  $z_{t,k} = (x_1^k y_1^k, x_1^k y_1^k, \dots, x_n^k y_{n-1}^k, x_n^k y_n^k)$ ;
6   for  $k \in [K]$  do
7      $p_{t,a} \leftarrow \alpha \sqrt{z_{t,k} A^{-1} x_{t,a}}$ 
8   end
9   Choose action pair  $k_t = \text{argmax}_a p_{t,a}$  with ties broken arbitrarily.:
10  Observe label  $r_t \in \{-1, 1\}$ ;
11   $A \leftarrow A + z_{t,k_t} z_{t,k_t}^\top$ ;
12   $b \leftarrow z_{t,j_t} r_t$ ;
13 end

```

Using this framework, each time we have to make a query we can sample a subset of points in the unlabeled dataset D and then we reveal the label of the pair with the highest uncertainty as measured by the bonus. We emphasize that r_t now references a label rather than a reward. Algorithm 2 describes this processes formally in the case of ActiveSim-LinUCB and similar modification applies for ActiveSim-NeuralUCB². In Algorithm 5 the most important change is line 5 and in algorithm 2 the most important change is line 7.

4 Empirical Evaluation

Below we describe the set of experiments that we performed. We test separately NeuralUCB and LinUCB based algorithms as we logically expect them to perform very differently due to the limitations of a linear approach.

4.1 NeuralUCB

Dataset Although we tested on various datasets we found the costs to train on non-toy datasets prohibitive for the neural version of the algorithms. As a result, we mainly tested on toy datasets and provide results only for the famous crescent moons dataset an implementation of which can be found here. We also provide results on MNIST dataset in section (A.2).

Neural Network For our experiments we used a 3 layer neural network with 25 hidden units in each layer and an output dimension of 2. In addition to the description of the algorithm provided above, we also added a dropout layer after each regular layer of the neural network with $p = 0.3$.

Optimizer We attempted to use SGD, Adam, and SGD with momentum with various different hyper parameters. Generally, We found that Adam was the best performing optimizer followed by SGD with momentum. We used a learning rate of 0.001, a momentum of 0.9, and the default hyperparameters in [5].

²A precise implementation can be found in the appendix

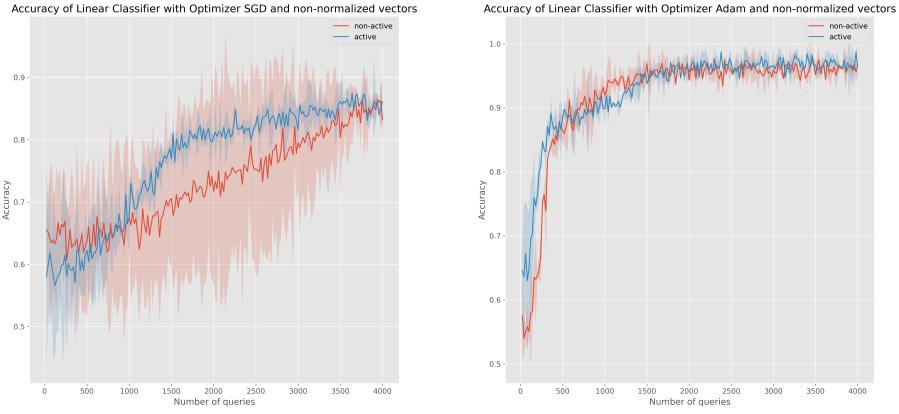


Figure 1: Performance SVM on non-normalized learned features Adam vs SGD

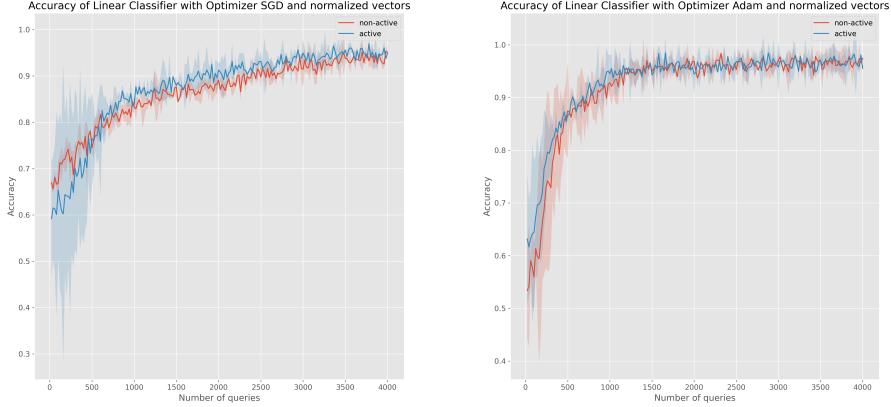


Figure 2: Performance SVM on normalized learned features Adam vs SGD

Additional Parameters We sampled ten datapoints at time for both the online and active version of the problem. Neural networks were trained after 100 queries (or timesteps) and trained for two epochs. Every 4 epochs we reset the matrices to their original states. We rotate the the data the algorithm sees every two time steps. The values reported for losses and accuracy are computed on a heldout set of the data of 1000 datapoints.

