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

## 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  $X$ :**

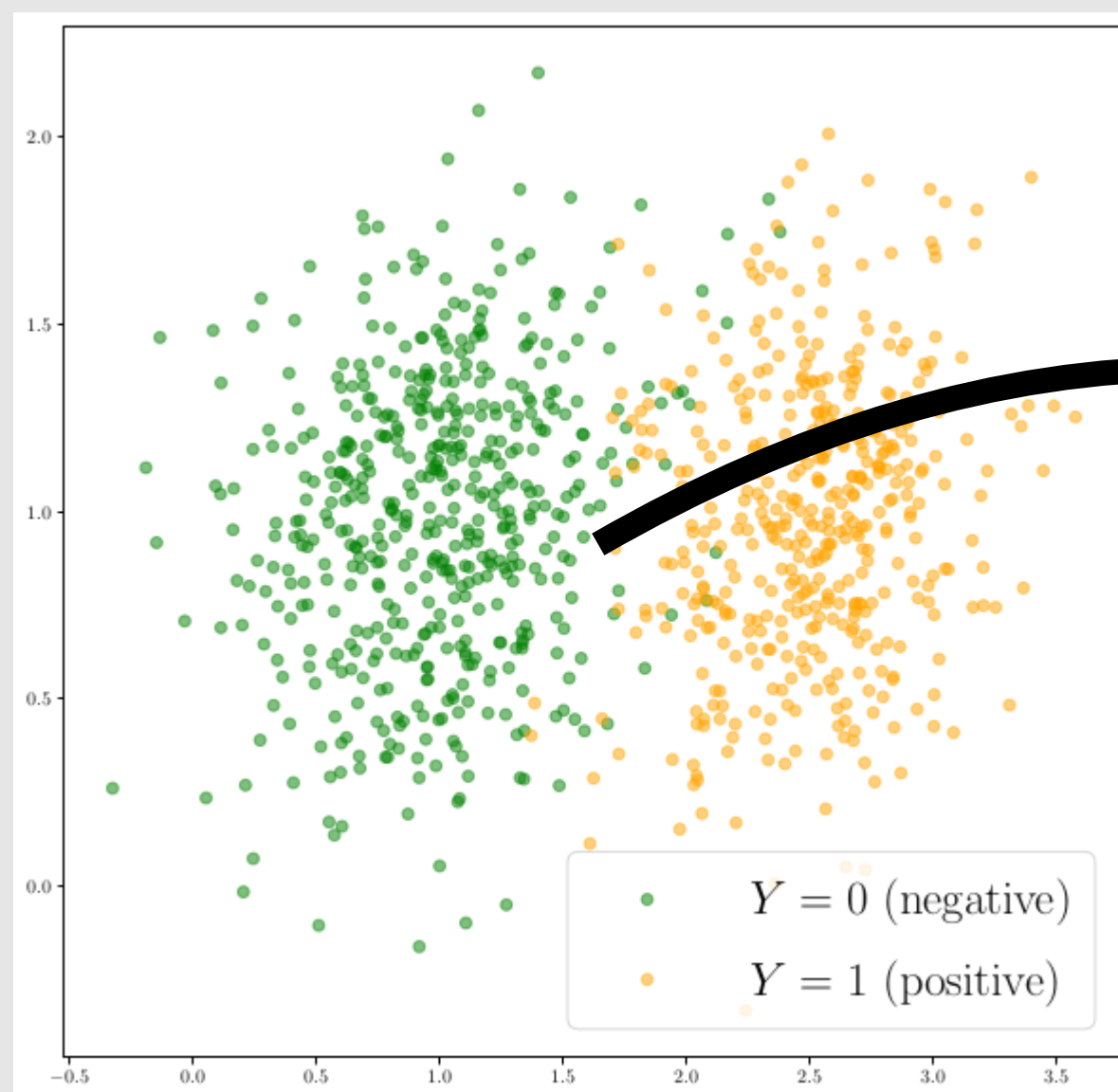
$$\mathbb{P}(Y = 1 | X = x) = \eta(x).$$

