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 similarity 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:

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

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

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:

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 linuch like methods.

Pros:

- Easy to reason about.
- Fast.

Cons:

• Can only learn linear similarities.

First idea Solution to problem 1:

```
Input: Rounds T and exploration parameter \alpha
A \leftarrow I_{n^2};
b \leftarrow 0_{n^2};
for t \in [T] do
      \theta_{+} \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, \dots, 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 = \operatorname{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_s}^{\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

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

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

$$\mathbf{for} \ t \in [T] \ \mathbf{do}$$

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

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

$$\mathbf{for} \ k \in [K] \ \mathbf{do}$$

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

$$\mathbf{end}$$

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

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

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

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

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.
- Proably correct regret bound of $\tilde{O}(\tilde{d}\sqrt{T})$.
- Slow due to the computation of a very wide matrix.

Second model

Assume that

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

or

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

where

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

Algorithm for solving Online Similarity Learning Problem

```
A \leftarrow I_n;
for t \in [T] do
       Observe K pairs of vectors x_t^k \in \mathbb{R}^n, y_t^k \in \mathbb{R}^{\times};
       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 = \operatorname{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 \operatorname{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_n
       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

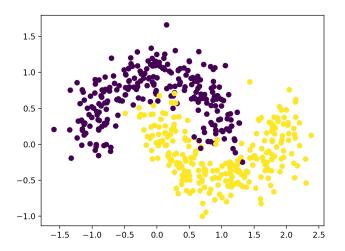
Algorithm for solving Active Learning Problem

```
A \leftarrow I_n;
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 = \operatorname{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 \operatorname{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_n
       end
       A \leftarrow A + \nabla_{\theta} \phi(x_t^k, y_t^k) (\nabla_{\theta} \phi(x_t^k, y_t^k))^{\top};
```

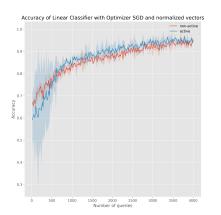
end

Algorithm 4: ActiveSim-NeuralUCB

Empirical Test with Crescent Moons:



Testing a SVM on learned features



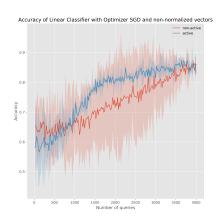
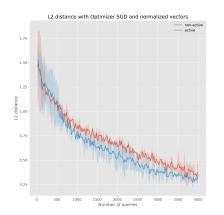


Figure: Performance SVM

Comparing L2 loss of learned features



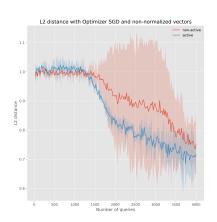
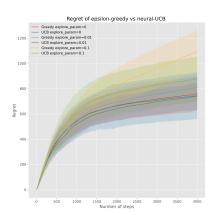


Figure: Performance SVM

Comparison of regret



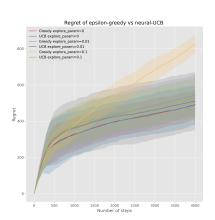


Figure: L2 Loss

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.