4.1.1 Experiment 1: Effectiveness of a linear classifier on learned features

To determine the quality of our embeddings we used an SVM to classify the learned features and observe these values per iteration. We report the results both for SGD with momentum and Adam. Additionally, we also report the performance of NeuralUCB using the unnormalized version of cosine similarity. All graphs contain the mean and a 95% confidence interval computed over 10 runs of the algorithm. The results are shown in Figures (1) and (2)

Clearly we see that on normalized version the performance of an active approach yields better results than non-active but when normalized features are used we see that this effect almost disappears completely. Moreover, it seems that using Adam reduces the difference between algorithms.

4.2 Experiment 2: Comparison of L2 loss through time

Using the exact setup as in Experiment 1, we report the results of the L2 loss through time for Active-NeuralUCB.

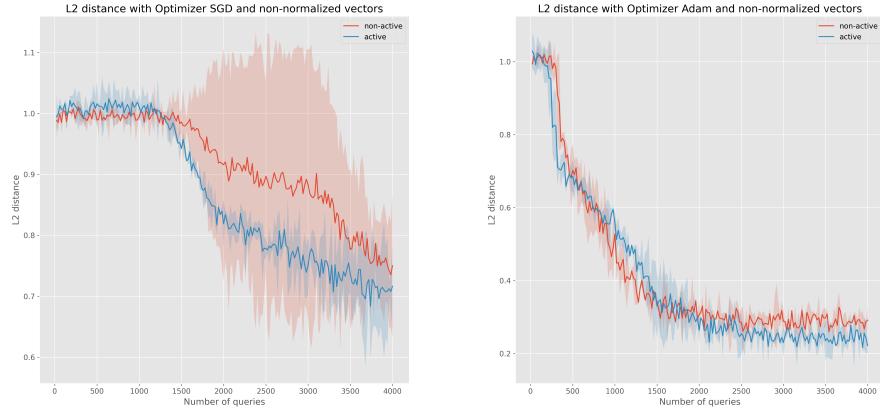


Figure 3: Performance SVM on non-normalized learned features Adam vs SGD

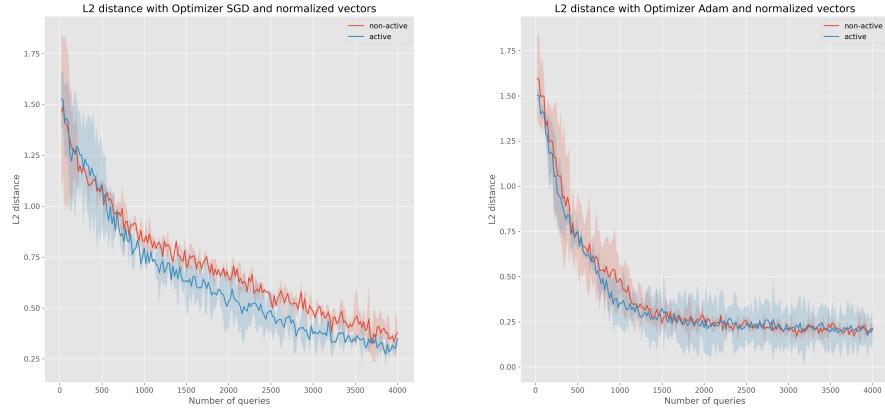


Figure 4: Performance SVM on normalized learned features Adam vs SGD

As before, we observe that adam erases to a large extent the differences between algorithms and that the performance of the active approach depends heavily on the particular optimizer used.

