KBYÖYO2019

June 25, 2019

Machine Learning from Weak Supervision:

Towards Accurate Classification with Low Labeling Costs



Slides: http://goo.gl/meiTwY

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About Myself

Affiliations:

- Director: RIKEN AIP
- Professor: University of Tokyo
- Consultant: several local startups

Research interests:

- Theory and algorithms of ML
- Real-world applications with partners (signal, image, language, brain, cars, robots, optics, ads, medicine, biology...)

Goal:

 Develop practically useful algorithms that have theoretical support

Sugiyama & Kawanabe, Machine Learning in Non-Stationary Environments, MIT Press, 2012

Sugiyama, Suzuki & Kanamori, Density Ratio Estimation in Machine Learning, Cambridge University Press, 2012

Sugiyama, Statistical Reinforcement Learning, Chapman and Hall/CRC, 2015

Sugiyama, Introduction to Statistical Machine Learning, Morgan Kaufmann, 2015

Cichocki, Phan, Zhao, Lee, Oseledets, Sugiyama & Mandic, Tensor Networks for Dimensionality Reduction and Large-Scale Optimizations, Now, 2017

Nakajima, Watanabe & Sugiyama, Variational Bayesian Learning Theory, Cambridge University Press, 2019



2











What Is This Tutorial about? ³

- Machine learning from big labeled data is highly successful.
 - Speech recognition, image understanding, natural language translation, recommendation...
- However, there are various applications where massive labeled data is not available.
 - Medicine, disaster, robots, brain, ...

What Is This Tutorial about? ⁴

- There are many approaches to coping with the label-cost problem:
 - Improve data collection (e.g., crowdsourcing)
 - Use a simulator to generate pseudo data
 - Use domain knowledge (i.e., engineering)
 - Use cheap but weak data (e.g., unlabeled)
- I introduce our recent advances in classification from weak supervision.



Unsupervised Classification ⁶

Gathering labeled data is costly. Let's use unlabeled data that are often cheap to collect:



- Unsupervised classification is typically clustering.
- This works well only when each cluster corresponds to a class.

Semi-Supervised Classification ⁷

Chapelle, Schölkopf & Zien (MIT Press 2006) and many

- Use a large number of unlabeled samples and a small number of labeled samples.
- Find a boundary along the cluster structure induced by unlabeled samples:
 - Sometimes very useful.
 - But not that different from unsupervised classification.







This Tutorial in a Nutshell

- 1. Background
- 2. PN Classification
- 3. PU Classification
- 4. PNU Classification
- 5. Pconf Classification
- 6. UU Classification
- 7. SU Classification
- 8. Comp Classification
- 9. Summary

Slides: http://goo.gl/meiTwY

- P: Positive
- N: Negative
- U: Unlabeled
- Conf: Confidence
- S: Similar
- Comp: Complementary

9

Method 1: PU Classification ¹⁰

du Plessis, Niu & Sugiyama (NIPS2014, ICML2015) Niu, du Plessis, Sakai, Ma & Sugiyama (NIPS2016) Kiryo, Niu, du Plessis & Sugiyama (NIPS2017)

Only PU data is available; N data is missing:

- Click vs. non-click
- Friend vs. non-friend

From PU data, PN classifiers are trainable!

Method 2: PNU Classification ¹¹ (Semi-Supervised Classification)

Sakai, du Plessis, Niu & Sugiyama (ICML2017)

Let's decompose PNU into PU, PN, and NU:

- Each is solvable.
- Let's combine them!
- Without cluster assumptions, PN classifiers are trainable!





Method 3: Pconf Classification ¹²

Ishida, Niu & Sugiyama (NeurIPS2018)

- Only P data is available, not U data:
 - Data from rival companies cannot be obtained.
 - Only positive results are reported (publication bias).
- "Only-P learning" is unsupervised.

From Pconf data, PN classifiers are trainable!

Positive confidence

Method 4: UU Classification ¹³

du Plessis, Niu & Sugiyama (TAAI2013) Nan, Niu, Menon & Sugiyama (ICLR2019)

From two sets of unlabeled data with different class priors, PN classifiers are trainable!



Method 5: SU Classification ¹⁴

Bao, Niu & Sugiyama (ICML2018)

Delicate classification (money, religion...):

- Highly hesitant to directly answer questions.
- Less reluctant to just say "same as him/her".

From SU data, PN classifiers are trainable!

 $1/\sqrt{n}$



Method 6: Comp Classification¹⁵

Ishida, Niu, Hu & Sugiyama (NIPS2017) Ishida, Niu, Menon & Sugiyama (ICML2019)

- Labeling patterns in multi-class problems:
 - Selecting a collect class from a long list of candidate classes is extremely painful.

Complementary labels:

- Specify a class that a pattern does not belong to.
- This is much easier and faster to perform!
- From complementary labels, classifiers are trainable!
 1/2/2





Contents

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16

PN Classification ¹⁷ (Ordinary Supervised Classification)

Labeled data: $\{(\boldsymbol{x}_i, y_i)\}_{i=1}^n \overset{\text{i.i.d.}}{\sim} p(\boldsymbol{x}, y)$

- Input $\boldsymbol{x} \in \mathbb{R}^d$: *d*-dimensional real vector
- Output $y \in \{+1, -1\}$: Binary class label



Some Definitions

Classifier: $f : \mathbb{R}^d \to \mathbb{R}$ • Label prediction by $\widehat{y} = \operatorname{sign}(f(\boldsymbol{x}))$ (e.g., linear, additive, kernel, deep models). Margin: m = yf(x) $y \in \{+1, -1\}$ • $m > 0 \implies \operatorname{sign}(f(\boldsymbol{x})) = y$ Classification is correct. • $m < 0 \implies \operatorname{sign}(f(\boldsymbol{x})) \neq y$ Classification is wrong.

Zero-one loss: $\ell_{0/1}(m) = \frac{1}{2} (1 - \operatorname{sign}(m))$

- 1 for correct prediction.
- 0 for wrong prediction.

