Similarity-based Learning via Data Driven Embeddings*

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Similarity-based Learning

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Outline

An Introduction to Learning

- A Brief History of Learning with Similarities
 - Learning with Suitable Similarities
 - Learning with a Suitable Similarity Function
 - Learning with a Suitable Distance Function
 - Data-sensitive Notions of Suitability
 - Learning with Data-sensitive Notions of Suitability
 - Learning the Best Notion of Suitability
 - Results

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Learning

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Dear Junta,

The Hall-8 mess will be closed for the occasion of Diwali at lunch & dinner time. The breakfast will be served along with Lunch packets tomorrow (26th October, 2011).

Please collect your Lunch Packet. The mess would resume its normal working from 27th October.

A legitimate mail

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DEPARTMENT OF COMPUTER SCIENCE AND ENGINEERING SEMINAR SERIES Departmental Colloquium

Title: Similarity-based Learning via Data Driven Embeddings

Speaker: Purushottam Kar

Affiliation: Ph.D. Scholar, CSE Dept., IIT Kanpur

To each his own ...

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- We are given *training points* S = {x₁, x₂,..., x_n} sampled from some distribution D over X and their true labels {ℓ(x₁),...,ℓ(x_n)}.
- Our goal is to output a classifier ℓ̂ : X → {−1, +1} such that it mostly gives out the true labels.

$$\Pr_{\mathbf{x}\sim\mathcal{D}}\left[\hat{\ell}(\mathbf{x})\neq\ell(\mathbf{x})\right]<\epsilon$$

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Learning with Suitable Similarities

- Learning with a Suitable Similarity Function
- Learning with a Suitable Distance Function

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- Perceptron algorithm : $\mathcal{X} \subset \mathbb{R}^d$
 - $\hat{\ell}(x) = \operatorname{sgn}(\langle w, x \rangle)$ for some $w \in \mathbb{R}^d$

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$$\hat{\ell}(x) = \operatorname{sgn}\left(\sum_{x' \in S} \alpha(x') \mathcal{K}(x, x') \ell(x')\right)$$
$$\mathcal{K}(x, x') = \langle x, x' \rangle$$
$$w = \sum_{x' \in S} \alpha(x') \ell(x')$$

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SVM allows use of arbitrary Positive semi-definite kernels

$$\hat{\ell}(x) = \operatorname{sgn}\left(\sum_{x' \in S} \alpha_{\operatorname{SVM}}(x') \mathcal{K}(x, x') \ell(x')\right)$$

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A lot of work was done in trying to incorporate various similarity measures, distance measures into such frameworks [Pękalska and Duin, 2001, Weinberger and Saul, 2009]

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- Some very nice work involving isometric embeddings to (pseudo)Hilbert / Banach spaces [Gottlieb et al., 2010, von Luxburg and Bousquet, 2004, Haasdonk, 2005]

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- A fair amount went into algorithms that did not require PSD kernels as SVMs do [Goldfarb, 1984]
- Some very nice work involving isometric embeddings to (pseudo)Hilbert / Banach spaces [Gottlieb et al., 2010, von Luxburg and Bousquet, 2004, Haasdonk, 2005]
- However, none addressed the issue of suitability of the similarity/distance measure to the learning task

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- Can we do the same for non-PSD similarities ?

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Definition ([Balcan and Blum, 2006])

A similarity $K : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is said to be (ϵ, γ) -good for a classification problem if for some weighing function $w : \mathcal{X} \to [-1, 1]$, at least a $(1 - \epsilon)$ probability mass of examples $x \sim \mathcal{D}$ satisfies

$$\underset{\substack{x' \sim \mathcal{D}, \ell(x') = \ell(x) \\ x'' \sim \mathcal{D}, \ell(x'') \neq \ell(x)}{\mathbb{E}} \left[w\left(x'\right) K(x, x') - w\left(x''\right) K(x, x'') \right] \geq \gamma$$