4.3 Experiment 3: Regret of OnSim-NeuralUCB

We observe the performance of OnSim-NeuralUCB by comprising the regret of the algorithm with the regret of an epsilon-greedy neural network with the same architecture and hyperparameters. We report the results only for Adam as it had a significantly better performance, but provide the comparison both for the normalized and unnormalized versions. Like in the previous experiment all graphs contain the mean and a 95% confidence interval. We also compare various values for the exploration parameter.

For this dataset we observe that there is no significant difference between using a simpler epsilon greedy approach and our neural-ucb based approach.

4.4 LinearUCB

Dataset: To test the linear version of our algorithm we created a blobs dataset. Every point is drawn from the following process. Assume that $x'_i \sim \mathcal{N}((0, 0)^\top, I_2)$ and $p_i \sim \text{Bernoulli}(p)$ where p is some parameter. Then the data point x_i is drawn from the following process

$$x_i = \begin{bmatrix} 3 & 0 \\ 0 & 1 \end{bmatrix} x'_i - (1 - p_i) \begin{bmatrix} 1 \\ 1 \end{bmatrix} + p_i \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

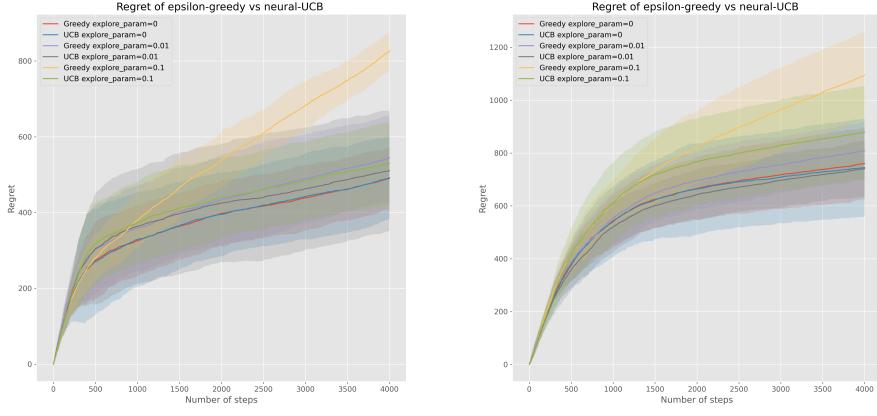


Figure 5: Performance OnSim-NeuralUCB on non-normalized and normalized features

which corresponds to two blobs one placed on the left axis and one on the right axis. We say that two points are similar if they share the same value of p . We refer to this dataset as the Blobs dataset.

4.4.1 Experiment 1: Effectiveness of active learning balanced and unbalanced dataset

We test the effectiveness of active learning on the balanced and unbalanced datasets. For the unbalanced instance we use $p = 0.1$ but provide the results of an L2 loss assuming that the real distribution of the data is balanced. This is done to simulate a situation in which our collected unlabeled data is based and to show the improvement in robustness of the algorithm. The plots in (6) and (7) contain the mean and the 95% confidence interval for the regret over 30 runs of each algorithm.

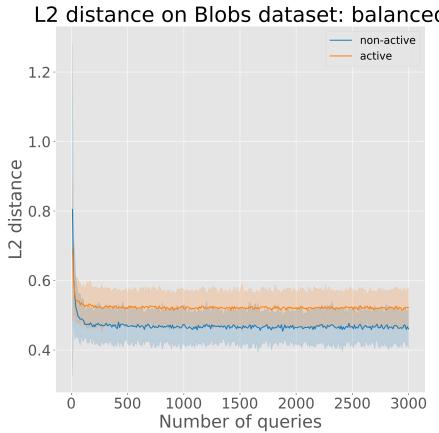


Figure 6: Balanced dataset

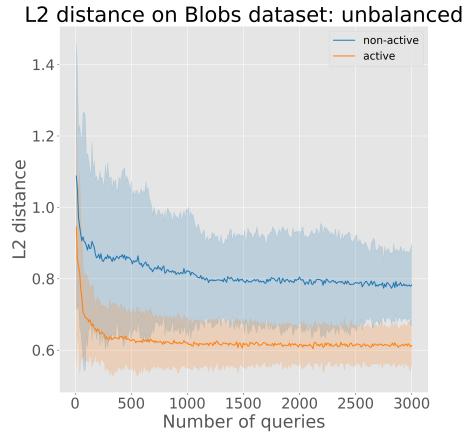


Figure 7: Unbalanced dataset

We observe that the performance of our active algorithm is slightly worse than the baseline in the balanced data regime but it is significantly better when we have unbalanced data. More importantly, we see that it is able to maintain low variance in an unbalanced regime while the non-active approach doesn't enjoy this property.