Classification Error 19
 and Empirical Approximation
 Classification error (expected zero-one loss over all test data): E: Expectation

 $R_{0/1}(f) = \mathbb{E}_{p(\boldsymbol{x},y)} \left[\ell_{0/1} \left(y f(\boldsymbol{x}) \right) \right] \qquad \ell_{0/1}(m) = \frac{1}{2} \left(1 - \text{sign}(m) \right)$

• Our goal: Find a minimizer of $R_{0/1}(f)$.

But this is impossible since p(x, y) is unknown:

• Let's use samples: $\{(\boldsymbol{x}_i, y_i)\}_{i=1}^n \overset{\text{i.i.d.}}{\sim} p(\boldsymbol{x}, y)$

i.i.d.: Independent and identically distributed

• Empirical approximation:

$$\widehat{R}_{0/1}(f) = \frac{1}{n} \sum_{i=1}^{n} \ell_{0/1} \left(y_i f(\boldsymbol{x}_i) \right) = R_{0/1}(f) + O_p \left(\frac{1}{\sqrt{n}} \right)$$

Minimization of Empirical Classification Error

$$\widehat{R}_{0/1}(f) = \frac{1}{n} \sum_{i=1}^{n} \ell_{0/1} \Big(y_i f(\boldsymbol{x}_i) \Big)$$

However, minimization of $\widehat{R}_{0/1}(f)$ is NP-hard, due to discrete nature of $\ell_{0/1}$:

 We may not be able to obtain a global minimizer in practice.

Let's use a smoother loss!

20

Surrogate Loss

Let's use a smoother loss as a surrogate:



PN Empirical Risk Minimization²²

Classification risk for loss ℓ :

$$R(f) = \mathbb{E}_{p(\boldsymbol{x},y)} \Big[\ell \Big(y f(\boldsymbol{x}) \Big) \Big]$$

- Empirical risk:
 - Expectation is approximated by sample average:

$$\widehat{R}_{\text{PN}}(f) = \frac{1}{n} \sum_{i=1}^{n} \ell\left(y_i f(\boldsymbol{x}_i)\right) = R(f) + O_p\left(\frac{1}{\sqrt{n}}\right)$$
$$\{(\boldsymbol{x}_i, y_i)\}_{i=1}^{n} \stackrel{\text{i.i.d.}}{\sim} p(\boldsymbol{x}, y)$$

 Minimize it within a certain model class (e.g., linear, additive, kernel, deep,...):

$$\widehat{f}_{\rm PN} = \operatorname*{argmin}_{f} \widehat{R}_{\rm PN}(f)$$



Contents

- - - - I
- 1. Background
- 2. PN Classification
- 3. PU Classification
- 4. PNU Classification
- 5. Pconf Classification
- 6. UU Classification
- 7. SU Classification
- 8. Comp Classification
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PU Classification: Setup

Given: Positive and unlabeled samples

$$\{oldsymbol{x}_i^{\mathrm{P}}\}_{i=1}^{n_{\mathrm{P}}} \stackrel{\mathrm{i.i.d.}}{\sim} p(oldsymbol{x}|y=+1)$$

 $\{oldsymbol{x}_i^{\mathrm{U}}\}_{i=1}^{n_{\mathrm{U}}} \stackrel{\mathrm{i.i.d.}}{\sim} p(oldsymbol{x})$

Goal: Obtain a PN classifier



PN Risk Decomposition 25



PU Risk Estimation ²⁶

$$R(f) = \pi \mathbb{E}_{p(\boldsymbol{x}|y=+1)} \left[\ell \left(f(\boldsymbol{x}) \right) \right] + (1-\pi) \mathbb{E}_{p(\boldsymbol{x}|y=-1)} \left[\ell \left(-f(\boldsymbol{x}) \right) \right]$$

U-density is a mixture of P- and N-densities:

$$p(x) = \pi p(x|y = +1) + (1 - \pi)p(x|y = -1)$$



PU Risk Estimation (cont.) 27

du Plessis, Niu & Sugiyama (ICML2015)

$$R(f) = \pi \mathbb{E}_{p(\boldsymbol{x}|\boldsymbol{y}=+1)} \left[\ell \left(f(\boldsymbol{x}) \right) \right] + (1-\pi) \mathbb{E}_{\boldsymbol{p}(\boldsymbol{x}|\boldsymbol{y}=-1)} \left[\ell \left(-f(\boldsymbol{x}) \right) \right]$$
$$p(\boldsymbol{x}) = \pi p(\boldsymbol{x}|\boldsymbol{y}=+1) + (1-\pi)p(\boldsymbol{x}|\boldsymbol{y}=-1)$$

This allow us to eliminate the N-density:

$$(1 - \pi)p(\boldsymbol{x}|\boldsymbol{y} = -1) = p(\boldsymbol{x}) - \pi p(\boldsymbol{x}|\boldsymbol{y} = +1)$$

$$R(f) = \pi \mathbb{E}_{p(\boldsymbol{x}|\boldsymbol{y}=+1)} \left[\ell \left(f(\boldsymbol{x}) \right) \right]$$

$$+ \mathbb{E}_{p(\boldsymbol{x})} \left[\ell \left(- f(\boldsymbol{x}) \right) \right] - \pi \mathbb{E}_{p(\boldsymbol{x}|\boldsymbol{y}=+1)} \left[\ell \left(- f(\boldsymbol{x}) \right) \right]$$

 Unbiased risk estimation is possible from PU data, just by replacing expectations by sample averages!