**Propensity or selection bias:**

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

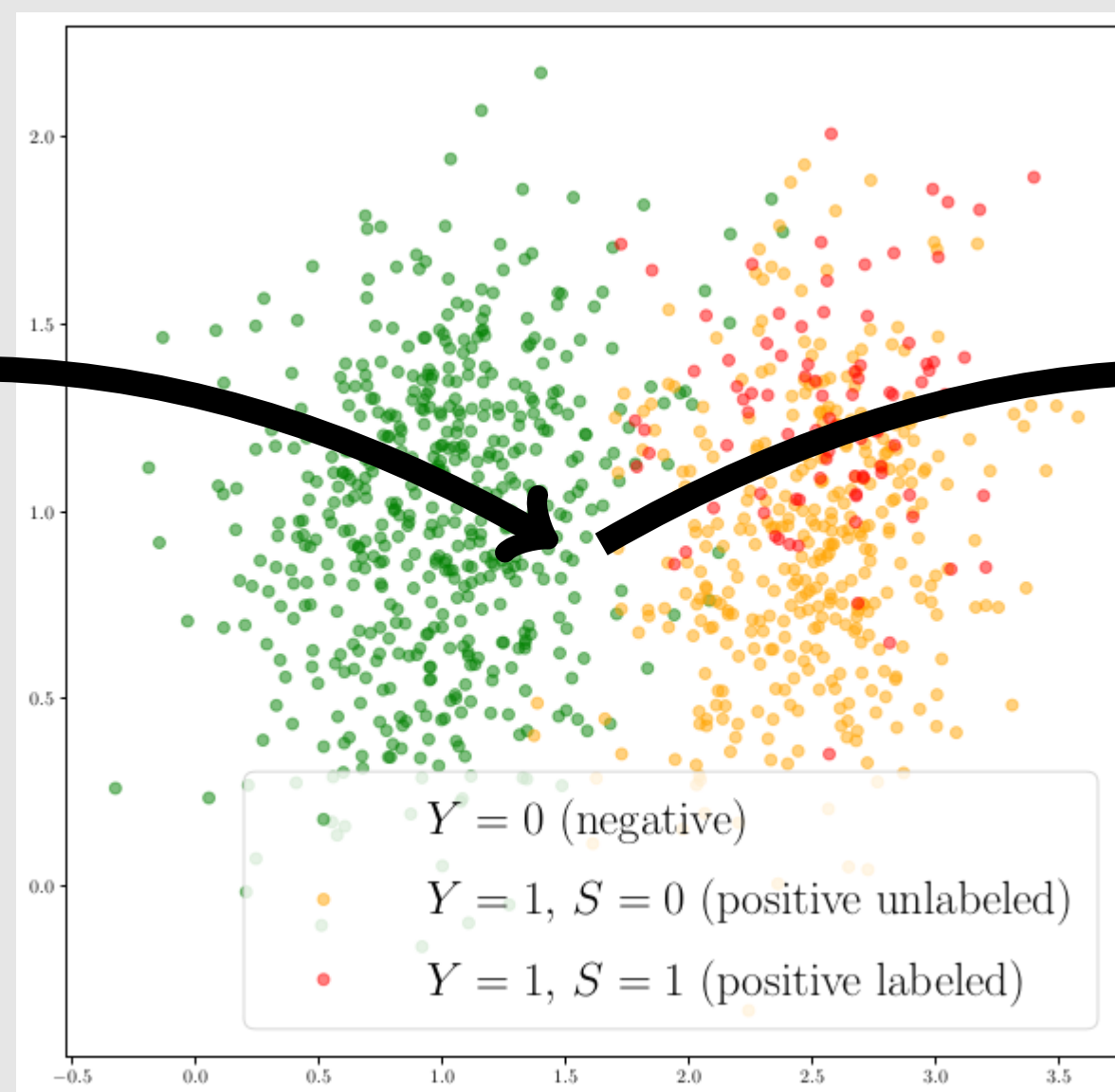
**Biased classification of  $S$  given  $X$ :**