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 In other words, according to the similarity function, most points, on an average, are more similar to points of the same label

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Learning with a good similarity function

Theorem ([Balcan and Blum, 2006])

Given an (ϵ, γ) -good similarity function, for any $\delta > 0$, given $n = \frac{16}{\gamma^2} \lg \frac{2}{\delta}$ labeled points $(x_i)_{i=1}^n$, the classifier $\hat{\ell}$ defined below has error at margin $\frac{\gamma}{2}$ no more than $\epsilon + \delta$ with probability greater than $1 - \delta$,

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- Notice that the classifier is very similar in form to the SVM and Perceptron classifiers
- Consequently one can use these algorithms to learn this classifier as well

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What is a good distance function

Definition ([Wang et al., 2007])

A distance function $d : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is said to be (ϵ, γ, B) -good for a classification problem if there exist two class conditional probability distributions $\tilde{\mathcal{D}}_+$ and $\tilde{\mathcal{D}}_-$ such that for all $x \in \mathcal{X}$, $\frac{\tilde{\mathcal{D}}_+(x)}{\mathcal{D}(x)} < \sqrt{B}$ and $\frac{\tilde{\mathcal{D}}_-(x)}{\mathcal{D}(x)} < \sqrt{B}$, such that at least a $(1 - \epsilon)$ probability mass of examples $x \sim \mathcal{D}$ satisfies

$$\Pr_{\substack{x'\sim \tilde{\mathcal{D}}_+\\ ''\sim \tilde{\mathcal{D}}_-}} \left[\ell(x)\left(\ell(x')d(x,x')-\ell(x'')d(x,x'')\right)<0\right]\geq \frac{1}{2}+\gamma$$

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- The definition expects the distance function to set dissimilarly labeled points farther off than similarly labeled points
- Yet again this yields a classifier with guaranteed generalization properties

Learning with a good distance function

Theorem ([Wang et al., 2007])

Given an (ϵ, γ, B) -good distance function, for any $\delta > 0$, given $n = \frac{4B^2}{\gamma^2} \lg \frac{1}{\delta}$ pairs of positive and negatively labeled points $(x_i^+, x_i^-)_{i=1}^n$, the classifier $\hat{\ell}$ defined below has error at margin $\frac{\gamma}{B}$ no more than $\epsilon + \delta$ with probability greater than $1 - \delta$,

$$\hat{\ell}(x) = sgn\left(\sum_{i=1}^n \beta_i sgn\left(d(x, x_i^+) - d(x, x_1^-)\right)\right), \sum_{i=1}^n \beta_i = 1, \beta_i \ge 0$$

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• Each of the pairs yields a stump sgn $(d(x, x_i^+) - d(x, x_1^-))$

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- A Brief History of Learning with Similarities
 - Learning with Suitable Similarities
 - Learning with a Suitable Similarity Function
 - Learning with a Suitable Distance Function

Data-sensitive Notions of Suitability

- Learning with Data-sensitive Notions of Suitability
- Learning the Best Notion of Suitability
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- Motivated by this observation we propose a notion of goodness that is data-sensitive
- This notion allows us to tune the goodness notion itself, allowing for better classifiers
- The resulting model subsumes the previous two models
- Consequently, the model does not require separate treatment for similarity and distance functions either

What is a good similarity/distance function

Definition (K. and Jain, 2011)

A similarity function $K : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is said to be (ϵ, γ, B) -good for a classification problem if for some antisymmetric *transfer* function $f : \mathbb{R} \to [-C_f, C_f]$ and some weighing function $w : \mathcal{X} \times \mathcal{X} \to [-B, B]$, at least a $(1 - \epsilon)$ probability mass of examples $x \sim \mathcal{D}$ satisfies

$$\mathop{\mathbb{E}}_{\substack{x'\sim\mathcal{D},\ell(x')=\ell(x)\\x''\sim\mathcal{D},\ell(x'')\neq\ell(x)}} \left[w\left(x',x''\right)f\left(K(x,x')-K(x,x'')\right)\right] \geq 2C_f \gamma$$

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• With appropriate setting of the weighing function and the transfer function, the previous two models can be recovered.

