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# 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:** $(X_i, Y_i, S_i)_{1\le i\le n}$ **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 $X$:**

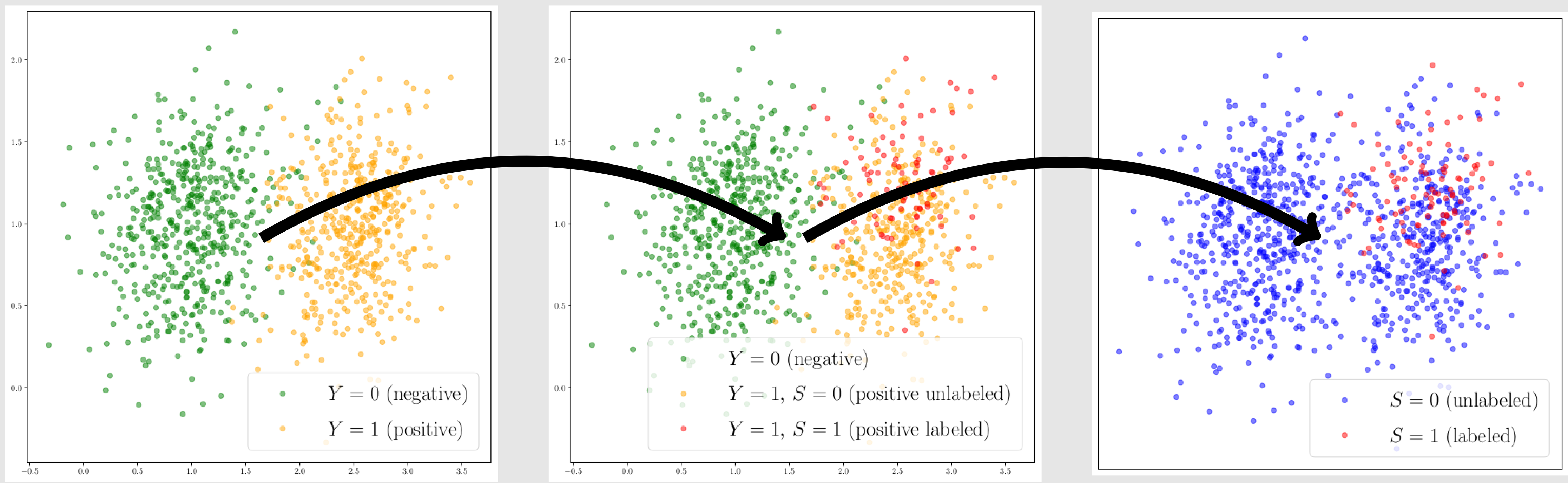
$$\mathbb{P}\left(Y = 1 \,|\, X = x\right) = \eta(x) \;.$$

**Propensity or selection bias:**

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

**Biased classification of $S$ given $X$:**

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




**Standard classification setting** $(X_i, Y_i) \to$ Estimate $\eta$

*Selection of positive instances through $e$*

**PU classification setting** $(X_i, S_i) \to$ Estimate $\eta$

## 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 $R(f) = \mathbb{E}\left[L\left(f(X), Y\right)\right]$.

$$f^* \in \underset{f}{\operatorname{Argmin}}\, R(f) \;.$$

**Estimation of $f^*$ using the training sample** $(X_i, S_i)_{1\le i\le n}$: 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 $(Y_i)_{1\le i\le n}$ are unobserved...

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

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

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

$\hookrightarrow$ 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.

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

## Theoretical risk bounds for PU learning[3]

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

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

**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 $\forall x \in \mathbb{R}^d$, $|2\,\mathbb{P}\left(Y = 1 \,|\, X = x\right) - 1| \ge h$ (Massart noise assumption[4]).
- $\exists\, e_m > 0$, $\forall x \in \mathbb{R}^d\; e(x) \ge e_m$.

**Result: two convergence rates**

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

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

## Simulation setting

- One-dimensional setting ($d = 1$)
- $\mathcal{F} = \{x \mapsto \mathbb{1}_{x\ge m},\; m \in \mathbb{R}\}$
- $X_i \sim \mathcal{N}(0, 1)$
- $Y_i \sim \mathcal{B}\left(\frac{1+h}{2}\mathbb{1}_{X_i\ge 0} + \frac{1-h}{2}\mathbb{1}_{X_i<0}\right)$, $h = 0.25$.
- $S_i \sim \mathcal{B}\left(e(x)\right)$ 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),
  $$e(x) = \max\left(e_m, \frac{1}{1 + e^{x-1}}\right), \text{ with } e_m > 0 \;.$$

