Convergence rates for PU learning under the SAR assumption: influence of propensity

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OpenLab AI between Stellantis and Inria

From standard classification to Positive Unlabeled (PU) classification setting

General setting: $(X_i, Y_i, S_i)_{1\leq i\leq n}$ **i.i.d.**

- $X_i \in \mathbb{R}^d$ *covariate vector*
- $Y_i \in \{0,1\}$ *class* of interest
- $S_i \in \{0,1\}$ observed *label*

Classification of Y given X:

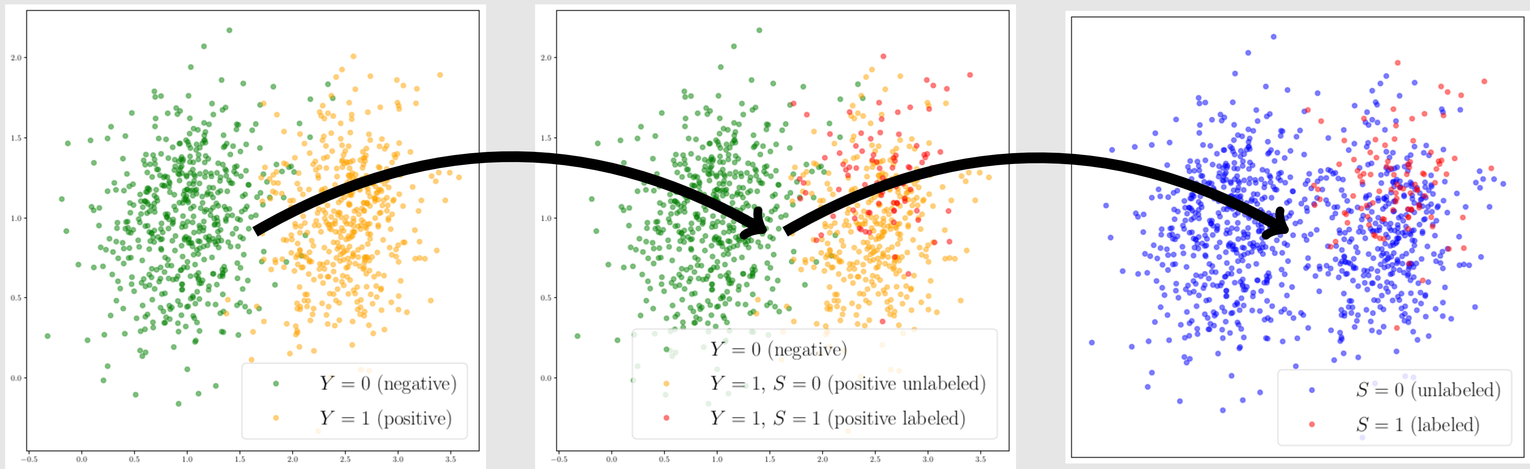
$$\mathbb{P}(Y=1 \,|\, X=x) = \eta(x) \ .$$

Propensity or selection bias:

$$\mathbb{P}(S=1 \,|\, X=x, Y=1) = e(x) \ .$$

Biased classification of S given X:

$$\mathbb{P}(S=1 \,|\, X=x) = \eta(x) \times e(x) \ .$$



Standard classification setting
$(X_i, Y_i) \rightarrow$ Estimate η

Selection of positive instances through e

PU classification setting
$(X_i, S_i) \rightarrow$ Estimate η

Estimating the classifier in PU learning setting

Objective: given a loss function $\boldsymbol{L}$, find the classification rule $f : \mathbb{R}^d \to \{0,1\}$ minimizing the associated risk $R(f) = \mathbb{E}[L(f(X), Y)]$.

$$f^* \in \operatorname*{Argmin}_f R(f) \ .$$

Estimation of f^* using the training sample $(X_i, S_i)_{1\leq i\leq n}$: find $f : \mathbb{R}^d \to \{0,1\}$ in a predefined class $\mathcal{F}$ minimizing an empirical risk.

Empirical risks:

1. Standard empirical risk: unavailable because the classes $(Y_i)_{1\leq i\leq n}$ are unobserved...

$$\widehat{R}_S(f) = \frac{1}{n}\sum_{i=1}^{n} L(f(X_i), Y_i)$$

2. Non traditional empirical risk: ignoring the propensity e.

$$\widehat{R}_{NT}(f) = \frac{1}{n}\sum_{i=1}^{n} L(f(X_i), S_i)$$

$\hookrightarrow$ biased estimate of the true risk.

