Active and Online Similarity Learning

An application of bandits to Similarity learning

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What we did:

Use bandit algorithms to solve the following problems:

- Online learning of a similarity measure.
- Active learning of a similiarity measure (i.e. by querying labels).

Definition

Similarity Measure: A function $\phi : \mathbb{R}^{2n} \to \mathbb{R}$ that maps datapoints $x, y \in \mathbb{R}^n$ to a real number in $\mathbb{R}$ according to how "similar" they are.

Problem: Online Similarity Learning

At round t the environment samples K pairs of points $(x_{t,k}, y_{t,k}) \in \mathbb{R}^{2n}$. We choose pair $k_t \in [K]$ and get reward $r_{t,k_t} \in \{1, -1\}$ based on whether they are similar.

We are trying to minimize:

$$R_T = \mathbb{E}\left[\sum_{t=1}^{T} r_{t,k_t^\star} - r_{t,k_t}\right]$$

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

Problem: Active Similarity Learning

Learner has access to a dataset $D = \{x_i \in \mathbb{R}^n | i \in [N]\}$ of unlabeled points. The learner can query T pairs of points in this set D to obtain a dataset $D_T = \{(x_t, y_t, r_t) \mid t \in [T]\}$. The learner mantains and estimate $\hat{\phi}_t \in \mathcal{F}$ of ϕ, where $\mathcal{F}$ is its function class. Denote the loss between an estimate $\hat{\phi}$ a ϕ as

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

Goal is to find

$$\min_{\hat{\phi}_T \in \mathcal{F}} \mathcal{L}(\hat{\phi}_T, \phi)$$

First idea: Solution to online learning problem

Assume that

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

and then use linucb like methods.

Pros:

- Easy to reason about.
- Fast.

Cons:

- Can only learn linear similarities.

First idea Solution to online learning problem

Input : Rounds T and exploration parameter α
$A \leftarrow I_{n^2}$;
$b \leftarrow 0_{n^2}$;
for $t \in [T]$ **do**
  $\theta_t \leftarrow A^{-1}b$;
  Observe K pairs of vectors $x^k \in \mathbb{R}^n$, $y^k \in \mathbb{R}^n$;
  Create $z_{t,k} = (x_1^k, y_1^k, x_1^k, y_1^k, \ldots, x_n^k y_{n-1}^k, x_n^k, y_n^k)$;
  for $k \in [K]$ **do**
    $p_{t,a} \leftarrow \theta_t^\top z_{t,k} + \alpha\sqrt{z_{t,k}^\top A^{-1} z_{t,a}}$
  end
  Choose action $k_t = \text{argmax}_a p_{t,a}$ with ties broken arbitrarily;
  Observe payoff $r_t \in \{-1, 1\}$;
  $A \leftarrow A + z_{t,k_t} z_{t,k_t}^\top$;
  $b \leftarrow z_{t,k_t} r_t$;
end

Algorithm 1: OnSim-LinUCB

Second idea: Solution to active learning problem

Use the ideas about optimist reward to encourage the learner to explore and chose points optimally.

We replace

$$p_{t,a} \leftarrow \theta_t^\top z_{t,k} + \alpha\sqrt{z_{t,k}^\top A^{-1} z_{t,a}}$$

by

$$p_{t,a} \leftarrow \sqrt{z_{t,k}^\top A^{-1} z_{t,a}}$$

Second Idea: Solution to active learning problem

Input : Rounds T and exploration parameter α

$A \leftarrow I_{n^2}$;

$b \leftarrow 0_{n^2}$;

for $t \in [T]$ **do**

  $\theta_t \leftarrow A^{-1}b$ Sample K pairs of vectors $x^k \in R^n$, $y^k \in R^n$;

  Create $z_{t,k} = (x_1^k y_1^k, x_1^k y_1^k, \ldots, x_n^k y_{n-1}^k, x_n^k y_n^k)$;

  for $k \in [K]$ **do**

    $p_{t,a} \leftarrow \alpha\sqrt{z_{t,k}A^{-1}x_{t,a}}$

  end

  Choose action pair $k_t = \text{argmax}_a p_{t,a}$ with ties broken arbitrarily.;

  Observe label $r_t \in \{-1, 1\}$;

  $A \leftarrow A + z_{t,k_t} z_{t,k_t}^\top$;

  $b \leftarrow z_{t,j_t} r_t$;

end

Algorithm 2: ActiveSim-LinUCB

More expressive model classes: Neural UCB

Method for solving the problem using a neural network to predict the rewards.

- Uses a Neural Network to model the rewards.
- Provably correct regret bound of $\tilde{O}(\tilde{d}\sqrt{T})$.
- Slow due to the computation of a very wide matrix.