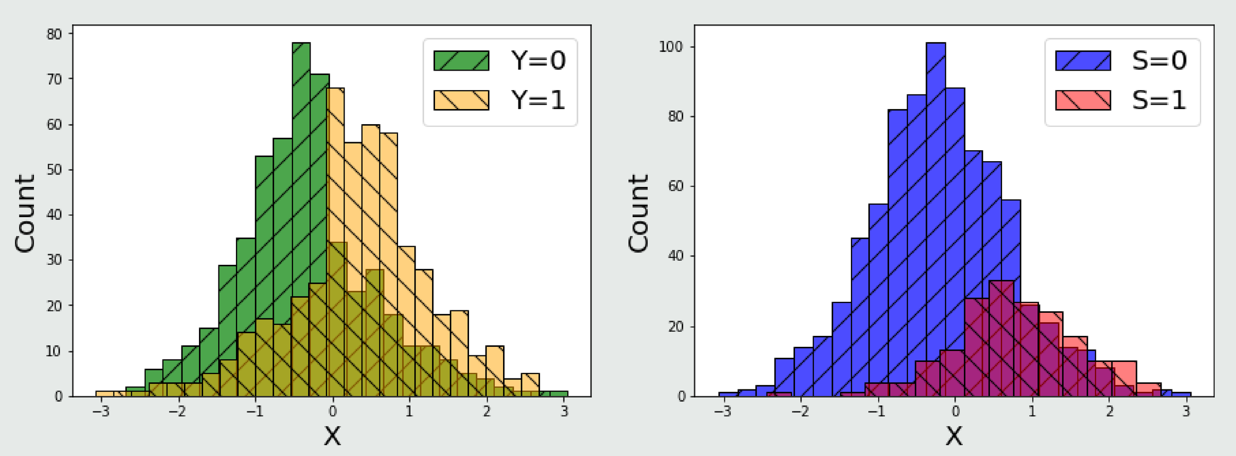
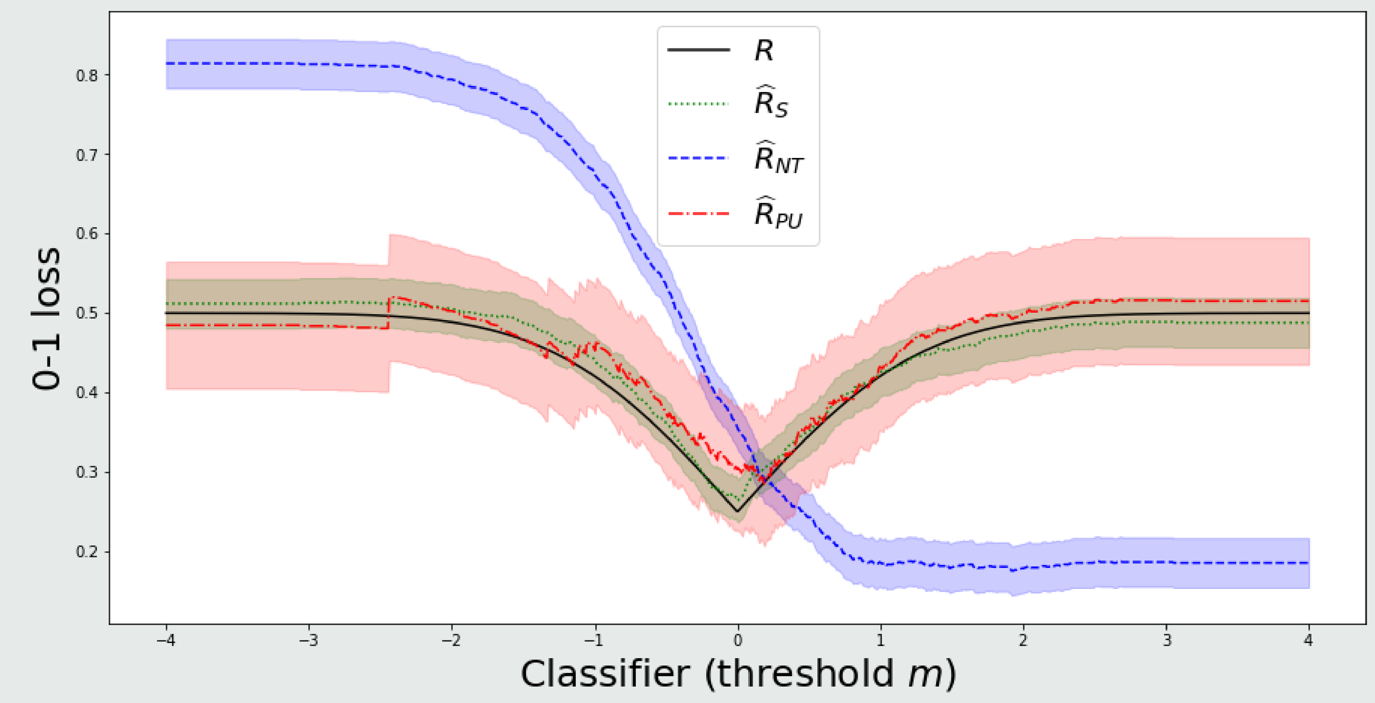