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- Let us first see how, given a (good) transfer function, can we learn a (good) classifier.
- We will later on plug in the routines to learn the transfer function as well.

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Algorithm 1 LEARN-DISSIM

Require: A similarity function *K*, landmark pairs $\mathcal{L} = (x_i^+, x_i^-)_{i=1}^n$, a good transfer function *f*. **Ensure:** A classifier $\hat{\ell} : \mathcal{X} \to \{-1, +1\}$ 1: Define $\Phi_{\mathcal{L}} : \mathcal{X} \to \mathbb{R}^n$ as $\Phi_{\mathcal{L}} : x \mapsto (f(\mathcal{K}(x, x_i^+) - \mathcal{K}(x, x_i^-)))_{i=1}^n)$

- 2: Get a labeled training set $T = \{t_j\}_{j=1}^{n'} \subset \mathcal{X}$ sampled from \mathcal{D} .
- 3: $T' \leftarrow \{\Phi_{\mathcal{L}}(t_j)\}_{j=1}^{n'} \subset \mathbb{R}^n$ be the data set embedded in \mathbb{R}^n
- 4: Learn a linear hyperplane over \mathbb{R}^n using T', $\ell_{lin} \leftarrow LEARN-LINEAR(T')$
- 5: Let $\hat{\ell} : \mathcal{X} \to \{-1, +1\}$ be defined as $\hat{\ell} : x \mapsto \ell_{\text{lin}} (\Phi_{\mathcal{L}}(x))$
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• LEARN-LINEAR may be taken to be any linear hyperplane learning algorithm such as Perceptron, SVM.

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- LEARN-LINEAR may be taken to be any linear hyperplane learning algorithm such as Perceptron, SVM.
- The above procedure essentially creates a *data-driven*, problem specific embedding of the domain \mathcal{X} into a Euclidean space

Learning with data-sensitive notions of suitability

 The results given earlier guarantee small classification error at large margin

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- Not amenable to efficient algorithms as hyperplane classification error is NP-hard to minimize [Garey and Johnson, 1979, Arora et al., 1997]

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- The results given earlier guarantee small classification error at large margin
- Not amenable to efficient algorithms as hyperplane classification error is NP-hard to minimize [Garey and Johnson, 1979, Arora et al., 1997]
- We provide our guarantees in terms of smooth Lipschitz losses like hinge-loss, log-loss etc that can be efficiently minimized over large datasets.

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Working with surrogate loss functions

Definition (K. and Jain, 2011)

A similarity function is said to be (ϵ, B) -good with respect to a loss function $L : \mathbb{R} \to \mathbb{R}^+$ if for some transfer function $f : \mathbb{R} \to \mathbb{R}$ and some weighing function $w : \mathcal{X} \times \mathcal{X} \to [-B, B], \underset{x \sim \mathcal{D}}{\mathbb{E}} [L(G(x))] \leq \epsilon$ where

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Theorem (K. and Jain, 2011)

If *K* is an (ϵ, B) -good similarity function with respect to a C_L -Lipschitz loss function *L* then for any $\epsilon_1 > 0$, with probability at least $1 - \delta$ over the choice of $d = (16B^2C_L^2/\epsilon_1^2)\ln(4B/\delta\epsilon_1)$ landmark pairs, the expected loss of the classifier $\hat{\ell}(x)$ returned by LEARN-DISSIM with respect to *L* satisfies $\mathbb{E}\left[L(\hat{\ell}(x))\right] \leq \epsilon + \epsilon_1$.

