Variance reduction for semi-supervised learning

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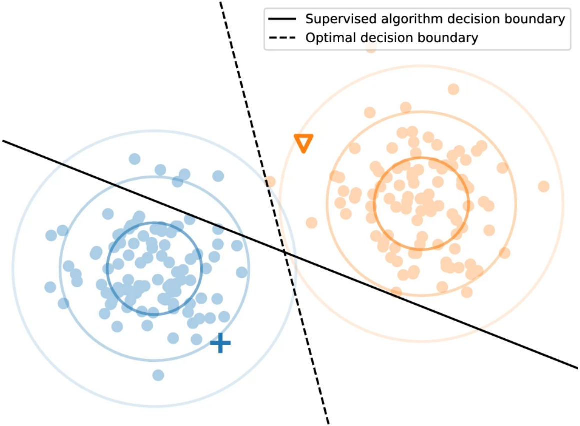
Deep semi-supervised learning ? What for ?

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



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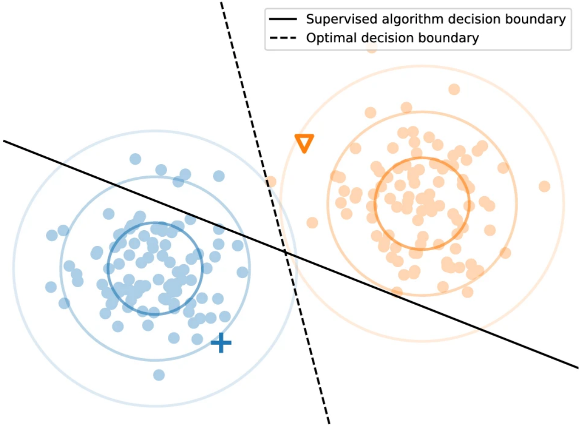

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Why bother ?

- 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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Complete case. Get rid of unlabelled data:

$$\hat{\mathcal{R}}_{CC}(\theta) = \frac{1}{n_l} \sum_{i=1}^{n_l} L(\theta; x_i, y_i)$$

$\longrightarrow$ Under MCAR, also unbiased $\Rightarrow$ basic property that is needed for the development of traditional learning theory and asymptotic statistics.

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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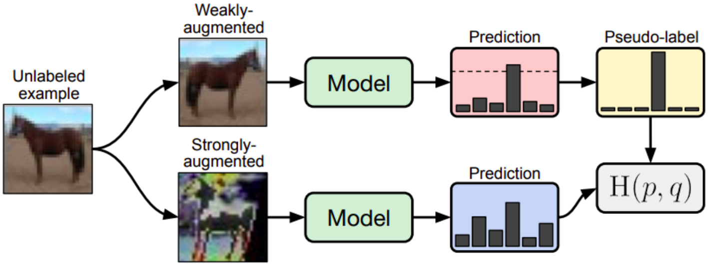
Examples:

- 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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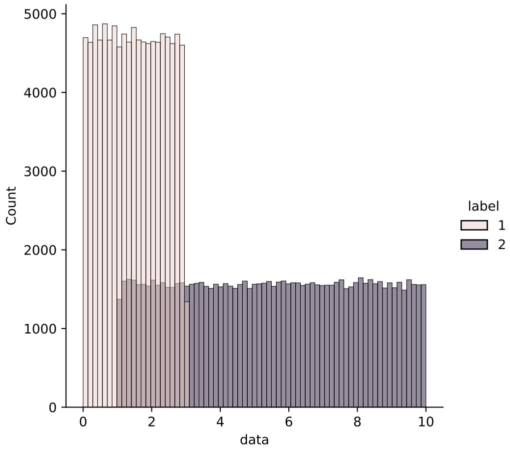
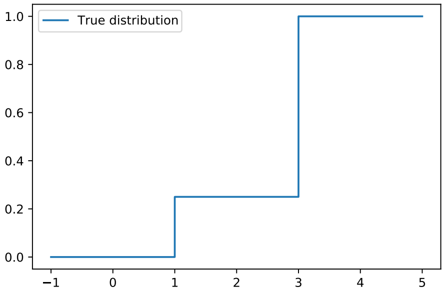
- An additional hyperparameter λ and no realistic validation (Oliver et al. [NeurIPS, 2018])

FEAR THE UNLABELLED !





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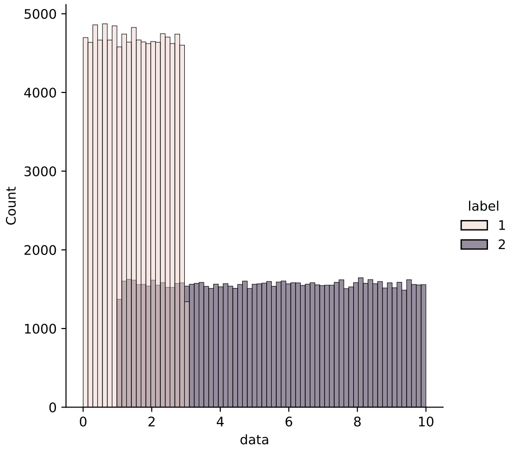
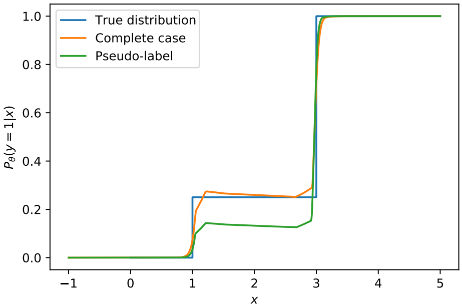
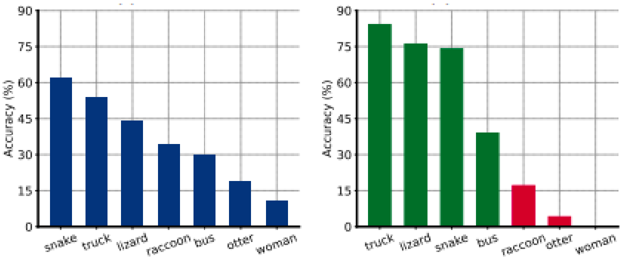




