Don't fear the unlabelled: safe semi-supervised learning via simple debiaising

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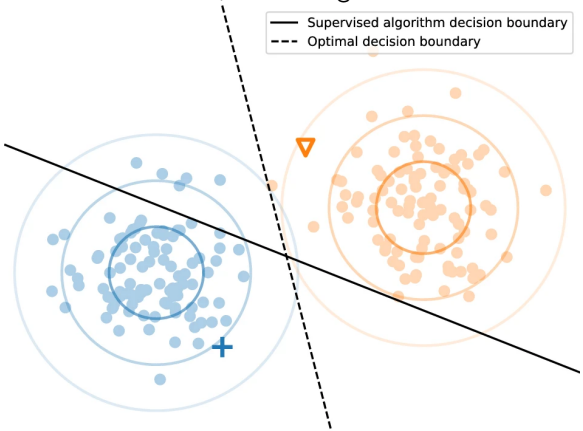
Deep semi-supervised learning ? What for ?

Goal: Using both labelled and unlabelled data to build better learners, than using each one alone



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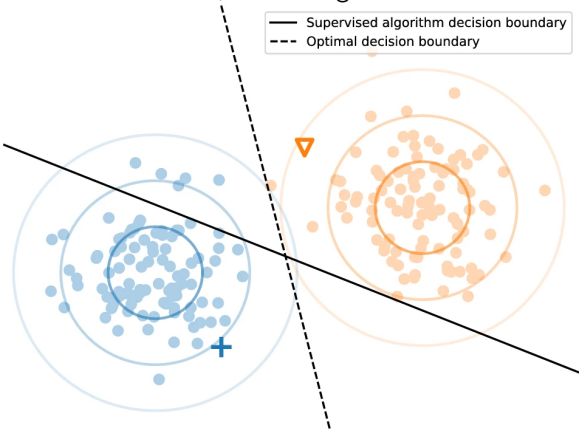

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Why bother ?

- unlabelled data are cheap
- labelled data can be hard to get

Learning theory relies on the unbiased estimator of the risk

We have two spaces of objects X and Y and would like to learn a function $f_\theta : X \to Y$.
L is a loss function which measures how different the prediction $f_\theta(x)$ is from the true outcome y.
We define the risk:

$$\mathcal{R}(\theta) = \mathbb{E}[L(\theta; x_i, y_i)]$$

The ultimate goal of a learning algorithm is to find θ^* among a fixed class of functions:

$$\theta^* = \arg\min_{\theta \in \Theta} \mathcal{R}(\theta)$$

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Empirical risk: Monte Carlo estimator of the risk

$$\hat{\mathcal{R}}(\theta) = \frac{1}{n} \sum_{i=1}^{n} L(\theta; x, y)$$

$\longrightarrow$ Unbiased estimator $\Rightarrow$ basic property that is needed for the development of traditional learning theory and asymptotic statistics.

The complete case, the simplest: get rid of unlabelled data

- labelled data: $\{(x_1, y_1), ..., (x_{n_l}, y_{n_l})\}$
- unlabelled data: $\{x_{n_l+1}, ..., x_{n_l+n_u}\}$
- $n_l + n_u = n$

Semi-supervised is a missing data problem. We consider the case missing completely at random (MCAR) i.e. y being missing is independent x.

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Using unlabelled data leads to biased estimator of the risk

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Including unlabelled data in the risk estimator:

$$\hat{\mathcal{R}}_{SSL}(\theta) = \frac{1}{n_l} \sum_{i=1}^{n_l} L(\theta; x_i, y_i) + \frac{\lambda}{n_u} \sum_{i=1}^{n_u} H(\theta; x_i)$$

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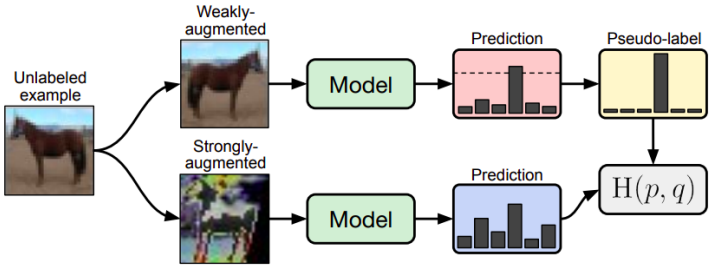
Examples:

