On Tree-based Methods for Similarity Learning

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Motivation

Biometric identification =
checks correspondance of two measurements (x, x').

Given a **similarity** s and a **threshold** t,

$$(x, x') \text{ is a match } \Leftrightarrow s(x, x') > t. \quad (1)$$

The ROC curve of s gives the **true positive rate** (TPR) given the **false positive rate** (FPR) associated to eq. (1) for all thresholds $t \in \mathbb{R}$.

An usual approach is to optimize the **Area under the ROC$_s$ curve** (AUC) of the similarity function s.

Biometric systems are deployed for a fixed, **low FPR**, which is hard to optimize in practice (see [1]).

Contributions

· **Extension of TreeRank** (see [2]) that learns a symmetric **similarity function** which optimizes the ROC curve for similarity ranking (see [1]).

· **Statistical guarantees** in $\|\cdot\|_\infty$ in the ROC space.

· Empirical illustration on synthetic data.

· Trials on real data.

Preliminaries

Classification setting. Assume $(X, Y) \sim P$, with:

- $Y \in \{1, \dots, K\}$ the output label,
- $X \in \mathcal{X} \subset \mathbb{R}^d$ the input random variable.

Similarity learning. Select similarity function S s.t.

the larger $S(X, X')$ the higher $\mathbb{P}\{Y = Y' \mid X, X'\}$,

with $(X, Y) \perp (X', Y') \sim P$.

Optimal similarities $\mathcal{S}^*$ are increasing transforms of:

$$\eta(x, x') = \mathbb{P}\{Y = Y' \mid (X, X') = (x, x')\}.$$

The accuracy of any $s \in \mathcal{S}$ can be measured by:

$$d_p(s, s^*) = \|\mathrm{ROC}_s - \mathrm{ROC}^*\|_p,$$

where $s^* \in \mathcal{S}^*$ and $p \in [1, +\infty]$.
With $p = 1$, d_p measures the AUC difference.

Given i.i.d. copies $\mathcal{D}_n = \{(X_i, Y_i)\}_{i=1}^n$ of (X, Y), one wants to *rank the dependent pairs*

$$\{((X_i, X_j), Z_{i,j}) : 1 \le i < j \le n\}.$$

TreeRank (see [2].) Recursive technique that builds a piecewise constant score s_{D_n} for *bipartite ranking*.

Bipartite ranking considers data $\{(X_i, Y_i)\}_{i=1}^n$, i.i.d. copies of $(X, Y) \in \mathcal{X} \times \{-1, +1\}$.

TreeRank **splits the input space recursively** for weighted classif. problems with a class $\mathcal{A} \subset \mathcal{P}(\mathcal{X})$.

Under assumptions on the distribution and $\mathcal{A}$, [2] (Corollary 16 therein), states that, given a tree of depth $D = D_n \underset{n\to\infty}{\sim} \log(\sqrt{n})$, $\forall \delta > 0, \exists \lambda$ s. t., w.p. $\ge 1 - \delta$, $\forall n \in \mathbb{N}$, for $i \in \{1, +\infty\}$,

$$d_i(s_{D_n}, s^*) \le \exp(-\lambda\sqrt{\log n}). \quad (2)$$

Similarity TreeRank

For $F_\sigma(\mathcal{C})$, $\sigma \in \{-, +\}$ and $\mathcal{C} \subset \mathcal{X} \times \mathcal{X}$, introduce :

$$\widehat{F}_{\sigma,n}(\mathcal{C}) = \frac{1}{n_\sigma} \sum_{i<j} \mathbb{I}\{(X_i, X_j) \in \mathcal{C},\ Z_{i,j} = \sigma 1\},$$

with $n_\sigma = (2/(n(n-1))) \sum_{i<j} \mathbb{I}\{Z_{i,j} = \sigma 1\}$.

The $\widehat{F}_{\sigma,n}$'s are not averages of i.i.d. observations, but ratios of **averages of pairs**, i.e. ratios of U-statistics, see [1].

Input. Maximal depth $D \ge 1$, class $\mathcal{A}$ of measurable symmetric subsets of $\mathcal{X} \times \mathcal{X}$, training dataset $\mathcal{D}_n$.