Figure 1. Simulation example (SAR)

## 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.

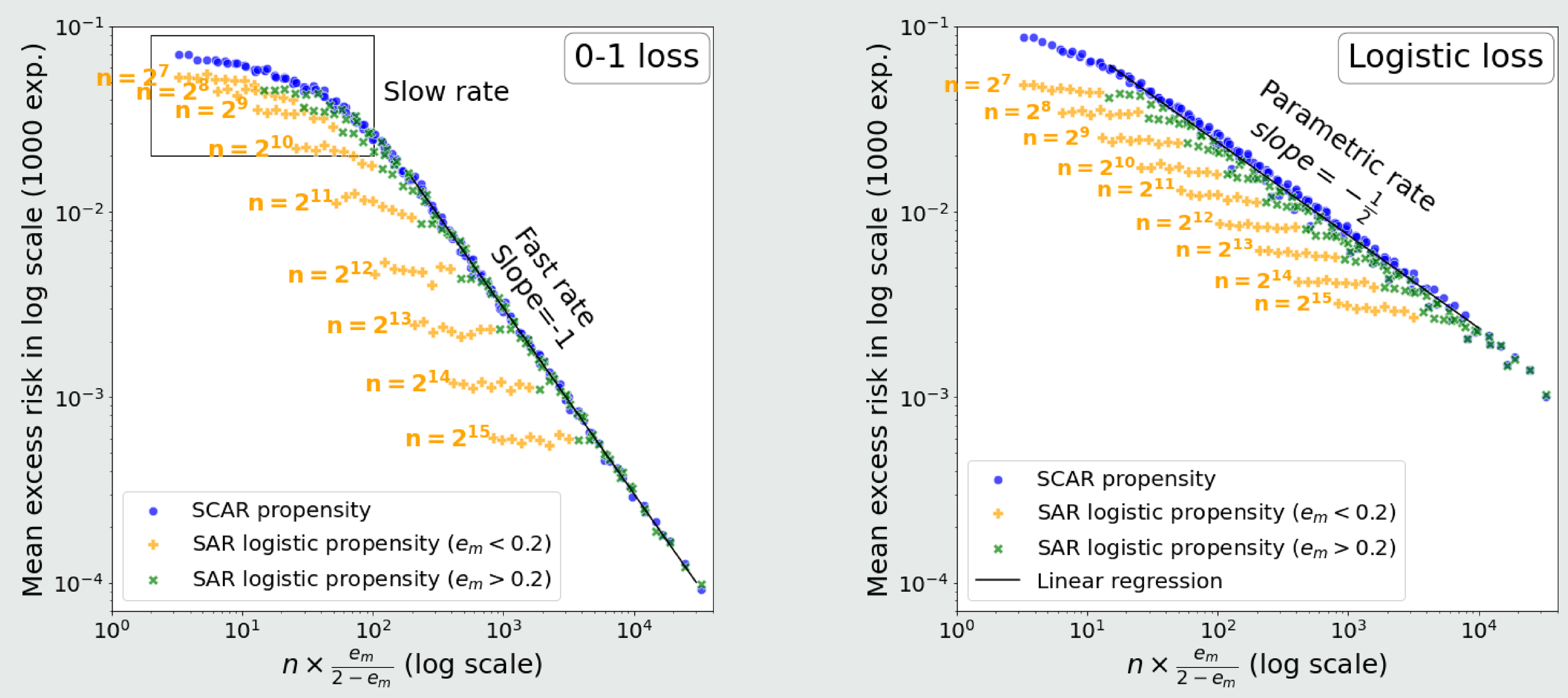
## Convergence rates: simulation study

**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 $n\,e_m/\left(2 - e_m\right) < 100$
  2. fast rate for $n\,e_m/\left(2 - e_m\right) \ge 100$: empirical rate in $\mathcal{O}\left(1/\left(n\,e_m\right)\right)$ 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 $\eta$ and the propensity $e$.
- Practical applications: fatigue design of mechanical parts.
- Extension of the theoretical study to convex loss functions.

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




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