PU Empirical Risk Minimization²⁸

 $R(f) = \pi \mathbb{E}_{p(\boldsymbol{x}|y=+1)} \left[\ell \left(f(\boldsymbol{x}) \right) \right] + \mathbb{E}_{p(\boldsymbol{x})} \left[\ell \left(-f(\boldsymbol{x}) \right) \right] - \pi \mathbb{E}_{p(\boldsymbol{x}|y=+1)} \left[\ell \left(-f(\boldsymbol{x}) \right) \right]$

Replacing expectations by sample averages gives an empirical risk:

$$\widehat{R}_{\mathrm{PU}}(f) = \frac{\pi}{n_{\mathrm{P}}} \sum_{i=1}^{n_{\mathrm{P}}} \ell\left(f(\boldsymbol{x}_{i}^{\mathrm{P}})\right) + \frac{1}{n_{\mathrm{U}}} \sum_{i=1}^{n_{\mathrm{U}}} \ell\left(-f(\boldsymbol{x}_{i}^{\mathrm{U}})\right) - \frac{\pi}{n_{\mathrm{P}}} \sum_{i=1}^{n_{\mathrm{P}}} \ell\left(-f(\boldsymbol{x}_{i}^{\mathrm{P}})\right)$$
$$\{\boldsymbol{x}_{i}^{\mathrm{P}}\}_{i=1}^{n_{\mathrm{P}}} \stackrel{\text{i.i.d.}}{\sim} p(\boldsymbol{x}|\boldsymbol{y} = +1) \qquad \{\boldsymbol{x}_{i}^{\mathrm{U}}\}_{i=1}^{n_{\mathrm{U}}} \stackrel{\text{i.i.d.}}{\sim} p(\boldsymbol{x})$$

Optimal convergence rate is attained:

Niu, du Plessis, Sakai, Ma & Sugiyama (NIPS2016)

$$R(\widehat{f}_{\rm PU}) - R(f^*) \le C(\delta) \left(\frac{2\pi}{\sqrt{n_{\rm P}}} + \frac{1}{\sqrt{n_{\rm U}}}\right)$$

with probability $1 - \delta$

 $\widehat{f}_{\rm PU} = \operatorname{argmin}_{f} \widehat{R}_{\rm PU}(f)$ $f^* = \operatorname{argmin}_{f} R(f)$

 $n_{\rm P}, n_{\rm U}~$: # of P, U samples

Theoretical Comparison with PN³⁹

Niu, du Plessis, Sakai, Ma & Sugiyama (NIPS2016)

Estimation error bounds for PU and PN:

 $\widehat{f}_{\rm PN} = \operatorname{argmin} \widehat{R}_{\rm PN}(f)$

$$R(\widehat{f}_{\rm PU}) - R(f^*) \le C(\delta) \left(\frac{2\pi}{\sqrt{n_{\rm P}}} + \frac{1}{\sqrt{n_{\rm U}}}\right)$$
$$R(\widehat{f}_{\rm PN}) - R(f^*) \le C(\delta) \left(\frac{\pi}{\sqrt{n_{\rm P}}} + \frac{1-\pi}{\sqrt{n_{\rm N}}}\right)$$

with probability $1 - \delta$

 $\widehat{R}_{PN}(f) = \frac{1}{n} \sum_{i=1}^{n} \ell(y_i f(\boldsymbol{x}_i))$ n_P, n_N, n_U : # of P, N, U samples

Comparison: PU bound is smaller than PN if

π	_ 1	$1-\pi$
$\sqrt{n_{\mathrm{P}}}$	$+ \frac{1}{\sqrt{n_{\rm U}}} > 1$	$\sqrt{n_{\rm N}}$

• PU can be better than PN, provided many PU data!

Further Correction ³⁰

$$R(f) = \pi \mathbb{E}_{p(\boldsymbol{x}|\boldsymbol{y}=+1)} \left[\ell \left(f(\boldsymbol{x}) \right) \right] + (1 - \pi) \mathbb{E}_{p(\boldsymbol{x}|\boldsymbol{y}=-1)} \left[\ell \left(- f(\boldsymbol{x}) \right) \right]$$

Risk for P data
Risk for N data $R^{-}(f)$

PU formulation: $p(\boldsymbol{x}) = \pi p(\boldsymbol{x}|\boldsymbol{y} = +1) + (1 - \pi)p(\boldsymbol{x}|\boldsymbol{y} = -1)$ $R^{-}(f) = \mathbb{E}_{p(\boldsymbol{x})} \left[\ell \left(-f(\boldsymbol{x}) \right) \right] - \pi \mathbb{E}_{p(\boldsymbol{x}|\boldsymbol{y}=+1)} \left[\ell \left(-f(\boldsymbol{x}) \right) \right]$

- If $\ell(m) \ge 0, \ \forall m$, $R^-(f) \ge 0$.
- However, its PU empirical approximation can be negative due to "difference of approximations".

$$\widehat{R}_{\mathrm{PU}}^{-}(f) = \frac{1}{n_{\mathrm{U}}} \sum_{i=1}^{n_{\mathrm{U}}} \ell \left(-f(\boldsymbol{x}_{i}^{\mathrm{U}}) \right) - \frac{\pi}{n_{\mathrm{P}}} \sum_{i=1}^{n_{\mathrm{P}}} \ell \left(-f(\boldsymbol{x}_{i}^{\mathrm{P}}) \right) \not\geq 0$$

• This problem is more critical for flexible models such as deep nets.

Non-Negative PU Classification³¹



Theoretical Analysis

Kiryo, Niu, du Plessis & Sugiyama (NIPS2017)

32

$$\widetilde{R}_{\mathrm{PU}}(f) = \frac{\pi}{n_{\mathrm{P}}} \sum_{i=1}^{n_{\mathrm{P}}} \ell\left(f(\boldsymbol{x}_{i}^{\mathrm{P}})\right) + \max\left\{\boldsymbol{0}, \ \frac{1}{n_{\mathrm{U}}} \sum_{i=1}^{n_{\mathrm{U}}} \ell\left(-f(\boldsymbol{x}_{i}^{\mathrm{U}})\right) - \frac{\pi}{n_{\mathrm{P}}} \sum_{i=1}^{n_{\mathrm{P}}} \ell\left(-f(\boldsymbol{x}_{i}^{\mathrm{P}})\right)\right\}$$

 $\widetilde{R}_{PU}(f) \text{ is still consistent and its bias decreases} \\ \text{exponentially: } \mathcal{O}(e^{-n_P - n_U}) \qquad n_P, n_U: \text{ # of P, U samples} \\ \end{array}$

- In practice, we can ignore the bias of $\widetilde{R}_{PU}(f)$!
- Mean-squared error of $\tilde{R}_{PU}(f)$ is not more than the original one.
 - In practice, $\widetilde{R}_{PU}(f)$ is more reliable!
- Risk of $\operatorname{argmin}_{f} \widetilde{R}_{PU}(f)$ for linear models attains optimal convergence rate: $\mathcal{O}_{p}\left(\frac{1}{\sqrt{n_{P}}} + \frac{1}{\sqrt{n_{U}}}\right)$
 - Learned function is optimal.