1. (Initialization.) Set $\mathcal{C}_{0,0} = \mathcal{X} \times \mathcal{X}$, $\alpha_{d,0} = \beta_{d,0} = 0$ and $\alpha_{d,2^d} = \beta_{d,2^d} = 1$ for $d \ge 0$.

2. (Iterations.)
For $d = 0, \dots, D-1$ and $k = 0, \dots, 2^d - 1$:

a) (Optimization step.)
Set the **entropic measure**:

$$\Lambda_{d,k+1}(\mathcal{C}) = (\alpha_{d,k+1} - \alpha_{d,k})\widehat{F}_{+,n}(\mathcal{C}) - (\beta_{d,k+1} - \beta_{d,k})\widehat{F}_{-,n}(\mathcal{C}).$$

Find the best subset $\mathcal{C}_{d+1,2k}$ of the cell $\mathcal{C}_{d,k}$ in the **AUC sense**:

$$\mathcal{C}_{d+1,2k} = \mathrm{argmax}_{\mathcal{C}\in\mathcal{A},\ \mathcal{C}\subset\mathcal{C}_{d,k}} \widehat{\Lambda}_{d,k+1}(\mathcal{C}).$$

Then, set $\mathcal{C}_{d+1,2k+1} = \mathcal{C}_{d,k} \setminus \mathcal{C}_{d+1,2k}$.

b) (Update.) Set

$$\alpha_{d+1,2k+1} = \alpha_{d,k} + \widehat{F}_{-,n}(\mathcal{C}_{d+1,2k}),$$
$$\beta_{d+1,2k+1} = \beta_{d,k} + \widehat{F}_{+,n}(\mathcal{C}_{d+1,2k}),$$

and $\alpha_{d+1,2k+2} = \alpha_{d,k+1}$, $\beta_{d+1,2k+2} = \beta_{d,k+1}$.

3. (Output.) After D iterations,
get the **piecewise constant similarity** function:

$$s_D(x, x') = \sum_{k=0}^{2^D-1} (2^D - k)\, \mathbb{I}\{(x, x') \in \mathcal{C}_{D,k}\}.$$

Guarantees

The theoretical guarantees of eq. (2) for bipartite ranking remain valid for similarity learning.

Assumption for Theorem 1 to hold:

- the feature space $\mathcal{X}$ is bounded,
- $\alpha \mapsto \mathrm{ROC}^*(\alpha)$ is twice differentiable with a bounded first order derivative,
- the class $\mathcal{A}$ is intersection stable, *i.e.* $\forall(\mathcal{C}, \mathcal{C}') \in \mathcal{A}^2, \mathcal{C} \cap \mathcal{C}' \in \mathcal{A}$,
- the class $\mathcal{A}$ has finite VC dimension $V < +\infty$,
- $\{(x, x') \in \mathcal{X}^2 : \eta(x, x') \ge q\} \in \mathcal{A}$ for all values of $q \in [0, 1]$.

Theorem 1.
Choose $D = D_n$ so that $D_n \underset{n\to\infty}{\sim} \sqrt{\log n}$. Then, for all $\delta > 0$, there exists a constant λ s.t., with probability at least $1 - \delta$, we have for all $n \ge 2$:

$$d_\infty(s_{D_n}, s^*) \le \exp(-\lambda\sqrt{\log n}).$$

Synthetic experiments

We generate data with a random tree of depth D_{gt} and fix $\mathcal{X} = \mathbb{R}^3$, $\delta = 0.01$, $n_{\text{test}} = 100,000$ and $n_{\text{train}} = 150 \cdot (5/4)^{D_{gt}^2}$, TreeRank outputs s_D.

Results feature 95% CI's based on 400 runs.

Class asymmetry		
p_+	$D_1(s_D, s^*)$	$D_\infty(s_D, s^*)$
0.5	$0.07(\pm0.07)$	$0.30(\pm0.07)$
10^{-1}	$0.08(\pm0.08)$	$0.31(\pm0.08)$
10^{-3}	$0.42(\pm0.17)$	$0.75(\pm0.17)$
$2 \cdot 10^{-4}$	$0.45(\pm0.08)$	$0.81(\pm0.08)$
Parameters: $D = D_{gt} = 3$.		