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

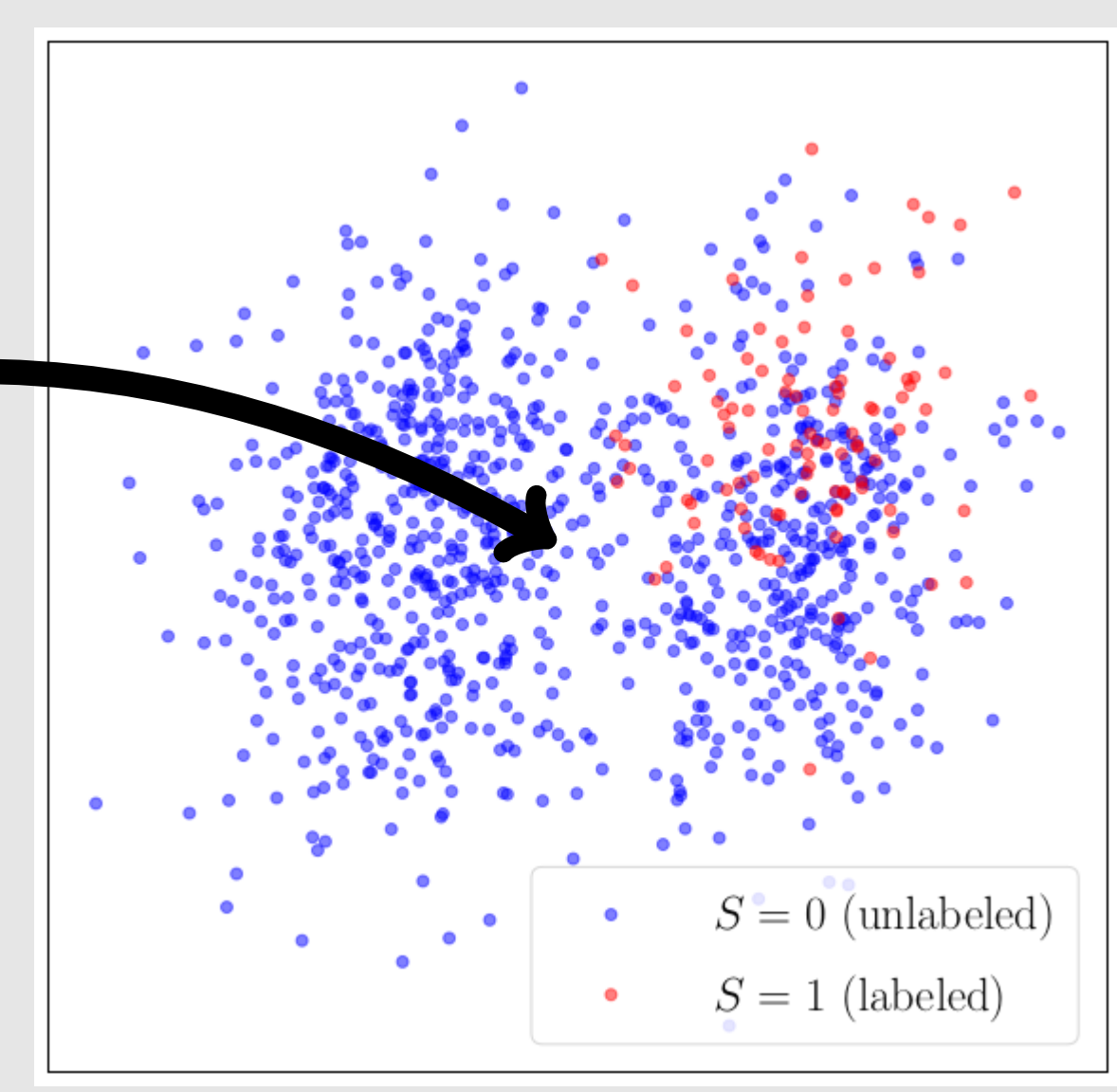


Standard classification setting

$(X_i, Y_i) \rightarrow$  Estimate  $\eta$



Selection of positive instances through  $e$



PU classification setting

$(X_i, S_i) \rightarrow$  Estimate  $\eta$

## Estimating the classifier in PU learning setting

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

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

