

Leveraging Ensemble Diversity for Robust Self-Training under Sample Selection Bias

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[Paper](#) - [Code](#)

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école —————
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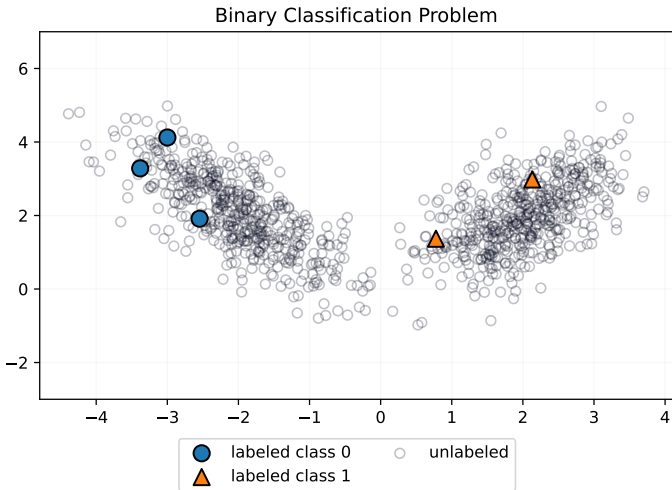
- ① Introduction
- ② Failure of Self-Training
- ③ Learning with the \mathcal{T} -similarity
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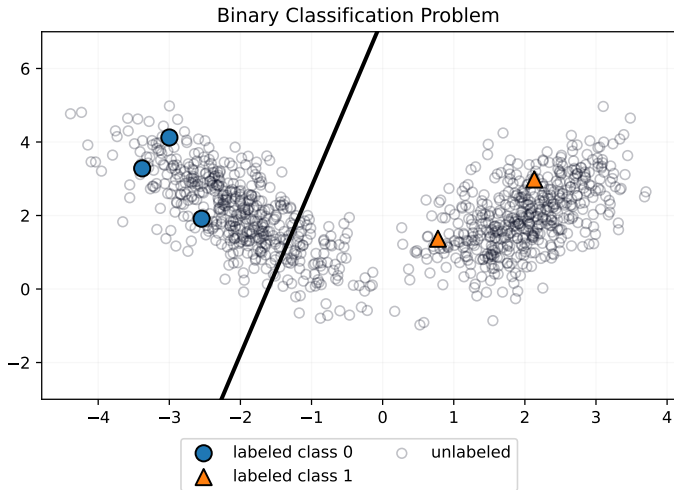


In some applications, data acquisition is cheaper than labeling ...





... and supervised learning is inefficient.

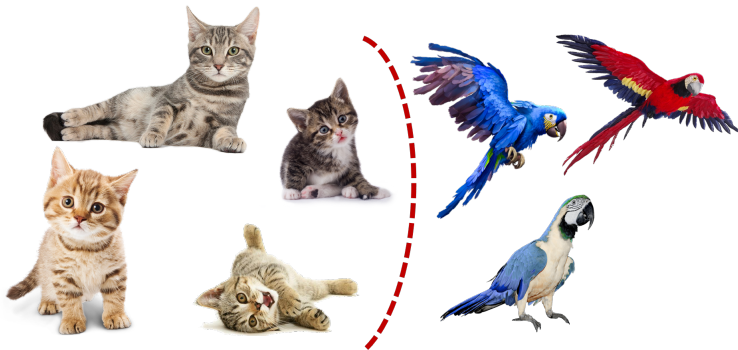




SSL → learn from a few labeled and many unlabeled examples.



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- ★ Pseudo-labeling (Amini et al., 2023):
 - Unlabeled regularization (Feofanov et al., 2023)
 - Self-training (Feofanov et al., 2019)
- ★ Graph-based algorithms (van Engelen and Hoos, 2020):
 - Label propagation
 - Label spreading
- ★ Unsupervised preprocessing (van Engelen and Hoos, 2020):
 - Cluster-then-label
 - Feature extraction: auto-encoders, PCA
 - Pre-training: self-supervised learning, stacked auto-encoders