4.4.2 Experiment 2: Regret of active similarity with regime shifts

To show that our approach leads to enhanced robustness we assume that we find ourselves in a situation where there might be regime shifts in the data in the sense that the underlying distribution at which the data is provided to the algorithm changes.

In particular, in the situation below we assume that initially the data is provided to us where there is an equal chance of getting a point from the left blob and right blob but there at every time-step there is a $1/3000$ chance that we will have a regime shift where the data is now sampled such that $p = 0.1$. Plots (8) and (9) indicate the mean regret of the algorithm at the end and the error bars depict the the 2.5 and 97.5 quantiles observed from 30 runs.

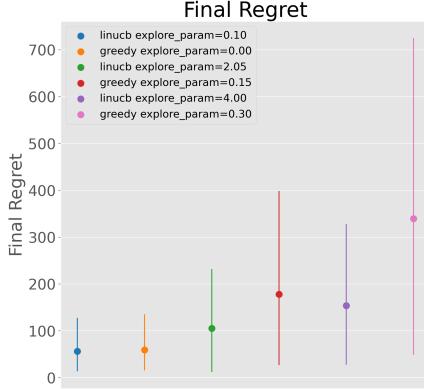


Figure 8: Regret without regime change

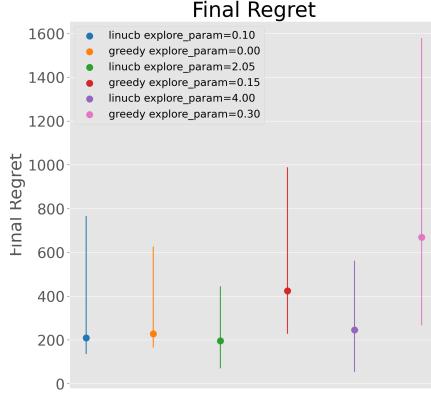


Figure 9: Regret with regime change

When there is no regime change we see that a purely greedy approach has a similar performance to an active approach with exploration parameter of 0.1. However, when we allow for regime changes we see that a linucb based approach with exploration parameter 2.05 beats all greedy algorithms, not only interms of a lower mean regret but also in terms of a significantly lower 97.5 quantile and lower 2.5 quantile.

5 Discussion of results

The results of the experiments show a mixed picture. On the one hand the results for Active-LinUCB and OnSim-LinUCB show the benefits that hour approach has compared to a naive use of the data or an epsilon greedy baseline. This is reasonable as the matrix used in the algorithm naturally favors a diversity of points which allows the algorithm to explore the two blobs more efficiently.

However, we observe that for our neural algorithms the performance varies significantly depending on the particular optimization strategy used and whether we use normalized or non-normalized features. This situation is aggravated further by $O(p^2)$ memory requirements (due to the matrix computation) of the algorithm and the $O(Tp^2)$ time requirements (due to the computation of the optimism). All of the above suggests that even if there is an advantage the algorithms are not feasible for practical settings.

Finally, it is important to note that even if the linear approach works, the reason why it performs so well is because it implicitly uses some notion of diversity implicit in the euclidean space. This is limiting and contradictory in that precisely such a notion of euclidean space is what we are trying to learn.

An interesting alternative which would solve the aformentioned issues realted to the complexity of the algorithms and the issues pertaining to the notion of space in the linear case is to use only a shallow notion of UCB as proposed in [10] or [7]. This way we can avoid the expensive matrix computations and optimize based on a diversity of vectors with respect to the notion of space used by the neural network, which is constantly changing.