3. Unbiased PU empirical risk[1],[2]: assuming the propensity scores $e(X_i)$ of labeled observations to be known.

$$\widehat{R}_{PU}(f) = \frac{1}{n}\sum_{i=1}^{n}\left[\frac{\mathbb{1}_{S_i=1}}{e(X_i)}\left(L(f(X_i),1) - L(f(X_i),0)\right) + L(f(X_i),0)\right]$$

Theoretical risk bounds for PU learning[3]

PU learning classifier using $0-1$ loss: $L(f(x),y) = \mathbb{1}_{f(x)\neq y}$.

$$\widehat{f}_{PU} = \operatorname*{Argmin}_{f\in\mathcal{F}} \widehat{R}_{PU}(f) \ .$$

Excess risk:

$$\ell\left(\widehat{f}_{PU}, f^*\right) = R(\widehat{f}) - R(f^*) \ .$$

Assumptions:

- $\mathcal{F}$ has finite VC dimension V (complexity)
- $f^* \in \mathcal{F}$
- $\exists\, h > 0$ such that $\forall\, x \in \mathbb{R}^d$, $|2\,\mathbb{P}(Y=1 \,|\, X=x) - 1| \geq h$ (Massart noise assumption[4]).
- $\exists\, e_m > 0$, $\forall x \in \mathbb{R}^d\ e(x) \geq e_m$.

Result: two convergence rates

$$\mathbb{E}\left[\ell\left(\widehat{f}, f^*\right)\right] \leq \kappa\sqrt{\frac{V}{n\,e_m}} \qquad \text{if } h \leq \sqrt{\frac{V}{n\,e_m}} \ ;$$

$$\leq \kappa\left[\frac{V\,(2-e_m)}{n\,e_m\,h}\left(1 + \log\left(\frac{n\,h^2}{V} \vee 1\right)\right)\right] \qquad \text{if } h \geq \sqrt{\frac{V}{n\,e_m}} \ .$$

Simulation setting

- One-dimensional setting $(d=1)$
- $\mathcal{F} = \{x \mapsto \mathbb{1}_{x\geq m},\ m \in \mathbb{R}\}$
- $X_i \sim \mathcal{N}(0,1)$
- $Y_i \sim \mathcal{B}\left(\frac{1+h}{2}\mathbb{1}_{X_i\geq 0} + \frac{1-h}{2}\mathbb{1}_{X_i<0}\right)$, $h = 0.25$.
- $S_i \sim \mathcal{B}(e(x))$ if $Y_i = 0$ (else $S_i = 0$)

- Propensity functions:
  1. SCAR constant propensity,
  $$e(x) = e_m, \text{ with } e_m > 0 \ ;$$
  2. SAR logistic propensity (cf. Fig. 1),
  $$e(x) = \max\left(e_m, \frac{1}{1+e^{x-1}}\right), \text{ with } e_m > 0 \ .$$

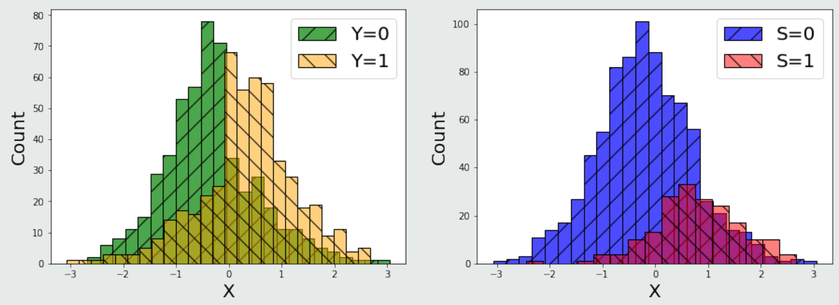
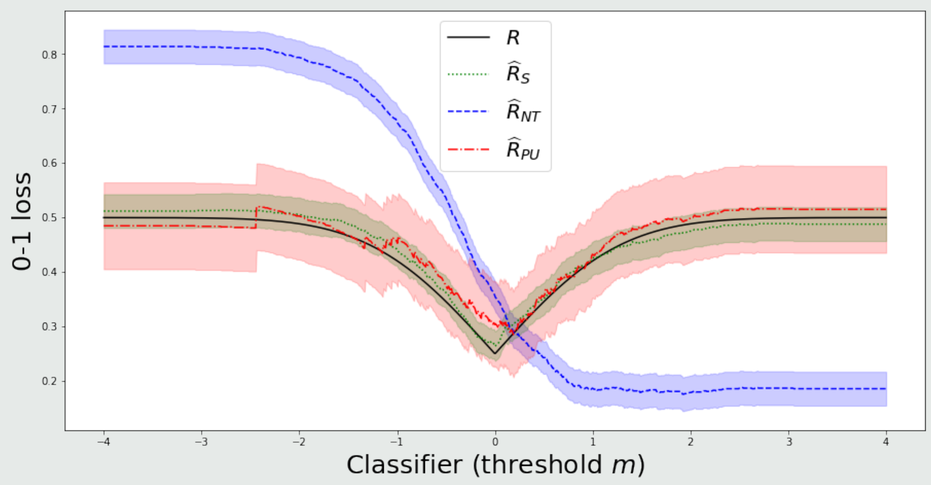