- Entropy minimization: $H(\theta; x_i) = -\sum f_\theta(x)_k \log(p_\theta(x)_k)$ (Grandvalet and Bengio 2005)
- Consistency based: $H(\theta; x_i) = Div(p_\theta(x), p_\theta(pert(x))$ (Sohn et al. 2020, Xie et al. 2020, Miyato et al. 2018, Laine and Aila 2017, ...)
- Pseudo-label (PL): $H(\theta; x_i) = -\log(\max p_\theta(u|x))\mathbb{1}[\max_y p_{\hat{\theta}}(y|x) > \tau]$ (Scudder 1965, Lee 2013, Rizve 2021)

Fixmatch (Sohn et al., NeurIPS [2020])



$$H(\theta; x) = \mathbb{E}_{x_1 \sim weak(x)} \left[\mathbb{1}[\max_y p_{\hat{\theta}}(y|x_1) > \tau] \mathbb{E}_{x_2 \sim strong(x)} [-\log(p_\theta(\arg\max_y p_{\hat{\theta}}(y|x_1)|x_2))] \right]$$

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Good performance on a various of (deep) learning tasks.

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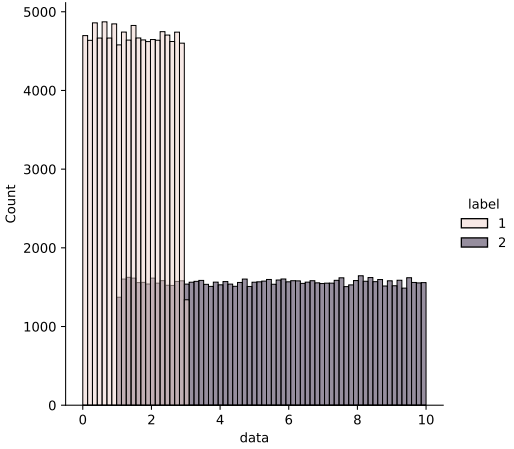
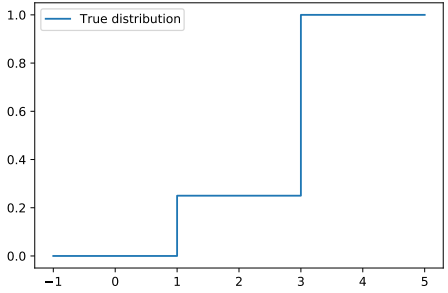
Safety: A SSL algorithm is safe if it has theoretical guarantees that are similar to or stronger than the complete case baseline.

FEAR THE UNLABELLED !





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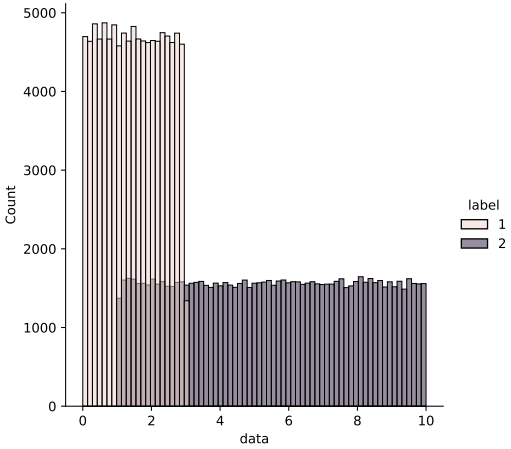
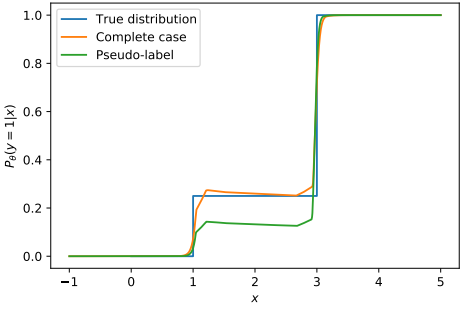
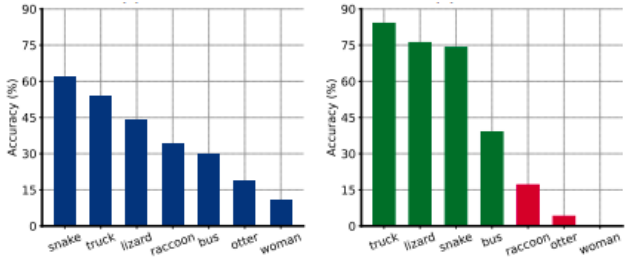