6 Conclusion and Future Work

In this work we studied a variety of approaches to solving the active learning and online versions of similarity learning using UCB based approaches. Although our work suggests that the methods proposed are not enough for practical use, we believe that the tests conducted suggests that there

is value in exploring these approaches, especially in situations where there might be shifts in the underlying distribution of the data and the amount of similar pairs that we get. As a future direction forward we propose to work with shallow methods of exploration to avoid expensive matrix computations while retaining the flexibility of neural based approaches.

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A Appendix

A.1 Algorithms omitted from main text

Algorithm 3: Train

Input : ϵ learning rate, E number of epochs, dataset $\{(x_i^{k_i}, y_i^{k_i}, r_i)\}_{i=1}^t$, b_s batch size

```

1 optimizer ← SGD( $\epsilon$ ,  $\theta$ );
2 for  $j = 1, \dots, E$  do
3    $\mathcal{D} \leftarrow \{(x_1^{k_1}, y_1^{k_1}, r_1), \dots, (x_t^{k_t}, y_t^{k_t}, r_t)\}$ ;
4   while  $\mathcal{D}$  is not empty do
5     Sample minibatch  $M$  of size  $b_s$  from the training examples;
6      $l = \frac{1}{M} \sum_{(x_i^{k_i}, y_i^{k_i}, r_i) \in M} (\phi(x_i^{k_i}, y_i^{k_i}) - r_i)^2$ ;
7      $\theta \leftarrow$  update using optimizer with loss  $l$ ;
8     Remove  $M$  from  $\mathcal{D}$ ;
9   end
10 end
```

Algorithm 4: OnSim-LinUCB

Input : Rounds T and exploration parameter α

```

1  $A \leftarrow I_{n^2}$ ;
2  $b \leftarrow 0_{n^2}$ ;
3 for  $t \in [T]$  do
4    $\theta_t \leftarrow A^{-1}b$  Observe  $K$  pairs of vectors  $x^k \in \mathbb{R}^n, y^k \in \mathbb{R}^n$ ;
5   Create  $z_{t,k} = (x_1^k, y_1^k, x_2^k, y_2^k, \dots, x_n^k, y_{n-1}^k, x_n^k, y_n^k)$ ;
6   for  $k \in [K]$  do
7      $p_{t,a} \leftarrow \theta_t^\top z_{t,k} + \alpha \sqrt{z_{t,k}^\top A^{-1} z_{t,a}}$ 
8   end
9   Choose action  $k_t = \text{argmax}_a p_{t,a}$  with ties broken arbitrarily;
10  Observe payoff  $r_t \in \{-1, 1\}$ ;
11   $A \leftarrow A + z_{t,k_t} z_{t,k_t}^\top$ ;
12   $b \leftarrow z_{t,k_t} r_t$ ;
13 end
```

A.2 Additonal experiments

This section contains additional experiments we ran but omit from the main text due to space considerations.

Algorithm 5: Active-NeuralUCB

Input : Queries T , exploration parameter α , τ_r frequency of resets, τ_T frequency of training,
 E epochs for training, b_s batch size for training, ϵ learning rate.

```
1  $A \leftarrow I_p$ ;
2 for  $t \in [T]$  do
3   Sample  $K$  pairs of vectors  $x_t^k \in \mathbb{R}^n$ ,  $y_t^k \in \mathbb{R}^n$  from dataset  $D$ ;
4   for  $k \in [K]$  do
5      $p_{t,k} \leftarrow \alpha \sqrt{(\nabla_\theta \phi(x_t^k, y_t^k))^\top A^{-1} \nabla_\theta \phi(x_t^k, y_t^k)}$ ;
6   end
7   Choose pair  $k_t = \text{argmax}_k p_{t,k}$  with ties broken arbitrarily;
8   Query label  $r_t \in \{-1, 1\}$ ;
9   if  $t \bmod \tau_r = 0$  then
10     $\theta \leftarrow \text{Train}(\epsilon, E, \{(x_i^{k_i}, y_i^{k_i}, r_i)\}_{i=1}^t, b_s)$ ;
11   end
12   if  $t \bmod \tau_T = 0$  then
13     $A \leftarrow I_p$ 
14   end
15    $A \leftarrow A + \nabla_\theta \phi(x_t^k, y_t^k) (\nabla_\theta \phi(x_t^k, y_t^k))^\top$ ;
16 end
```