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- We give uniform convergence guarantees that enable standard ERM-based routines to recover the best transfer from any compact class of antisymmetric functions.
- This will yield a nested learning problem with the ERM-based transfer function learning algorithm calling the classifier learning algorithm as a subroutine.
- For any transfer function *f* and arbitrary set of landmarks \mathcal{L} , let $L(f) = \underset{x \sim \mathcal{D}}{\mathbb{E}} [L(G(x))]$ and let $L(f, \mathcal{L})$ denote the generalization loss of the best classifier that uses the embedding $\Phi_{\mathcal{L}}$ defined by the landmarks \mathcal{L} .

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- The earlier result shows that for a *fixed* f, for a large enough random \mathcal{L} , $L(f, \mathcal{L}) \leq L(f) + \epsilon_1$.

Theorem (K. and Jain, 2011)

Let \mathcal{F} be a compact class of transfer functions with respect to the infinity norm and $\epsilon_1, \delta > 0$. Let $\mathcal{N}(\mathcal{F}, r)$ be the size of the smallest ϵ -net over \mathcal{F} with respect to the infinity norm at scale $r = \frac{\epsilon_1}{4C_LB}$. Taking $n = \frac{64B^2C_L^2}{\epsilon_1^2} \ln\left(\frac{16B\cdot\mathcal{N}(\mathcal{F},r)}{\delta\epsilon_1}\right)$ random landmark pairs, we have with probability greater than $(1 - \delta)$

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$$\sup_{f\in\mathcal{F}}\left[|L(f,\mathcal{L})-L(f)|\right]\leq\epsilon_1$$

Algorithm 2 FTUNE

Require: A family of transfer functions \mathcal{F} , a similarity function K, a loss function L.

Ensure: An optimal transfer function $f^* \in \mathcal{F}$.

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- 1: Select *d* landmark pairs \mathcal{L} .
- 2: for all $f \in \mathcal{F}$ do

3:
$$w_f \leftarrow \text{LEARN-DISSIM}(K, \mathcal{L}, f), L_f \leftarrow L(f, \mathcal{L})$$

- 4: end for
- 5: $f^* \leftarrow \underset{f \in \mathcal{F}}{\operatorname{arg\,min}} L_f$
- 6: return f*.

 If landmarks are clumped together, then all points will get a similar embedding and linear separation would be impossible

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Algorithm 3 DSELECT **Require:** A training set T. Ensure: A set of *n* landmark pairs. 1: $S \leftarrow \text{RANDOM-ELEMENT}(T), \mathcal{L} \leftarrow \emptyset$ 2: for *j* = 2 to *n* do 3: $z \leftarrow \operatorname*{arg\,min}_{x \in T} \sum_{x' \in S} K(x, x').$ 4: $S \leftarrow S \cup \{z\}, T \leftarrow T \setminus \{z\}$ 5 end for 6: for j = 1 to *n* do 7: Sample z_1, z_2 from S with replacement s.t. $\ell(z_1) = 1, \ \ell(z_2) = -1$ 8: $\mathcal{L} \leftarrow \mathcal{L} \cup \{(z_1, z_2)\}$ 9. end for 10: return L

Outline

- An Introduction to Learning
- A Brief History of Learning with Similarities
 - Learning with a Suitable Similarity Function
 - Learning with a Suitable Distance Function

Data-sensitive Notions of Suitability

- Learning with Data-sensitive Notions of Suitability
- Learning the Best Notion of Suitability
- Results

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Results



Discussion

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Discussion

- BBS performs reasonably well for small landmarking sizes while DBOOST performs well for large landmarking sizes.
- In contrast, our method consistently outperforms the existing methods in both the scenarios.
- Since FTUNE selects its output by way of validation, it is susceptible to over-fitting on small datasets.
- In these cases, DSELECT (intuitively) removes redundancies in the landmark points thus allowing FTUNE to recover the best transfer function.

Thanks

Preprint available at

http://www.cse.iitk.ac.in/users/purushot/

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