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

**Empirical risks:**

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

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

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

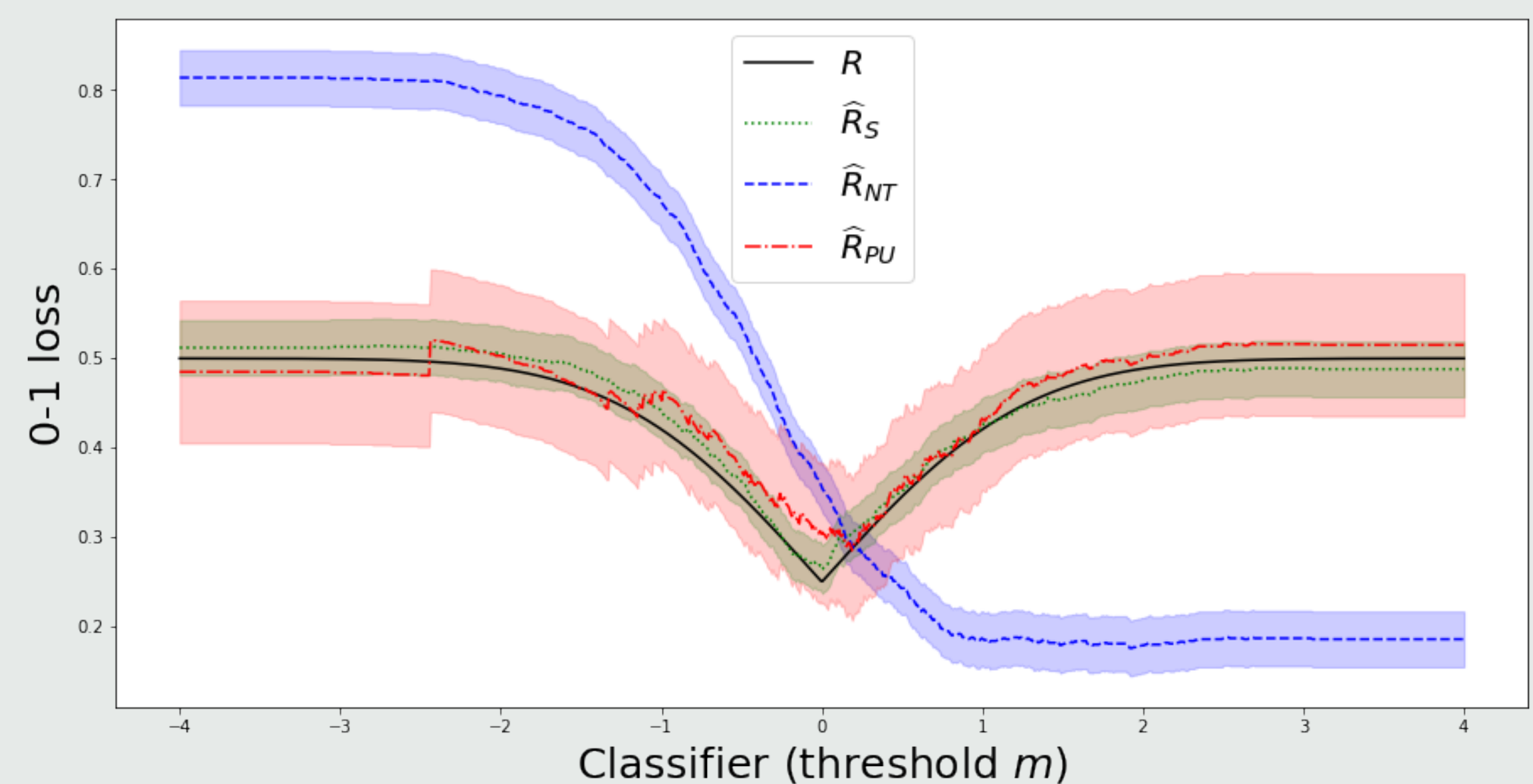
$$\widehat{R}_{NT}(f) = \frac{1}{n} \sum_{i=1}^n L(f(X_i), S_i)$$

$\Leftrightarrow$  **biased** estimate of the true risk.