The rich get richer ! (Zhu et al. [ICLR, 2022])



Top-1 accuracy of 7 randomly selected categories with different training methods on CIFAR-100. (Left) Complete case. (Right) FixMatch

FixMatch largely increases the bias of poor-behaved categories. (Chen et al., [arXiv:2202.07136])

DeSSL: Debiased version of SSL

$$\hat{\mathcal{R}}_{DeSSL}(\theta) = \frac{1}{n_l}\sum_{i=1}^{n_l} L(\theta; x_i, y_i) + \frac{\lambda}{n_u}\sum_{i=1}^{n_u} H(\theta; x_i) - \frac{\lambda}{n_l}\sum_{i=1}^{n_l} H(\theta; x_i)$$

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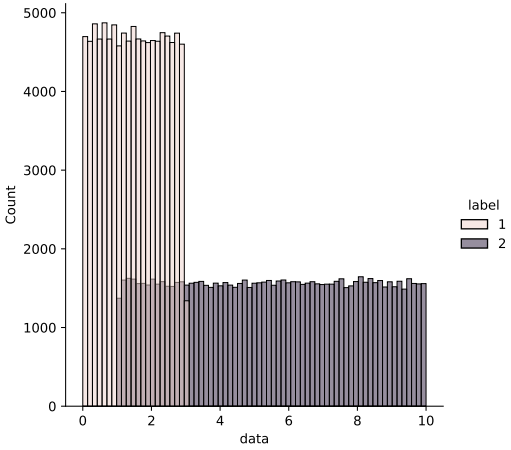
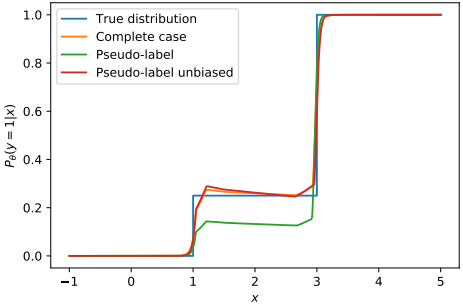
- Under the MCAR assumption, estimator is unbiased estimator of the true risk.
- Close relationship with control variates (Owen [2013]).
- Other motivations:
  - Penalising the confidence of a model on labelled data (Pereyra et al., [2017])
  - Maximising the plausibility (Barndorff-Nielsen [1976]).
  - The risk estimate is a Lagrangian!

Pseudo-label unbiased success under the cluster assumption





DeSSL is calibrated and benefits from generalisation error bounds

Variance:

- It exists λ such as the variance of the risk estimate is lower than the one of the complete case.
- We expect DeSSL to be a **more accurate** risk estimate than the complete case.
- Formula for λ_{opt}.
- Justification on the heuristic idea that H should be a surrogate of L.

Calibration:

- We can expect DeSSL to be as **well-calibrated** as the complete case, while SSL will generally overfit.

Generalisation error bound:

- Under classical assumptions on L and H, DeSSL benefits of generalisation error bounds derived from the **Rademacher complexity**.

DeSSL is consistent and improves the supervised baseline

Consistency:

- Under classical assumptions on L and H, DeSSL provides **asymptotically consistent** models.
- SSL may fail with an infinite number of labelled data when DeSSL will not

Asymptotic normality:

- Under classical assumptions on L and H, the parameter estimated using DeSSL is asymptotically normal.
- It exists λ such as the asymptotic variance of the estimated parameters is lower than the one of the complete case.
- **DeSSL outperforms the complete case baseline in term of parameters estimation**

DeFixmatch improves Fixmatch accuracy and calibration

Table: Test accuracy, worst class accuracy and cross-entropy of Complete Case, Fixmatch and DeFixmatch on 5 folds of CIFAR-10 and one fold of CIFAR-100.