Experiments

With a large number of unlabeled data, non-negative PU can even outperform PN!

- Binary CIFAR-10: Positive (airplane, automobile, ship, truck) Negative (bird, cat, deer, dog, frog, horse)
- 13-layer CNN with ReLU

$$n_{\rm P} = 1000$$

 $n_{\rm U} = 50000$
 $\pi = 0.4$



PU Classification: Summary ³⁴

Just separating P and U is biased.

To be unbiased, use composite loss $\tilde{\ell}(m) = \ell(m) - \ell(-m)$ for P data.

Natarajan, Dhillon, Ravikumar & Tewari (NIPS2013)

• Optimal convergence rate achieved. Niu, du Plessis, Sakai, Ma & Sugiyama (NIPS2016)

If
$$\ell(m) + \ell(-m) = \text{Const.}$$

the same loss for P and U data. du Plessis, Niu & Sugiyama (NIPS2014)

If
$$\widetilde{\ell}(m) = am + b$$

optimization becomes convex. du Plessis, Niu & Sugiyama (ICML2015)

For deep nets, roundup the empirical false negative error to zero. Kiryo, Niu, du Plessis & Sugiyama (NIPS2017)









Contents

- 1. Background
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- 4. PNU Classification
- 5. Pconf Classification
- 6. UU Classification
- 7. SU Classification
- 8. Comp Classification
- 9. Summary

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PNU Classification: Setup ³⁶

Given: Positive, negative & unlabeled samples

$$\begin{aligned} \{\boldsymbol{x}_{i}^{\mathrm{P}}\}_{i=1}^{n_{\mathrm{P}}} & \stackrel{\text{i.i.d.}}{\sim} p(\boldsymbol{x}|y=+1) \\ \{\boldsymbol{x}_{i}^{\mathrm{N}}\}_{i=1}^{n_{\mathrm{N}}} & \stackrel{\text{i.i.d.}}{\sim} p(\boldsymbol{x}|y=-1) \\ \{\boldsymbol{x}_{i}^{\mathrm{U}}\}_{i=1}^{n_{\mathrm{U}}} & \stackrel{\text{i.i.d.}}{\sim} p(\boldsymbol{x}) \end{aligned}$$

Goal: Obtain a PN classifier

• PNU classification is semi-supervised learning.



PNU Decomposition

Sakai, du Plessis, Niu & Sugiyama (ICML2017)

37

Let's decompose PNU into PU, PN, and NU:

- Each can be solved easily.
- Combine them!



Theoretical risk analysis:

Niu, du Plessis, Sakai, Ma & Sugiyama (NIPS2016)

- When PU<NU: PU<PN<NU or PN<PU<NU.
- When NU<PU: NU<PN<PU or PN<NU<PU.

PU+NU is not the best possible combination.PU+PN & NU+PN are the best combinations.

PN+PU & PN+NU Classification³⁹

Proposed method: Combine two best methods.



• PN+PU classification:

 $R_{\rm PN+PU}^{\gamma}(f) = (1-\gamma)R_{\rm PN}(f) + \gamma R_{\rm PU}(f) \quad 0 \le \gamma \le 1$

• PN+NU classification:

 $R_{\rm PN+NU}^{\gamma}(f) = (1-\gamma)R_{\rm PN}(f) + \gamma R_{\rm NU}(f) \quad 0 \le \gamma \le 1$

- without cluster assumptions!
- 680 880 880 We use unlabeled data for loss evaluation, not for regularization (as manifold smoothing).

 - Label information is extracted from unlabeled data!

Experiments

Misclassification error rate: average (std)

5% t-tes	st			(Gra	ndvalet & Ben NIPS2004)	gio, (Belkin et JMLR200	al., (Niu et a)6) ICML201	I., (Li et al., 3) JMLR2013)
Dataset	$n_{ m u}$	π	$\widehat{\pi}$	Proposed	EntReg	LapSVM	SMIR	WellSVM
	1000	0.50	0.49(0.01)	27.4(1.3)	26.6(0.5)	$26.1 \ (0.7)$	40.1(3.9)	27.5(0.5)
Arts	5000	0.50	0.50(0.01)	24.8 (0.6)	26.1 (0.5)	26.1 (0.4)	30.1(1.6)	N/A
	10000	0.50	0.52(0.01)	25.6(0.7)	25.4(0.5)	$25.5 \ (0.6)$	N/A	N/A
	1000	0.73	$0.67 \ (0.01)$	$13.0 \ (0.5)$	15.3(0.6)	16.7(0.8)	17.2(0.8)	18.2(0.7)
Deserts	5000	0.73	0.67(0.01)	$13.4 \ (0.4)$	$13.3 \ (0.5)$	16.6(0.6)	24.4(0.6)	N/A
	10000	0.73	0.68(0.01)	$13.3 \ (0.5)$	$13.7 \ (0.6)$	16.8(0.8)	N/A	N/A
	1000	0.65	0.57(0.01)	22.4(1.0)	26.2(1.0)	26.6(1.3)	28.2(1.1)	26.6(0.8)
Fields	5000	0.65	0.57(0.01)	$20.6 \ (0.5)$	22.6(0.6)	24.7(0.8)	29.6(1.2)	N/A
	10000	0.65	0.57(0.01)	$21.6 \ (0.6)$	$22.5 \ (0.6)$	25.0(0.9)	N/A	N/A
	1000	0.50	$0.50\ (0.01)$	$11.4 \ (0.4)$	$11.5 \ (0.5)$	12.5(0.5)	$17.4 \ (3.6)$	$11.7 \ (0.4)$
Stadiums	5000	0.50	0.50(0.01)	$11.0 \ (0.5)$	10.9 (0.3)	$11.1 \ (0.3)$	13.4(0.7)	N/A
	10000	0.50	0.51 (0.00)	$10.7 \ (0.3)$	$10.9 \ (0.3)$	$11.2 \ (0.2)$	N/A	N/A
	1000	0.27	0.33(0.01)	$21.8 \ (0.5)$	23.9(0.6)	24.1 (0.5)	30.1(2.3)	26.2(0.8)
Platforms	5000	0.27	0.34(0.01)	23.3 (0.8)	$24.4\ (0.7)$	24.9(0.7)	26.6(0.3)	N/A
	10000	0.27	0.34(0.01)	$21.4 \ (0.5)$	24.3 (0.6)	24.8(0.5)	N/A	N/A
	1000	0.55	$0.51 \ (0.01)$	43.9(0.7)	43.9(0.6)	$43.4 \ (0.6)$	50.7(1.6)	44.3(0.5)
Temples	5000	0.55	0.54(0.01)	43.4(0.9)	43.0 (0.6)	$43.1 \ (1.0)$	43.6(0.7)	N/A
	10000	0.55	$0.50 \ (0.01)$	45.2 (0.8)	$44.4 \ (0.8)$	$44.2 \ (0.7)$	N/A	N/A