- **Unbiased** PU empirical risk<sup>[1],[2]</sup>: assuming the propensity scores  $e(X_i)$  of labeled observations to be known.

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

## Comparison of the empirical risk functions



**Conclusion**

- The non-traditional loss  $\widehat{R}_{NT}$  is a **biased** estimate of the true risk  $R$   
 $\Leftrightarrow$  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.

## Theoretical risk bounds for PU learning<sup>[3]</sup>

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

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

**Excess risk:**

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

**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<sup>[4]</sup>).
- $\exists e_m > 0, \forall x \in \mathbb{R}^d e(x) \geq e_m$ .

**Result: two convergence rates**

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

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

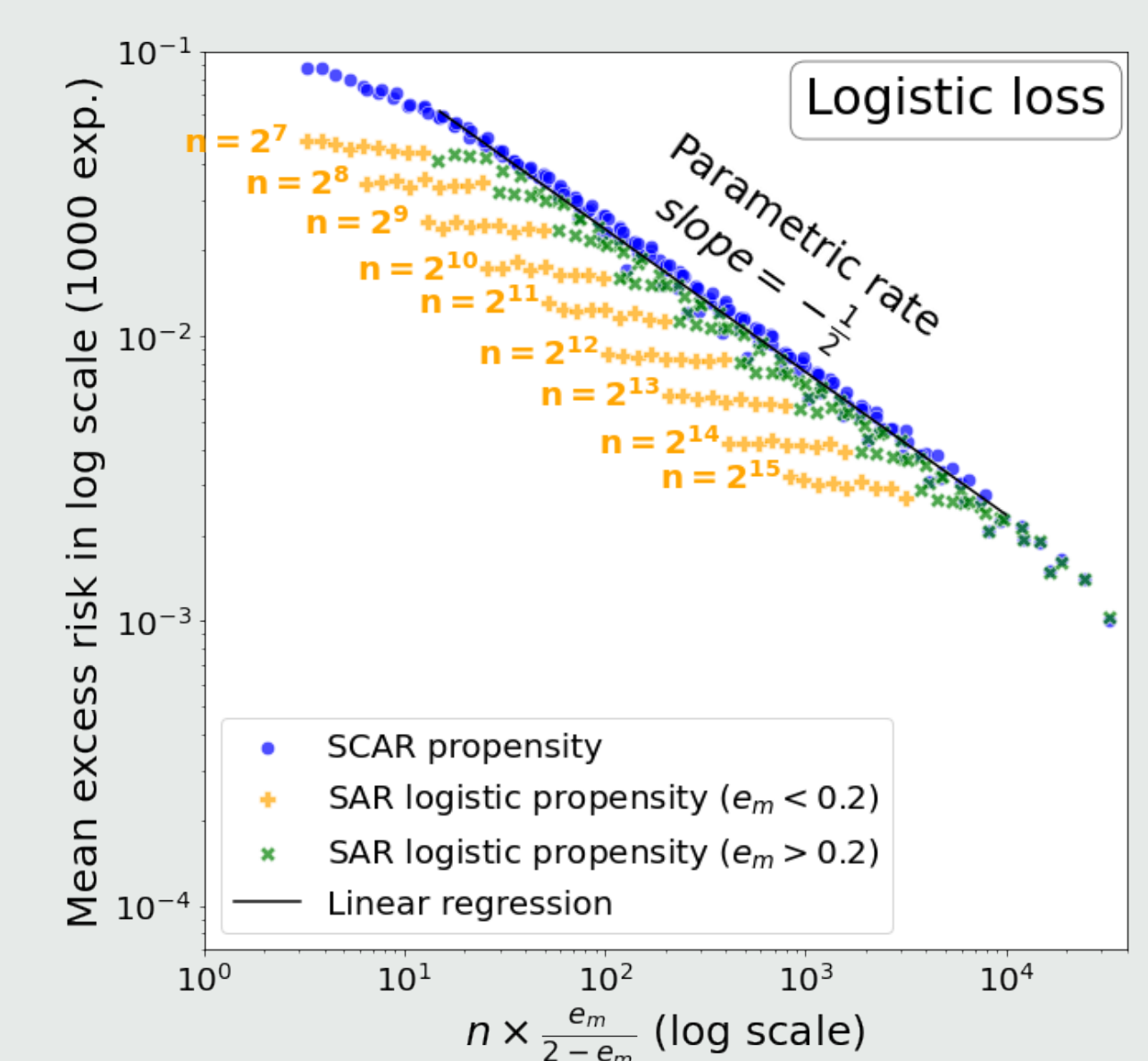
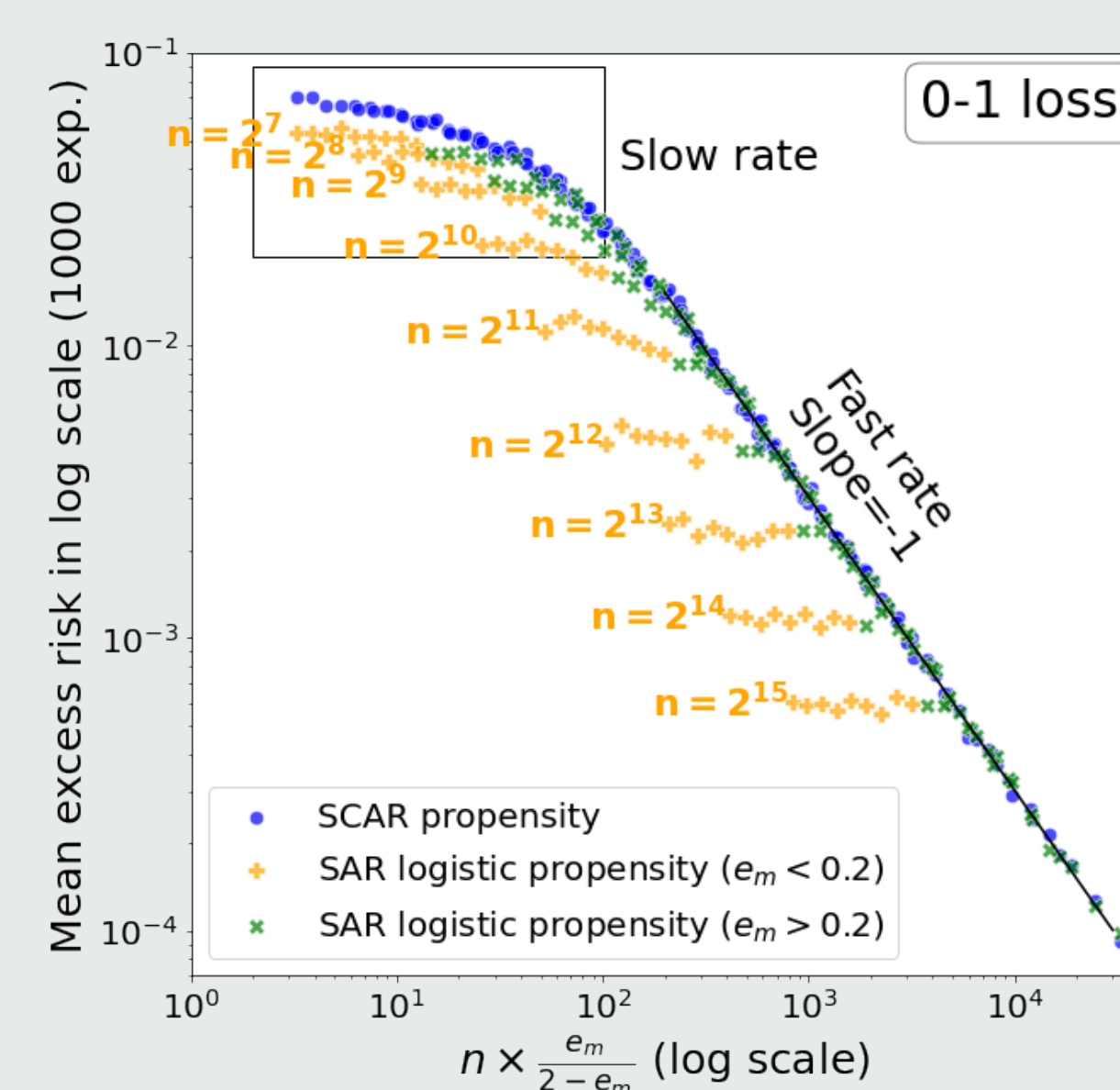
## Convergence rates: simulation study