	CIFAR-10 ($n_l = 4000$)			CIFAR-100 ($n_l = 10000$)		
	Complete Case	Fixmatch	DeFixmatch	Complete Case	Fixmatch	DeFixmatch
Accuracy	87.27 $\pm$ 0.25	93.87 $\pm$ 0.13	**95.44 $\pm$ 0.10**	62.62	69.28	**71.22**
Worst class accuracy	70.08 $\pm$ 0.93	82.25 $\pm$ 2.27	**87.16 $\pm$ 0.46**	28.00	23.00	**31.00**
Cross entropy	0.60 $\pm$ 0.01	0.27 $\pm$ 0.01	**0.20 $\pm$ 0.01**	1.87	1.52	**1.42**
Brier score	0.214 $\pm$ 0.005	0.101 $\pm$0.003	**0.076 $\pm$ 0.001**	0.56	0.47	**0.44**

DeSSL mitigates the disparact effect of SSL

Table: Mean accuracy per class and mean benefit ratio ($\mathcal{BR}$, Zhu et al. [2022]) on 5 splits.

	Complete Case	Fixmatch		DeFixmatch	
	Accuracy	Accuracy	$\mathcal{BR}$	Accuracy	$\mathcal{BR}$
airplane	86.94	95.94	0.88	96.62	0.94
automobile	95.26	97.54	0.68	98.22	0.89
bird	**80.46**	**90.80**	**0.68**	**92.64**	**0.80**
cat	**70.08**	**82.50**	**0.56**	**87.16**	**0.78**
deer	88.88	95.86	0.78	97.26	0.94
dog	**79.66**	**87.16**	**0.53**	**90.98**	**0.81**
frog	93.12	97.84	0.80	98.62	0.94
horse	90.96	96.94	0.83	97.64	0.92
ship	94.12	97.26	0.67	98.06	0.84
truck	93.18	96.82	0.84	97.20	0.93

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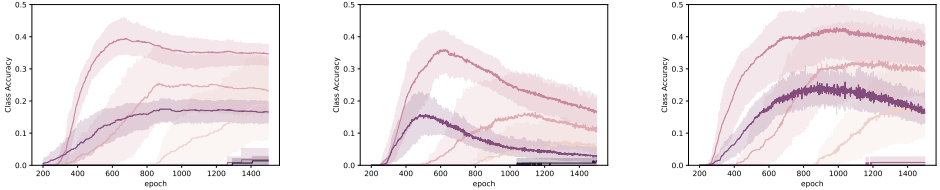

Class accuracies (without the majority class) on DermaMNIST trained with $n_l = 1000$ labelled data on five folds. (Left) CompleteCase (B-Acc: 26.88 $\pm$ 2.26%); (Middle) PseudoLabel (B-Acc: 22.03 $\pm$ 1.45%); (Right) DePseudoLabel (B-Acc: **28.84** $\pm$ 1.02%), with 95% CI.

Conclusion

More results on CIFAR-100, SVHN, STL10, UCI datasets and MedMNIST datasets in the paper.

- DeSSL come with theoretical guarantees using only the MCAR assumption
- Estimator unbiased, reduction of variance, asymptotically consistent, well calibrated
- Formula for the hyperparameter
- Mitigates the disparact effect of SSL
- Performs better than the biased estimator on various datasets (see our paper)

Future directions:

- Compute of λ_{opt}
- Extend to non MCAR settings.
- Extend to segmentation
- Stratified sampling to select autmatically the number of labelled and unlabelled data per batch

Is $\hat{\mathcal{R}}_{DeSSL}(\theta)$ an accurate risk estimator ?

Theorem: The function $\lambda \mapsto \mathbb{V}(\hat{\mathcal{R}}_{DeSSL}(\theta))$ reaches its minimum for:

$$\lambda_{opt} = \frac{n_u}{n} \frac{\mathrm{Cov}(L(\theta; x, y), H(\theta; x))}{\mathbb{V}(H(\theta; x))} \tag{1}$$

and

$$\begin{aligned} \mathbb{V}(\hat{\mathcal{R}}_{DeSSL}(\theta))|_{\lambda_{opt}} &= (1 - \frac{n_u}{n}\rho^2_{L,H})\mathbb{V}(\hat{\mathcal{R}}_{CC}(\theta)) \\ &\leq \mathbb{V}(\hat{\mathcal{R}}_{CC}(\theta)) \end{aligned} \tag{2}$$

where $\rho_{L,H} = \mathrm{Corr}(L(\theta; x, y), H(\theta; x))$.

Justification on the heuristic idea that H should be a surrogate of L.