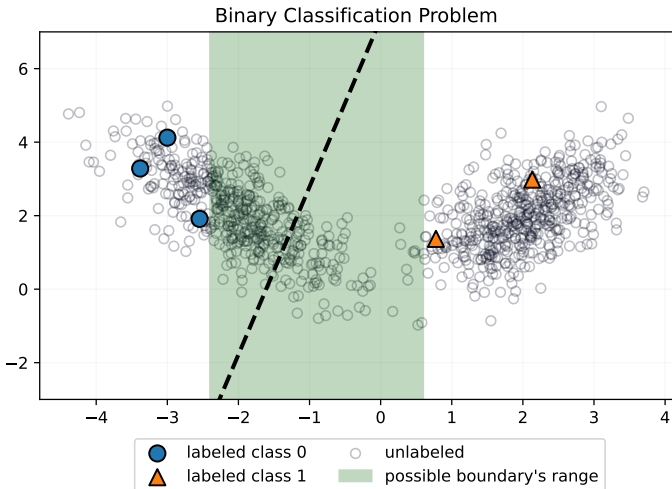
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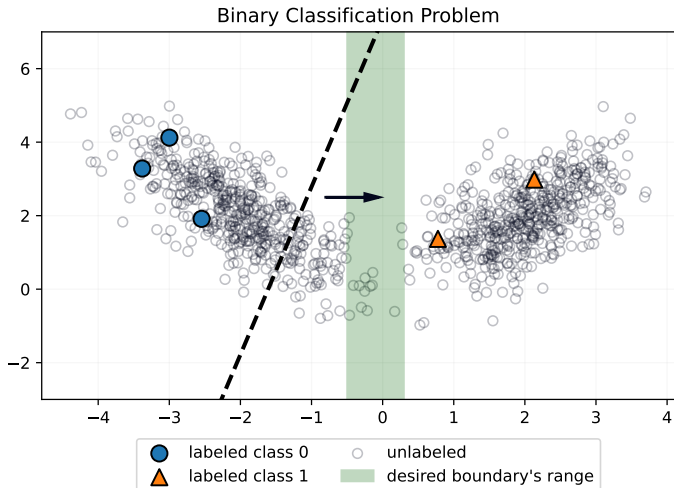


Range of possible supervised classifiers is vast: we need to make assumptions.





Low Density Separation (LDS) assumption: push boundary away from regions of unlabeled data.

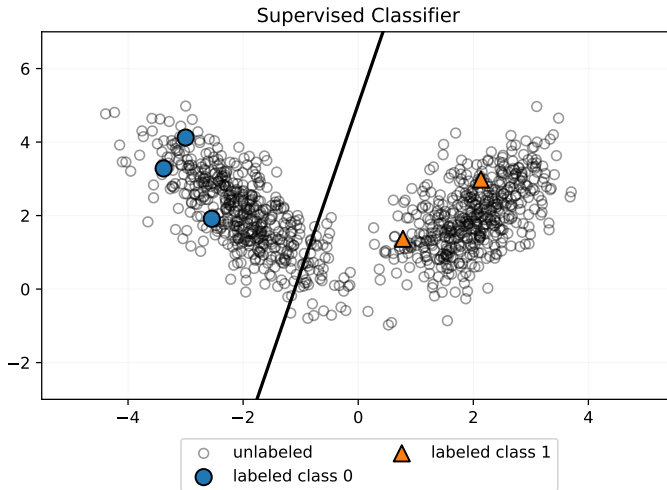




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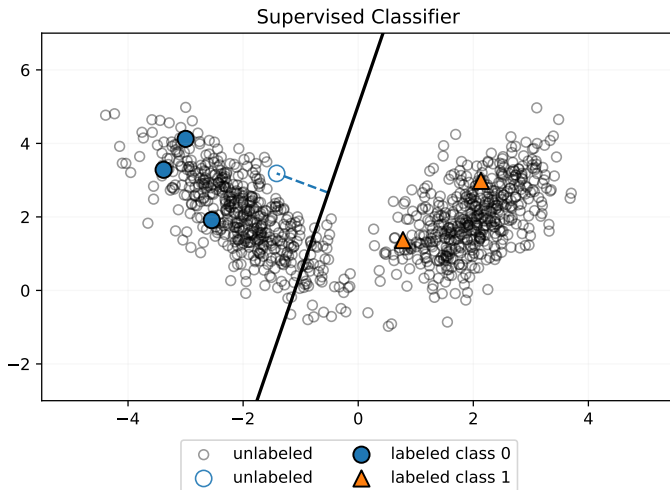


Start from a supervised classifier trained on the labeled set.