**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:**

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



**Conclusion**

- Illustration of theoretical risk bounds for PU learning under 0-1 loss:
  - **slow rate** for  $n e_m / (2 - e_m) < 100$
  - **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  $\mathcal{O}(1/\sqrt{n e_m})$

## 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  $Y_i = 1$  (else  $S_i = 0$ )

**Propensity functions:**

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

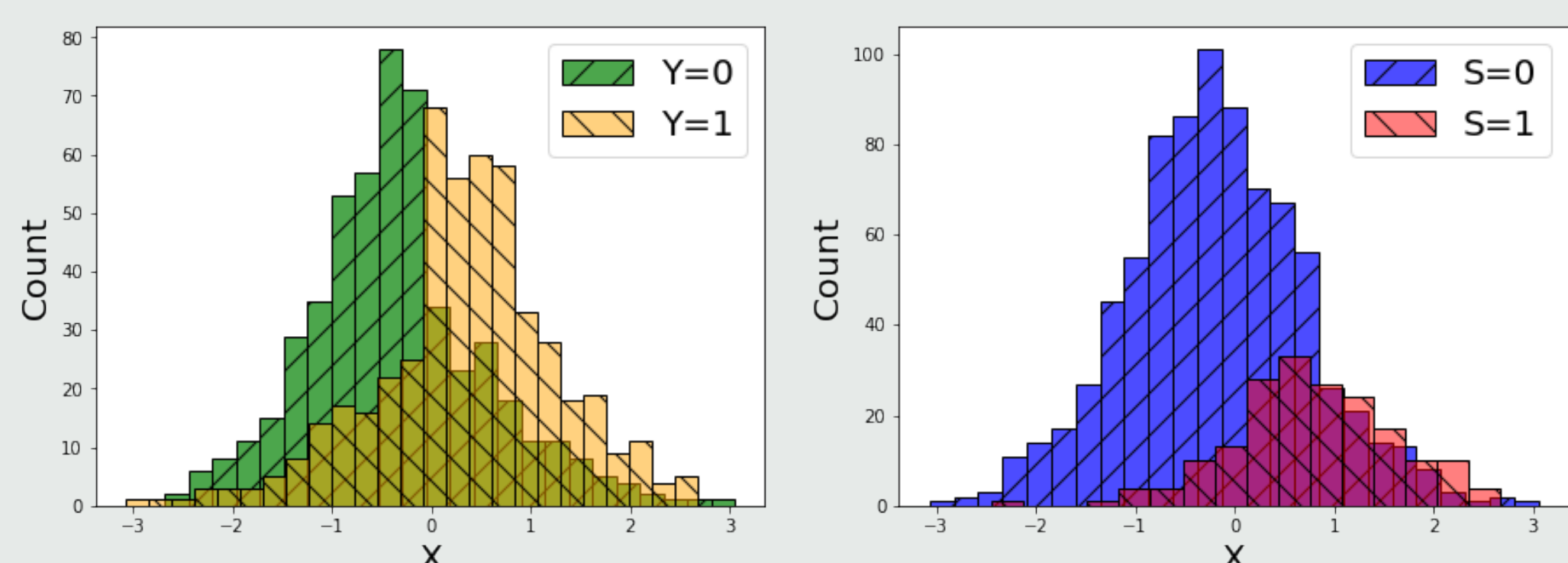


Figure 1. Simulation example (SAR)

## 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

- [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.
- [2] M. C. Du Plessis, G. Niu, and M. Sugiyama. "Analysis of learning from positive and unlabeled data". In: *NIPS* 1 (Jan. 2014), pp. 703-711.
- [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  . N d lec. "Risk bounds for statistical learning". In: *Annals of Statistics* 34.5 (Oct. 2006).