The rich get richer ! (Zhu et al. [ICLR, 2022])



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

Don't fear the unlabelled: Safe semi-supervised learning via debiasing, Schmutz et al., ICLR 2023

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

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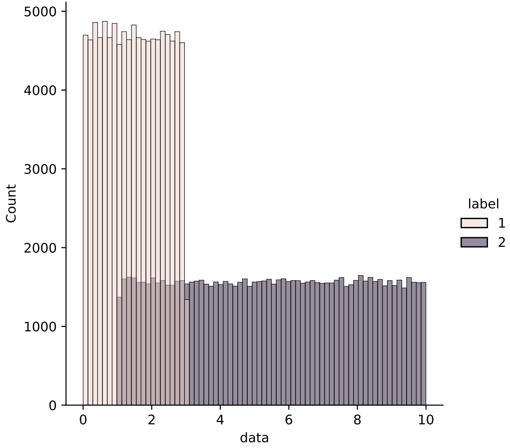
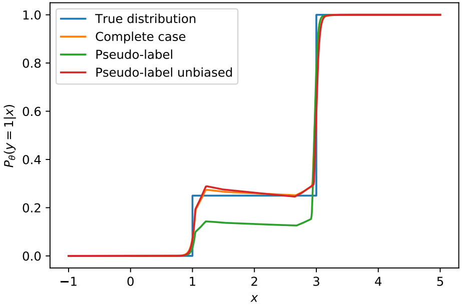
- Under the MCAR assumption, estimator is unbiased estimator of the true risk.
- Close relationship with control variates (Owen [2013]).
- Other motivations:
  - Penalising the confidence of a model on labelled data (Pereyra et al., [2017])
  - Maximising the plausibility (Barndorff-Nielsen [1976]).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

Pseudo-label unbiased success under the cluster assumption





$\hat{\mathcal{R}}_{DeSSL}(\theta)$ is unbiased but is it 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

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

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

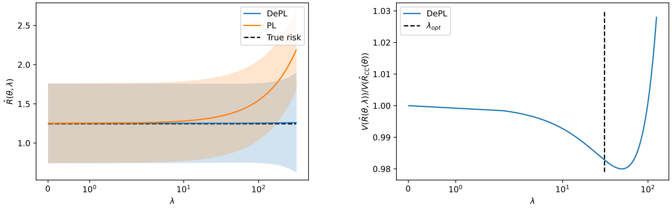


Figure: (Left) Risk estimate value for PseudoLabel (PL) and DePseudoLabel (DePL) compared to the true value of the risk. (Right) The influence of λ on the ratio $\mathbb{V}(\hat{\mathcal{R}}_{DePL}(\theta)|r)/\mathbb{V}(\hat{\mathcal{R}}_{CC}(\theta)|r)$. (Down) The influence of λ on the ratio $\mathbb{V}(\nabla\hat{\mathcal{R}}_{DePL}(\theta)|r)/\mathbb{V}(\nab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

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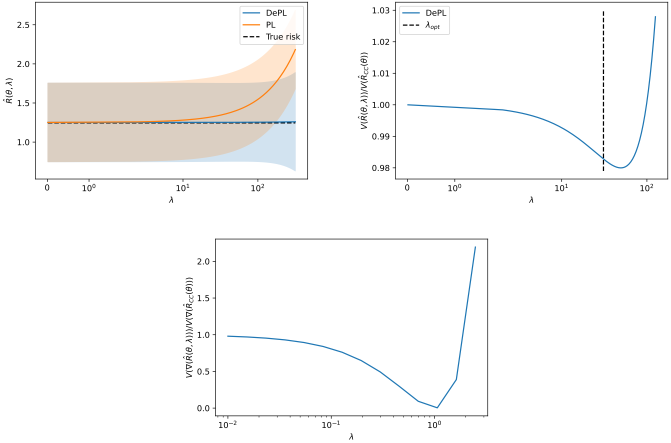

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DeSSL is calibrated and benefits from generalisation error bounds

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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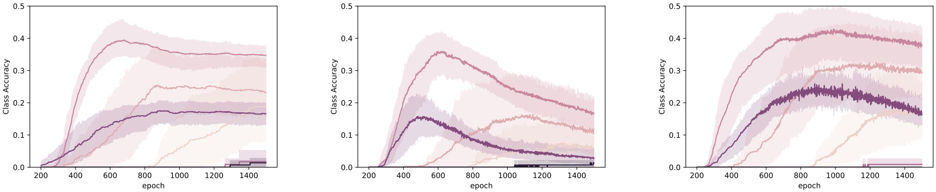

Class accuracies (without the majority class) on DermaMNIST trained with $n_l = 1000$ labelled data on five folds. (Left) CompleteCase (B-Acc: $26.88 \pm 2.26\%$); (Middle) PseudoLabel (B-Acc: $22.03 \pm 1.45\%$); (Right) DePseudoLabel (B-Acc: $\mathbf{28.84} \pm 1.02\%$), with 95% CI.

Conclusion

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

- DeSSL comes 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)

On going works:

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

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Monte Carlo theory, methods and examples , Art B. Owen, 2013