Figure 1. Simulation example (SAR)

Comparison of the empirical risk functions



Conclusion

- The non-traditional loss $\widehat{R}_{NT}$ is a biased estimate of the true risk R
  $\hookrightarrow$ fails to provide a good estimate of the optimal classifier f^*.
- Despite a higher variance, the PU loss function $\widehat{R}_{PU}$ provides a better estimate of the true risk.

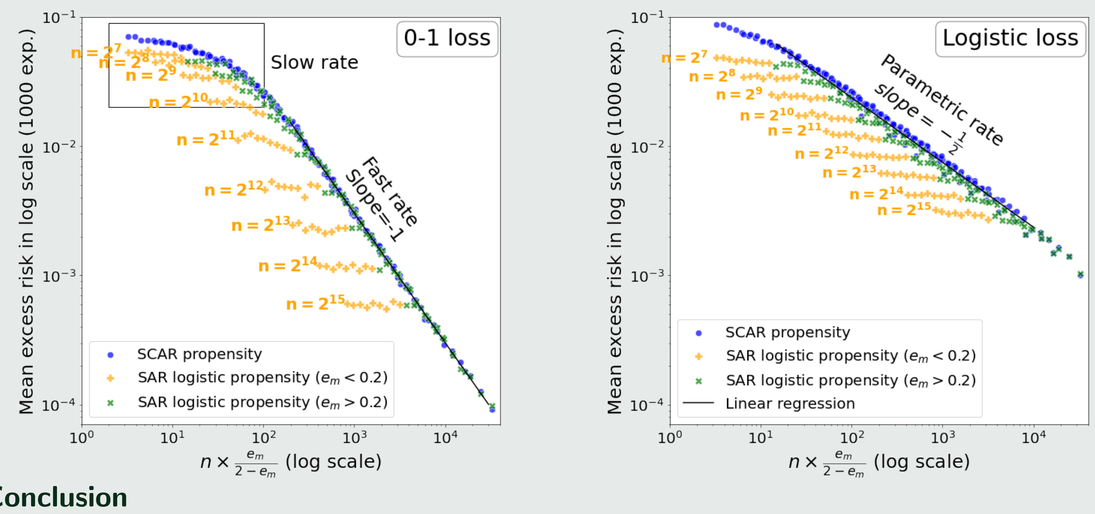
Convergence rates: simulation study

Estimation of the mean excess risk for:

- n ranging from 100 to $30{,}000$
- e constant propensity or logistic propensity
- e_m ranging from 0.05 to 1.

Two series of experiments:

1. using the PU unbiased $0-1$ loss function
2. using a PU unbiased logistic loss function.



Conclusion

- Illustration of theoretical risk bounds for PU learning under $0-1$ loss:
  1. slow rate for $n\,e_m/(2-e_m) < 100$
  2. fast rate for $n\,e_m/(2-e_m) \geq 100$: empirical rate in $\mathcal{O}(1/(n\,e_m))$ matching the theory
- Extension to a tractable logistic loss highlighting a unique parametric convergence rate $\mathcal{O}\left(1/\sqrt{n\,e_m}\right)$

Perspectives

Ongoing / future work

- Dealing with an unknown propensity: joint estimation of the classifier η and the propensity e.
- Practical applications: fatigue design of mechanical parts.
- Extension of the theoretical study to convex loss functions.

Main references

[1] J. Bekker, P. Robberechts, and J. Davis. "Beyond the Selected Completely at Random Assumption for Learning from Positive and Unlabeled Data". In: *Machine Learning and Knowledge Discovery in Databases*. Vol. 11907. 2020, pp. 71–85.

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[3] O. Coudray, C. Keribin, P. Massart, and P. Pamphile. "Risk bounds for PU learning under Selected At Random assumption". Preprint. Jan. 2022. URL: https://hal.inria.fr/hal-03526889.

[4] P. Massart and É. Nédélec. "Risk bounds for statistical learning". In: *Annals of Statistics* 34.5 (Oct. 2006).