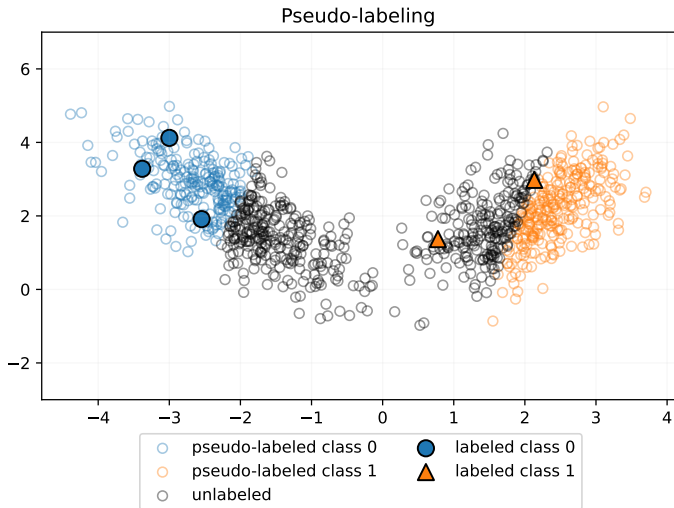


Predict labels and confidence scores for unlabeled data.





Pseudo-label most confident data and include in the labeled set.





Retrain the model and repeat the same procedure again.





And again...

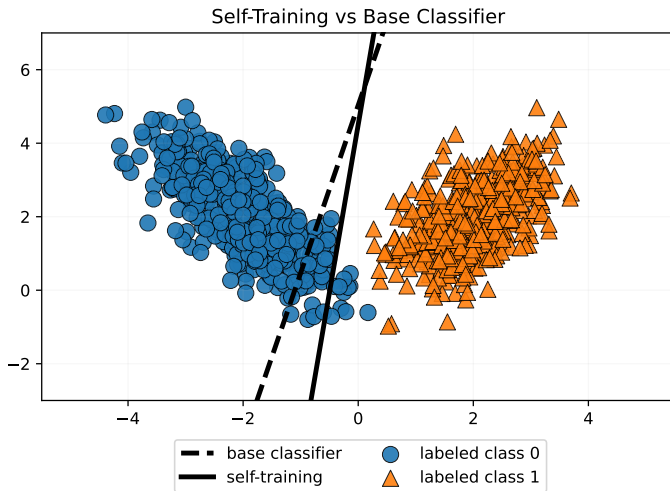




Until there are no data to pseudo-label.



Self-training pushed the boundary away from the confident data.





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★ *Confidence Estimation* → How to rank unlabeled data?



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- ★ *Pseudo-Labeling Policy* → How to select unlabeled data for pseudo-labeling at each iteration?

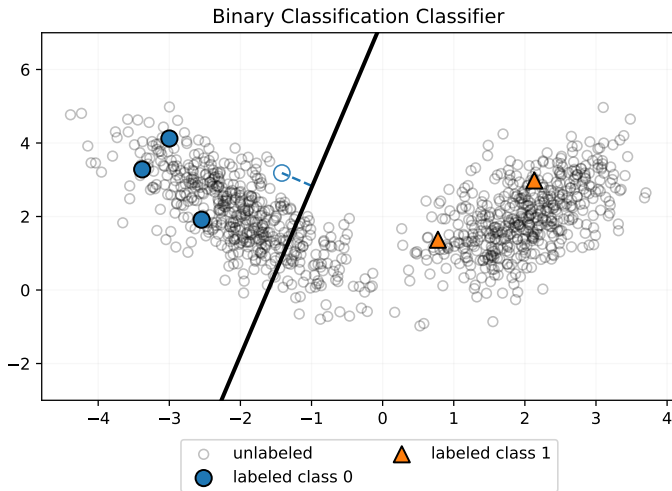


- ★ *Confidence Estimation* → How to rank unlabeled data?
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In this work, we focus on *Confidence Estimation*.