$\hat{\mathcal{R}}_{DeSSL}(\theta)$ is an accurate risk estimator but $\nabla\hat{\mathcal{R}}_{DeSSL}(\theta)$ is even better

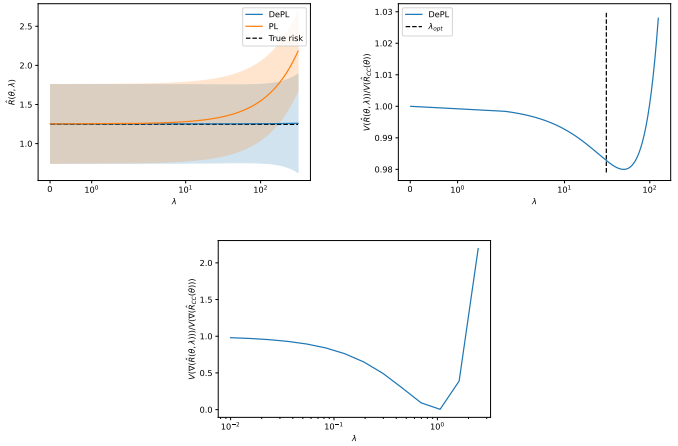

Figure: (Left) Risk estimate value for PseudoLabel (PL) and DePseudoLabel (DePL) compared to the true value of the risk. (Right) The influence of λ on the ratio $\mathbb{V}(\hat{\mathcal{R}}_{DePL}(\theta)|r)/\mathbb{V}(\hat{\mathcal{R}}_{CC}(\theta)|r)$. (Down) The influence of λ on the ratio $\mathbb{V}(\nabla\hat{\mathcal{R}}_{DePL}(\theta)|r)/\mathbb{V}(\nabla\hat{\mathcal{R}}_{CC}(\theta)|r)$.

DeSSL models are calibrated

Theorem: If the original loss is a proper scoring rule, then DeSSL is also a proper scoring rule.

- We can expect DeSSL to be as well-calibrated as the complete case.
- What if the model is non probabilistic ? Fisher consistency

Asymptotic consistency

$\hat{\theta}$ is asymptotically consistent with respect to n if $d(\hat{\theta}, \theta^*) \xrightarrow{p} 0$.

Theorem: Under usual regularity conditions of M-estimators for both L and H, $\hat{\theta} = \arg\min \hat{\mathcal{R}}_{DeSSL}$ is asymptotically consistent with respect to n.

SSL may fail with an infinite number of labelled data when DeSSL will not.

Asymptotic normality

Theorem:

Suppose L and H are smooth functions in $\mathcal{C}^2(\Theta, \mathbb{R})$. Assume $\mathcal{R}(\theta)$ admit a second-order Taylor expansion at θ^* with a non-singular second order derivative V_{θ^*}. Under the MCAR assumption, we have that $\hat{\theta}_{DeSSL}$ is asymptotically normal and we can minimise the trace of the asymptotic covariance. Indeed, $\mathrm{Tr}(\Sigma_{DeSSL})$ reaches its minimum at

$$\lambda_{opt} = (1-\pi)\frac{\mathrm{Tr}(V_{\theta^*}^{-1} K_{\theta^*} V_{\theta^*}^{-1})}{\mathrm{Tr}(V_{\theta^*}^{-1}\mathbb{E}\left[\nabla H(\theta^*; x)\nabla H(\theta^*; x)^T\right] V_{\theta^*}^{-1})}, \tag{3}$$

and at λ_{opt} :

$$\mathrm{Tr}(\Sigma_{DeSSL}) - \mathrm{Tr}(\Sigma_{CC}) = -\frac{1-\pi}{\pi}\frac{\mathrm{Tr}(V_{\theta^*}^{-1} K_{\theta^*} V_{\theta^*}^{-1})^2}{\mathrm{Tr}(V_{\theta^*}^{-1}\mathbb{E}\left[\nabla H(\theta^*; x)\nabla H(\theta^*; x)^T\right] V_{\theta^*}^{-1})} \leq 0. \tag{4}$$

DeSSL does benefit of generalisation error bounds

Theorem: We assume that labels are MCAR and that both L and H are bounded. Then, there exists a constant $\kappa > 0$, that depends on λ, L, H, and the ratio of observed labels, such that, with probability at least $1 - \delta$, for all $\theta \in \Theta$,

$$\mathcal{R}(\theta) \leq \hat{\mathcal{R}}_{DeSSL}(\theta) + 2R_n + \kappa\sqrt{\frac{\log(4/\delta)}{n}}. \tag{5}$$