Proposed PN+PU & PN+NU works well!



Contents

42

- 1. Background
- 2. PN Classification
- 3. PU Classification
- 4. PNU Classification
- 5. Pconf Classification
- 6. UU Classification
- 7. SU Classification
- 8. Comp Classification
- 9. Summary

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Pconf Classification: Setup ⁴³

Ishida, Niu & Sugiyama (NeurIPS2018)

Given: Positive-confidence samples

• Positive patterns: $\{\boldsymbol{x}_i\}_{i=1}^n \stackrel{\text{i.i.d.}}{\sim} p(\boldsymbol{x}|y=+1)$

 $\{(x_i, r_i)\}_{i=1}^n$

• Their confidence: $r_i = P(y = +1|\boldsymbol{x}_i)$

Goal: Obtain a PN classifier



Pconf Risk Estimation

44

Classification risk: $R(f) = \mathbb{E}_{p(\boldsymbol{x},y)} \left[\ell \left(yf(\boldsymbol{x}) \right) \right]$

Naïve "confidence-weighting" is not correct. $R(f) \neq \mathbb{E}_{p(\boldsymbol{x}|y=+1)} \left[r(\boldsymbol{x})\ell(f(\boldsymbol{x})) + (1 - r(\boldsymbol{x}))\ell(-f(\boldsymbol{x})) \right]$ $r(\boldsymbol{x}) = P(y = +1|\boldsymbol{x})$

Right form is given by importance sampling:

$$R(f) = \pi \mathbb{E}_{p(\boldsymbol{x}|y=+1)} \left[\ell \left(f(\boldsymbol{x}) \right) + \frac{1 - r(\boldsymbol{x})}{r(\boldsymbol{x})} \ell \left(- f(\boldsymbol{x}) \right) \right]$$

resulting in an empirical risk:

$$\widehat{R}_{\text{Pconf}}(f) \propto \sum_{i=1}^{n} \left[\ell \left(f(\boldsymbol{x}_{i}) \right) + \frac{1 - r_{i}}{r_{i}} \ell \left(- f(\boldsymbol{x}_{i}) \right) \right]$$
$$\{\boldsymbol{x}_{i}\}_{i=1}^{n} \stackrel{\text{i.i.d.}}{\sim} p(\boldsymbol{x}|\boldsymbol{y} = +1) \quad r_{i} = P(\boldsymbol{y} = +1|\boldsymbol{x}_{i})$$

Theoretical Analysis

Estimation error:

$$R(f^*) - R(\widehat{f}_{Pconf}) = \mathcal{O}_p\left(\frac{1}{\sqrt{n}}\right)$$
$$f^* = \underset{f}{\operatorname{argmin}} R(f) \quad \widehat{f}_{Pconf} = \underset{f}{\operatorname{argmin}} \widehat{R}_{Pconf}(f)$$
$$R(f) = \mathbb{E}_{p(\boldsymbol{x}, y)} \left[\ell\left(yf(\boldsymbol{x})\right)\right]$$
$$\widehat{R}_{Pconf}(f) \propto \sum_{i=1}^n \left[\ell\left(f(\boldsymbol{x}_i)\right) + \frac{1 - r_i}{r_i}\ell\left(-f(\boldsymbol{x}_i)\right)\right]$$

Optimal parametric convergence rate is attained!

Experiments

Correct classification rate: average (std)

5% t-test

Positive	vs.	Negative	Pconf	Weighted	Supervised
airplane	vs.	automobile	84.34 ± 0.84	79.32 ± 2.74	93.82 ± 0.21
airplane	vs.	bird	82.50 ± 3.19	81.38 ± 0.48	89.24 ± 0.50
airplane	vs.	cat	89.10 ± 0.47	86.98 ± 1.20	92.78 ± 0.49
airplane	vs.	deer	87.44 ± 1.43	82.00 ± 2.39	92.08 ± 0.50
airplane	vs.	dog	$\textbf{90.24} \pm \textbf{1.27}$	86.86 ± 1.41	94.42 ± 0.89
airplane	vs.	frog	91.44 ± 0.86	85.12 ± 1.66	95.52 ± 0.42
airplane	vs.	horse	89.26 ± 2.20	87.72 ± 1.99	95.58 ± 0.56
airplane	vs.	ship	$\overline{74.36\pm2.00}$	$\overline{70.82 \pm 1.80}$	89.04 ± 1.06
airplane	vs.	truck	84.98 ± 0.47	83.22 ± 0.58	91.84 ± 1.19

Works better than naïve "weighted" baseline!