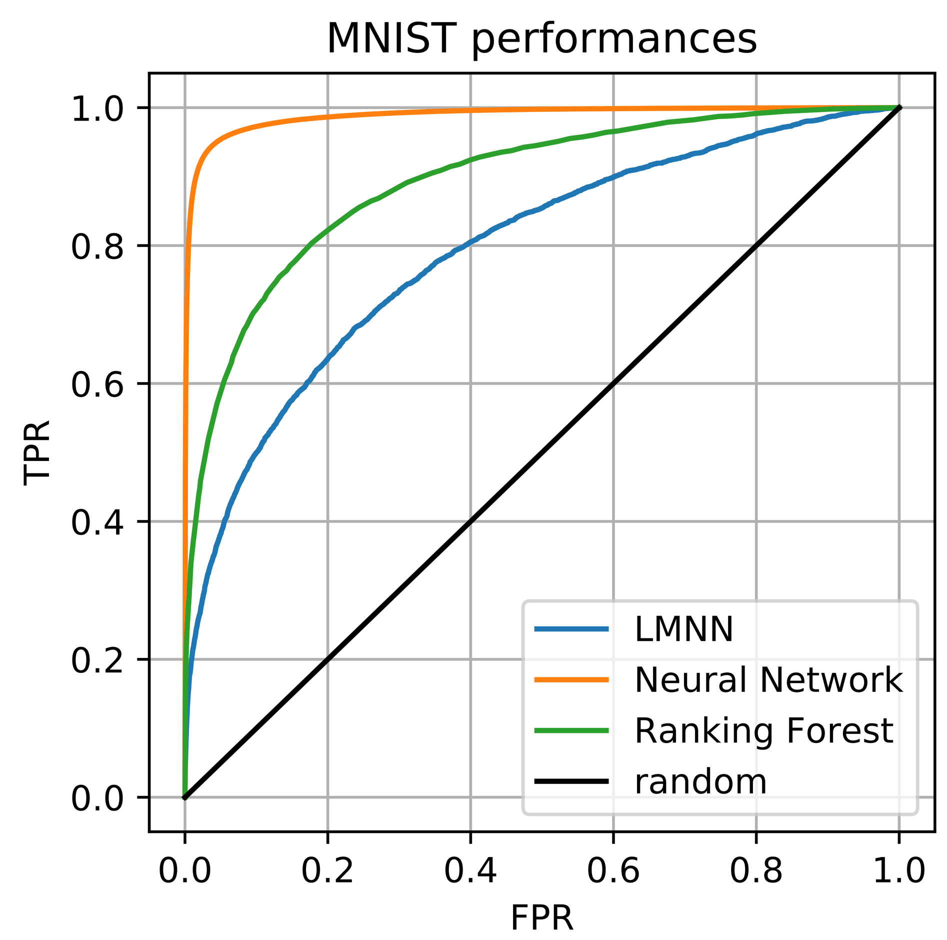
Model bias		
D	$D_1(s_D, s^*)$	$D_\infty(s_D, s^*)$
1	$0.21(\pm0.13)$	$0.65(\pm0.13)$
2	$0.11(\pm0.10)$	$0.43(\pm0.10)$
3	$0.07(\pm0.07)$	$0.30(\pm0.07)$
8	$0.06(\pm0.06)$	$0.28(\pm0.06)$
Parameters: $D_{gt} = 3$, $p = 0.5$.		

This illustrate two factors impairing generalization:
· pronounced **class asymmetry**,
· **underspecified models**.

Real data experiments

We try validating our model by learning similarities on MNIST, reduced by PCA. We test three models:

· A **linear metric learning** algorithm: LMNN [3],
· A simple metric on a **neural network encoding**, trained for classification,
· **Similarity TreeRank** with decision stumps as $\mathcal{A}$.



Conclusions:
TreeRank with decision stumps is limited.
→ $\mathcal{A}$ is not expressive enough ?
Future work: **Treerank with neural networks** as $\mathcal{A}$.

References

[1] Robin Vogel, Aurélien Bellet, and Stéphan Clémençon. A probabilistic theory of supervised similarity learning for pointwise ROC curve optimization. In *ICML*, 2018.

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[3] Kilian Q. Weinberger and Lawrence K. Saul. Distance Metric Learning for Large Margin Nearest Neighbor Classification. *JMLR*, 2009.