Second model

Assume that

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

or

$$\phi(x,y) = \langle f(x;\theta), f(y;\theta)\rangle$$

where

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

Algorithm for solving Online Similarity Learning Problem

$A \leftarrow I_p$;
for $t \in [T]$ **do**
  Observe K pairs of vectors $x_t^k \in \mathbb{R}^n$, $y_t^k \in \mathbb{R}^\ltimes$;
  for $k \in [K]$ **do**
    $p_{t,k} \leftarrow \phi(x, y) + \alpha\sqrt{(\nabla_\theta \phi(x_t^k, y_t^k))^\top A^{-1} \nabla_\theta \phi(x_t^k, y_t^k)}$;
  end
  Choose pair $k_t = \mathrm{argmax}_k p_{t,k}$ with ties broken arbitrarily;
  Observe payoff $r_t \in \{-1, 1\}$;
  if $t \mod \tau_r = 0$ **then**
    $\theta \leftarrow \mathrm{Train}(\epsilon, E, \{(x_i^{k_i}, y_i^{k_i}, r_i)\}_{i=1}^t, b_s)$;
  end
  if $t \mod \tau_T = 0$ **then**
    $A \leftarrow I_p$
  end
  $A \leftarrow A + \nabla_\theta \phi(x_t^k, y_t^k)(\nabla_\theta \phi(x_t^k, y_t^k))^\top$;
end

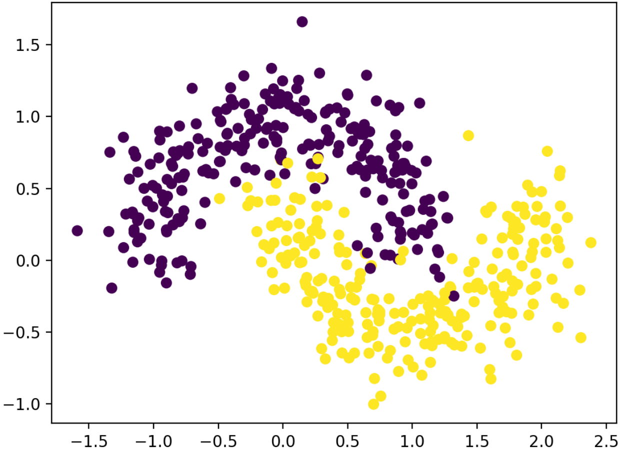
Algorithm 3: OnSim-NeuralUCB

Algorithm for solving Active Learning Problem

$A \leftarrow I_p$;
for $t \in [T]$ **do**
  Sample K pairs of vectors $x_t^k \in \mathbb{R}^n$, $y_t^k \in \mathbb{R}^n$ from dataset D;
  for $k \in [K]$ **do**
    $p_{t,k} \leftarrow \alpha\sqrt{(\nabla_\theta \phi(x_t^k, y_t^k))^\top A^{-1} \nabla_\theta \phi(x_t^k, y_t^k)}$;
  end
  Choose pair $k_t = \mathrm{argmax}_k p_{t,k}$ with ties broken arbitrarily;
  Query label $r_t \in \{-1, 1\}$;
  if $t \mod \tau_r = 0$ **then**
    $\theta \leftarrow \mathrm{Train}(\epsilon, E, \{(x_i^{k_i}, y_i^{k_i}, r_i)\}_{i=1}^t, b_s)$;
  end
  if $t \mod \tau_T = 0$ **then**
    $A \leftarrow I_p$
  end
  $A \leftarrow A + \nabla_\theta \phi(x_t^k, y_t^k)(\nabla_\theta \phi(x_t^k, y_t^k))^\top$;
end

Algorithm 4: ActiveSim-NeuralUCB

Empirical Test with Crescent Moons:



Testing a SVM on learned features

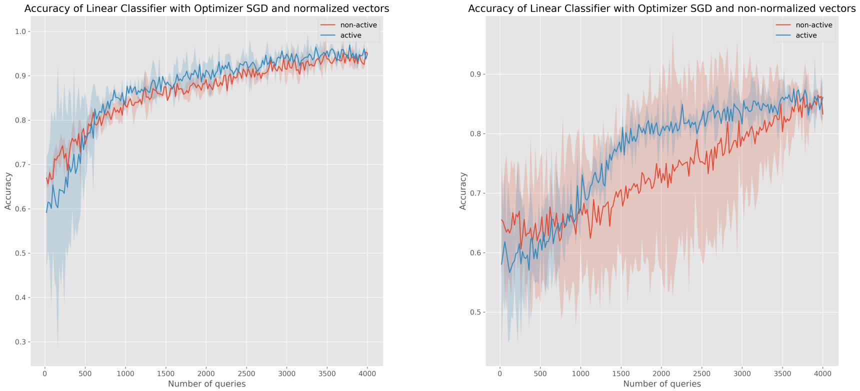


Figure: Performance SVM

Comparing L2 loss of learned features

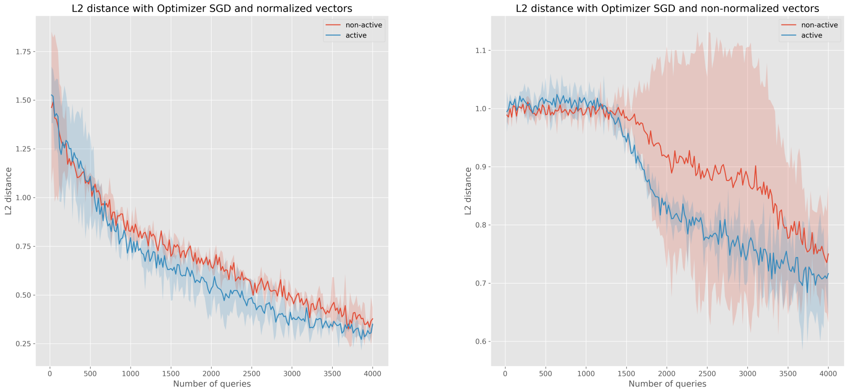


Figure: Performance SVM

Empirical test on blobs:

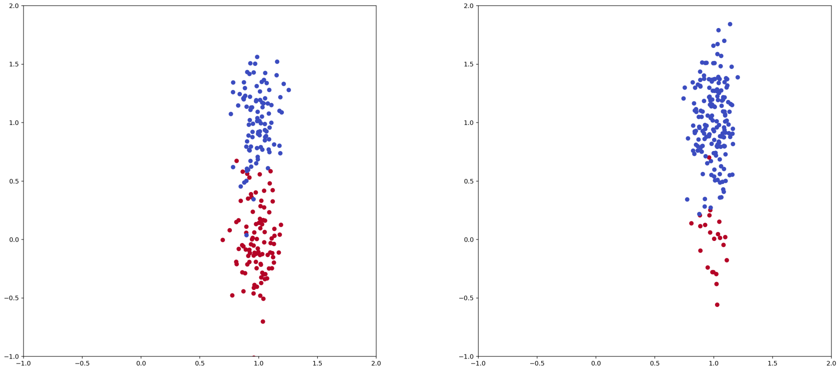


Figure: Performance SVM

Results

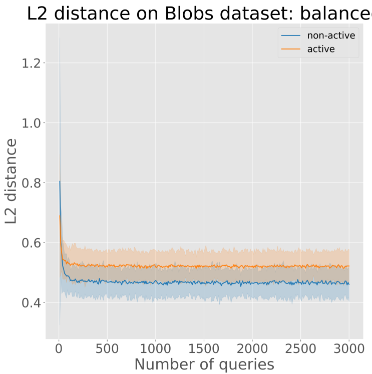


Figure: Balanced dataset

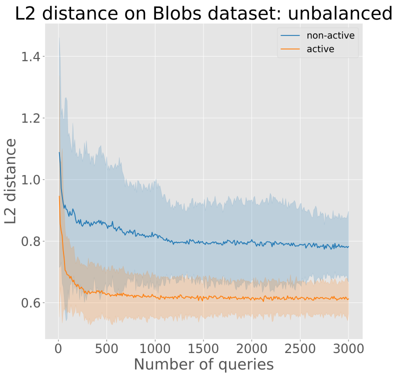


Figure: Unbalanced dataset

Results

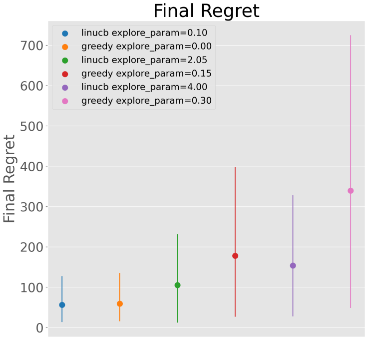


Figure: Regret without regime change

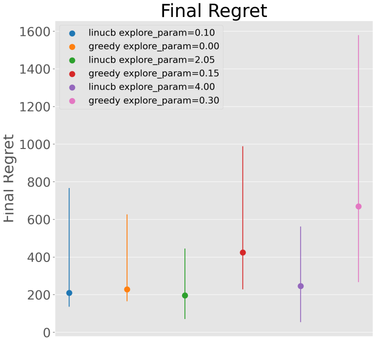


Figure: Regret with regime change

Caveats:

- The algorithm is really slow (we tried using on raw MNIST/CIFAR10 etc and it was unusable).
- The results seem to be sensitive with respect to the optimizer (see next slide).
- We currently don't have theoretical guarantees on the regret.

Conclusion: Is this the right approach?

Maybe but not exactly like this.