Contents

- Background
- 2. PN Classification
- 3. PU Classification
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- 5. Pconf Classification
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- 8. Comp Classification
- 9. Summary

Slides: http://goo.gl/meiTwY

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UU Classification: Setup ⁴⁸

du Plessis, Niu & Sugiyama (TAAI2013) Nan, Niu, Menon & Sugiyama (ICLR2019)

Given: Two sets of unlabeled data

$$\{\boldsymbol{x}_i\}_{i=1}^n \overset{\text{i.i.d.}}{\sim} p(\boldsymbol{x}) \ \{\boldsymbol{x}'_i\}_{i=1}^{n'} \overset{\text{i.i.d.}}{\sim} p'(\boldsymbol{x})$$

Assumption: Only class-priors are different

$$p(y) \neq p'(y)$$
 $p(\boldsymbol{x}|y) = p'(\boldsymbol{x}|y)$

Goal: Obtain a PN classifier



Optimal UU Classifier ⁴⁹

du Plessis, Niu & Sugiyama (TAAI2013)

Boundary

Sign of the difference of class-posteriors:

$$g(\boldsymbol{x}) = \operatorname{sign}[p(y = +1|\boldsymbol{x}) - p(y = -1|\boldsymbol{x})]$$

Under uniform test class-prior,

$$g(\boldsymbol{x}) = C \operatorname{sign}[p(\boldsymbol{x}) - p'(\boldsymbol{x})]$$
$$C = \operatorname{sign}[p(y = +1) - p'(y = +1)]$$

Sign of *C* is unknown, but just knowing sign[p(x) - p'(x)]still allows optimal separation!

UU Risk Estimation ⁵⁰

Nan, Niu, Menon & Sugiyama (ICLR2019)

For

r

- uniform test class-prior: $\pi = 1/2$
- symmetric loss: $\ell(m) + \ell(-m) = \text{Const.}$

the classification risk can be expressed as

$$\begin{split} R(f) &= \mathbb{E}_{p(\boldsymbol{x},y)} \left[\ell \Big(yf(\boldsymbol{x}) \Big) \right] \\ &\propto \mathbb{E}_{p(\boldsymbol{x})} \left[\ell \Big(f(\boldsymbol{x}) \Big) \right] + \mathbb{E}_{p'(\boldsymbol{x}')} \left[\ell \Big(-f(\boldsymbol{x}') \Big) \right] + \text{Const.} \\ \text{esulting an empirical risk (up to label flip):} \end{split}$$

$$\widehat{R}_{\mathrm{UU}}(f) \propto \frac{1}{n} \sum_{i=1}^{n} \ell\left(f(\boldsymbol{x}_{i})\right) + \frac{1}{n'} \sum_{i=1}^{n} \ell\left(-f(\boldsymbol{x}_{i}')\right)$$
$$\{\boldsymbol{x}_{i}\}_{i=1}^{n} \stackrel{\text{i.i.d.}}{\sim} p(\boldsymbol{x}) \quad \{\boldsymbol{x}_{i}'\}_{i=1}^{n'} \stackrel{\text{i.i.d.}}{\sim} p'(\boldsymbol{x})$$

Theoretical Analysis

Estimation error:

$$R(f^*) - R(\widehat{f}_{UU}) = \mathcal{O}_p\left(\frac{1}{\sqrt{n}} + \frac{1}{\sqrt{n'}}\right)$$

$$f^* = \underset{f}{\operatorname{argmin}} R(f) \quad \widehat{f}_{UU} = \underset{f}{\operatorname{argmin}} \widehat{R}_{UU}(f)$$

$$R(f) = \mathbb{E}_{p(\boldsymbol{x},y)}\left[\ell\left(yf(\boldsymbol{x})\right)\right]$$

$$\widehat{R}_{UU}(f) \propto \frac{1}{n} \sum_{i=1}^n \ell\left(f(\boldsymbol{x}_i)\right) + \frac{1}{n'} \sum_{i=1}^{n'} \ell\left(-f(\boldsymbol{x}'_i)\right)$$

Optimal parametric convergence rate is attained!

Experiments

Dataset	# Train	# Test	# Feature	$\pi_{ m p}$	Model $g(x; \theta)$	Optimizer
MNIST	60,000	10,000	784	0.49	FC with ReLU (depth 5)	SGD
Fashion-MNIST	60,000	10,000	784	0.50	FC with ReLU (depth 5)	SGD
SVHN	100,000	26,032	3,072	0.27	AllConvNet (depth 12)	Adam
CIFAR-10	50,000	10,000	3,072	0.60	ResNet (depth 32)	Adam





Contents

- . Background
- 2. PN Classification
- 3. PU Classification
- 4. PNU Classification
- 5. Pconf Classification
- 6. UU Classification
- 7. SU Classification
- 8. Comp Classification
- 9. Summary

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SU Classification 54

Bao, Niu & Sugiyama (ICML2018)

Given: Similar and unlabeled samples

$$\{(\boldsymbol{x}_i, \boldsymbol{x}'_i)\}_{i=1}^{n_{\mathrm{S}}} \stackrel{\mathrm{i.i.d.}}{\sim} p(\boldsymbol{x}, \boldsymbol{x}'|y=y') \ \{\boldsymbol{x}_i^{\mathrm{U}}\}_{i=1}^{n_{\mathrm{U}}} \stackrel{\mathrm{i.i.d.}}{\sim} p(\boldsymbol{x})$$

Goal: Obtain a PN classifier

This is a special case of UU classification:

 $p(y = +1) = \pi^2 / (2\pi^2 - 2\pi + 1)$ $p'(y = +1) = \pi$

Classification from dissimilar data is also possible (DU, SD, SDU)!

Shimada, Bao, Sato & Sugiyama (arXiv2019)





Contents

- 1. Background
- 2. PN Classification
- 3. PU Classification
- 4. PNU Classification
- 5. Pconf Classification
- 6. UU Classification
- 7. SU Classification
- 8. Comp Classification
- 9. Summary

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55

Multiclass Labeling is Costly ⁵⁶

Labeling in multi-class classification:

• What is the robot in this image?



https://www.bostondynamics.com/atla

- 1. Amazon Kiva
- 2. Aldebaran Nao
- 3. Softbank Pepper
- 4. Sony Aibo
- 5. iRobot Roomba
- 83. Boston Dynamics Atlas
- 100. Rethink Robotics Baxter

Selecting the correct class from a long list of candidates is extremely time-consuming!

Complementary Classification ⁵⁷

Ishida, Niu, Hu & Sugiyama (NIPS2017) Ishida, Niu, Menon & Sugiyama (ICML2019)

Given: Complementarily labeled data

$$\{(\boldsymbol{x}_i, \bar{y}_i)\}_{i=1}^n \stackrel{\text{i.i.d.}}{\sim} \bar{p}(\boldsymbol{x}, \bar{y}) \quad \bar{p}(\boldsymbol{x}, \bar{y}) = \frac{1}{c-1} \sum_{y \neq \bar{y}} p(\boldsymbol{x}, y)$$

• Pattern x does not belong to class $\overline{y} \in \{1, 2, ..., c\}$. Goal: Obtain a multiclass classifier



Possible Approaches $\{(x_i, \bar{y}_i)\}_{i=1}^n \overset{\text{i.i.d.}}{\sim} \bar{p}(x, \bar{y})$

58

- Approach 1: Classification from partial labels Cour, Sapp & Taskar (JMLR2011)
 - Multiple candidate classes are provided for each x_i .
 - Complementary labels are the extreme case of partial labels given to all c-1 classes other than \bar{y}_i .
- Approach 2: Multi-label classification
 - Each x_i can belong to multiple classes.
 - Negative label for \bar{y}_i and positives for the rest.

We want a more direct approach!

Multi-Class Classification ⁵⁹

C-class classifier: $f(\mathbf{x}) = \underset{y \in \{1,...,c\}}{\operatorname{argmax}} g_y(\mathbf{x})$

 $g_y(oldsymbol{x})$: one-vs-rest classifier for y

c-class loss: L(y, g(x))

$$oldsymbol{g}(oldsymbol{x}) = (g_1(oldsymbol{x}), \dots, g_c(oldsymbol{x}))^ op$$

• One-versus-rest:

$$L_{\text{OVR}}\left(y, \boldsymbol{g}(\boldsymbol{x})\right) = \ell\left(g_{y}(\boldsymbol{x})\right) + \frac{1}{c-1}\sum_{y' \neq y}\ell\left(-g_{y'}(\boldsymbol{x})\right)$$

• Pairwise comparison:

$$L_{\mathrm{PC}}\Big(y, \boldsymbol{g}(\boldsymbol{x})\Big) = \sum_{y' \neq y} \ell\Big(g_y(\boldsymbol{x}) - g_{y'}(\boldsymbol{x})\Big)$$

c-class classification risk:

$$R(\boldsymbol{g}) = \mathbb{E}_{p(\boldsymbol{x},y)} \Big[L\Big(y, \boldsymbol{g}(\boldsymbol{x})\Big) \Big]$$

Complementary Risk Estimation⁶⁰

Ishida, Niu, Menon & Sugiyama (ICML2019)

$$R(\boldsymbol{g}) = \mathbb{E}_{p(\boldsymbol{x},y)} \Big[L\Big(y, \boldsymbol{g}(\boldsymbol{x})\Big) \Big]$$

Risk can be equivalently expressed as

$$R(\boldsymbol{g}) = \mathbb{E}_{\overline{\boldsymbol{p}}(\boldsymbol{x}, \overline{\boldsymbol{y}})} \Big[\overline{\boldsymbol{L}} \Big(\overline{\boldsymbol{y}}, \boldsymbol{g}(\boldsymbol{x}) \Big) \Big]$$

• Complementary loss:

$$\bar{L}\left(\bar{y}, \boldsymbol{g}(\boldsymbol{x})\right) = -(c-1)L\left(\bar{y}, \boldsymbol{g}(\boldsymbol{x})\right) + \sum_{y=1}^{c} L\left(y, \boldsymbol{g}(\boldsymbol{x})\right)$$

Empirical risk estimation is possible from complementary data!

$$\widehat{R}_{\text{Comp}}(\boldsymbol{g}) = \frac{1}{n} \sum_{i=1}^{n} \overline{L}\left(\overline{y}_{i}, \boldsymbol{g}(\boldsymbol{x}_{i})\right) \quad \{(\boldsymbol{x}_{i}, \overline{y}_{i})\}_{i=1}^{n} \overset{\text{i.i.d.}}{\sim} \overline{p}(\boldsymbol{x}, \overline{y})$$

Theoretical Analysis⁶¹

Ishida, Niu, Hu & Sugiyama (NIPS2017)

Estimation error:

Optimal parametric convergence rate is attained!

Experiments

Correct classification rate: average (std)

5% t-	test
-------	------

Dataset	Class	Dim	# train	# test	Proposed	Partial-label	Multi-label	
WAVEFORM1	$1 \sim 3$	21	1226	398	85.8(0.5)	85.7(0.9)	79.3(4.8)	
WAVEFORM2	$1 \sim 3$	40	1227	408	84.7(1.3)	84.6(0.8)	74.9(5.2)	
SATIMAGE	$1 \sim 7$	36	415	211	68.7(5.4)	60.7(3.7)	33.6(6.2)	
PENDIGITS	$1 \sim 5$ $6 \sim 10$ even # odd # $1 \sim 10$	16	719 719 719 719 719 719	336 335 336 335 335	$\begin{array}{c} 87.0(2.9)\\ 78.4(4.6)\\ 90.8(2.4)\\ 76.0(5.4)\\ 38.0(4.3) \end{array}$	76.2(3.3) 71.1(3.3) 76.8(1.6) 67.4(2.6) 33.2(3.8)	$\begin{array}{r} 44.7(9.6) \\ 38.4(9.6) \\ 43.8(5.1) \\ 40.2(8.0) \\ 16.1(4.6) \end{array}$	
DRIVE	$1 \sim 5$ $6 \sim 10$ even # odd # $1 \sim 10$	48	3955 3923 3925 3939 3925	1326 1313 1283 1278 1269	$\begin{array}{c} 89.1(4.0)\\ 88.8(1.8)\\ 81.8(3.4)\\ 85.4(4.2)\\ 40.8(4.3)\end{array}$	77.7(1.5)78.5(2.6)63.9(1.8)74.9(3.2)32.0(4.1)	$\begin{array}{c} 31.1(3.5) \\ 30.4(7.2) \\ 29.7(6.3) \\ 27.6(5.8) \\ 12.7(3.1) \end{array}$	
LETTER	$ \begin{array}{r} 1 \sim 5 \\ 6 \sim 10 \\ 11 \sim 15 \\ 16 \sim 20 \\ 21 \sim 25 \\ 1 \sim 25 \end{array} $	16	565 550 556 550 585 550	171 178 177 184 167 167	$79.7(5.3) \\76.2(6.2) \\78.3(4.1) \\77.2(3.2) \\80.4(4.2) \\5.1(2.1)$	$\begin{array}{c} \textbf{75.1(4.4)} \\ 66.8(2.5) \\ 67.4(3.3) \\ 68.4(2.1) \\ \textbf{75.1(1.9)} \\ \textbf{5.0(1.0)} \end{array}$	$28.3(10.4) \\34.0(6.9) \\28.6(5.0) \\32.7(6.4) \\32.0(5.7) \\5.2(1.1)$	Proposed method works
USPS	$1 \sim 5$ $6 \sim 10$ even # odd # $1 \sim 10$	256	652 542 556 542 542	166 147 147 147 127	$\begin{array}{c} \textbf{79.1(3.1)} \\ \textbf{69.5(6.5)} \\ \textbf{67.4(5.4)} \\ \textbf{77.5(4.5)} \\ \textbf{30.7(4.4)} \end{array}$	$\begin{array}{r} 70.3(3.2) \\ \hline 66.1(2.4) \\ 66.2(2.3) \\ \hline 69.3(3.1) \\ 26.0(3.5) \end{array}$	$\begin{array}{c} 44.4(8.9)\\ 37.3(8.8)\\ 35.7(6.6)\\ 36.6(7.5)\\ 13.3(5.4)\end{array}$	well!

Incorporating Ordinary Labels ⁶³

Convert multiclass labeling into yes-no labeling:



http://www.softbank.jp/corp/group/ sbr/news/press/2014/20141029_01/



https://www.bostondynamics.com/atlas

Is this Softbank Pepper? Yes! (ordinary label)

Is this iRobot Roomba? No! (complementary label)

Use both of ordinary and complementary labels! $R(\boldsymbol{g}) = \boldsymbol{\alpha} \mathbb{E}_{p(\boldsymbol{x},y)} \left[L\left(y, \boldsymbol{g}(\boldsymbol{x})\right) \right] + (1 - \boldsymbol{\alpha}) \mathbb{E}_{\bar{p}(\boldsymbol{x},\bar{y})} \left[\bar{L}\left(\bar{y}, \boldsymbol{g}(\boldsymbol{x})\right) \right]$ $\alpha \in [0, 1]$

Experiments

64

	$\begin{array}{l} \text{OL \& CL} \\ (\alpha = \frac{1}{2}) \end{array}$	$\begin{array}{c} \text{CL} \\ (\alpha = 0) \end{array}$	$\begin{vmatrix} \text{OL} \\ (\alpha = 1) \end{vmatrix}$	# test	# train	Dim	Class	Dataset
	86.9(0.5)	86.0(0.4)	85.3(0.8)	408	413/826	21	$1 \sim 3$	WAVEFORM1
	84.7(0.6)	82.0(1.7)	82.7(1.3)	411	411/821	40	$1 \sim 3$	WAVEFORM2
5% t-test	81.2(1.1)	70.1(5.6)	74.9(4.9)	211	69/346	36	$1 \sim 7$	SATIMAGE
	$\frac{93.1(2.0)}{87.8(2.8)}$	84.7(3.2) 78.3(6.2)	$\begin{array}{ c c c } 91.3(2.1) \\ \hline 86.3(3.5) \end{array}$	336 335	144/575 144/575		$\begin{array}{c} 1\sim5\\ 6\sim10 \end{array}$	
Incorpo-	$\begin{array}{c} 95.8(0.6)\\ 86.9(1.1)\\ 66.9(2.0)\end{array}$	$91.0(4.3) \\75.9(3.1) \\41.1(5.7)$	94.3(1.7) 85.6(2.0) 61.7(4.3)	336 335 335	144/575 144/575 72/647	16	even # odd # $1 \sim 10$	PENDIGITS
rating comple-	$\begin{array}{c} 94.2(1.0)\\ 89.5(2.1)\\ 91.8(3.3)\\ 93.4(0.5)\\ 77.6(2.2) \end{array}$	$\begin{array}{c} 89.0(2.1)\\ 86.5(3.1)\\ 81.8(4.6)\\ 86.7(2.9)\\ 40.5(7.2)\end{array}$	92.1(2.6) 87.0(3.0) 91.4(2.9) 91.1(1.5) 75.2(2.8)	1305 1290 1314 1255 1292	780/3121 795/3180 657/3284 790/3161 397/3570	48	$1 \sim 5$ $6 \sim 10$ even # odd # $1 \sim 10$	DRIVE
labels Improves	$\begin{array}{c} 89.5(1.6)\\ 84.6(1.0)\\ 87.3(1.6)\\ 84.7(2.0)\\ 91.1(1.0)\\ 31.0(1.7)\end{array}$	77.2(6.1) 77.6(3.7) 76.0(3.2) 77.9(3.1) 81.2(3.4) $6.5(1.7)$	$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	171 178 177 184 167 167	113/452 110/440 111/445 110/440 117/468 22/528	16	$ \begin{array}{r} 1 \sim 5 \\ 6 \sim 10 \\ 11 \sim 15 \\ 16 \sim 20 \\ 21 \sim 25 \\ 1 \sim 25 \end{array} $	LETTER
the accuracy!	$\begin{array}{c} 89.5(1.3)\\ 85.5(2.4)\\ 84.8(1.4)\\ 87.3(2.2)\\ 59.3(2.2)\end{array}$	76.5(5.3) 67.6(4.3) 67.4(4.4) 72.9(6.2) 28.5(3.6)	$ \begin{vmatrix} 83.8(1.7) \\ 79.2(2.1) \\ 79.6(2.7) \\ 82.7(1.9) \\ 43.7(2.6) \end{vmatrix} $	166 147 166 147 147	130/522 108/434 108/434 111/445 54/488	256	$1 \sim 5$ $6 \sim 10$ even # odd # $1 \sim 10$	USPS



Contents

- Background
- 2. PN Classification
- 3. PU Classification
- 4. PNU Classification
- 5. Pconf Classification
- 6. UU Classification
- 7. SU Classification
- 8. Comp Classification
- 9. Summary

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65

Model vs. Learning Methods ⁶⁶