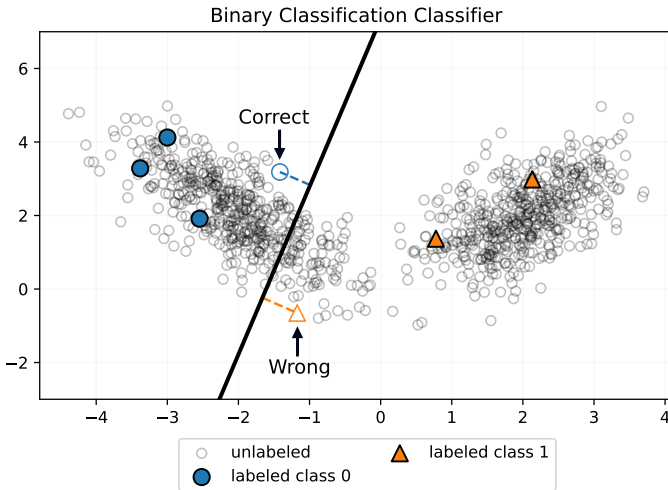


Requirements → trust the classifier's predictions.



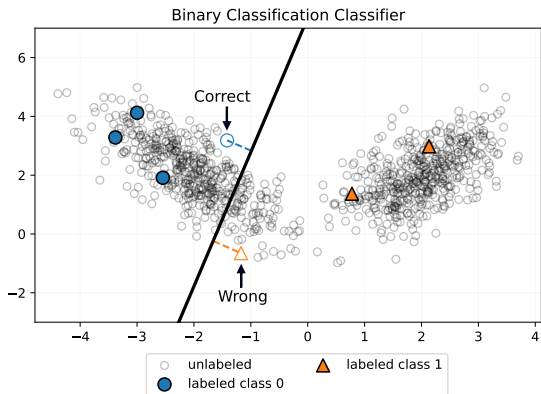


Problem → not safe since the prediction can be wrong.





Biased prediction confidence \Rightarrow wrong direction can be chosen.
 \rightarrow This can occur when there is a distribution shift in the data.





- ★ SSL assumption: labeled and unlabeled data are i.i.d.
- ★ Confidence can be biased when this assumption does not hold



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- ★ **Sample Selection Bias (SSB)**: data labeling subject to constraints
 - Creation of group study in clinical trials;
 - People with poor mobility less likely to be in street surveys;
 - Labeling can be constrained for privacy reasons.

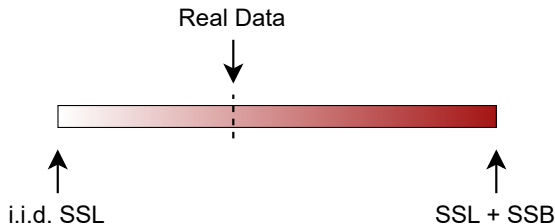


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 - Creation of group study in clinical trials;
 - People with poor mobility less likely to be in street surveys;
 - Labeling can be constrained for privacy reasons.
- ★ SSB has been studied but not in the case of SSL.



SSL + SSB combines SSL and Sample Selection Bias (SSB):

- 1 Few labeled examples (SSL)
- 2 Biased labeling procedure (SSB)



Goal → obtain a method good on **both** i.i.d. SSL and SSL + SSB.



Select the labeled set to violate the i.i.d. assumption.

- Binary selection variable s_i for each \mathbf{x}_i ;
- $s_i = 1$ if \mathbf{x}_i is labeled, $s_i = 0$ otherwise;
- Model $\mathbb{P}(s_i = 1 | \mathbf{x}_i, y_i)$ to violate i.i.d. assumption.



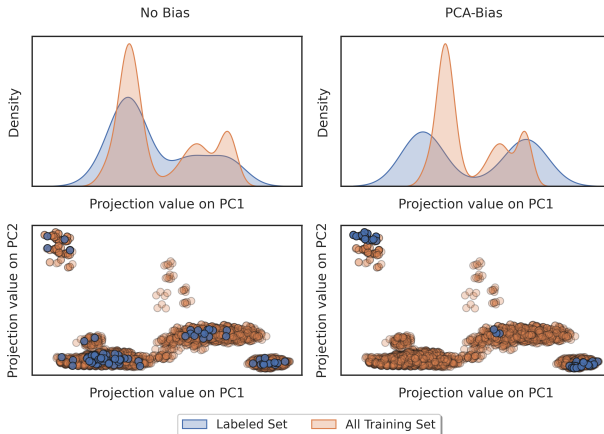
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PCA-Bias \rightarrow for each class c ,

- 1 Apply PCA on training data of class c ;
- 2 Compute $\text{proj}_1(\mathbf{x}_i)$, projection value on PC1;
- 3 $\mathbb{P}(s_i = 1 | \mathbf{x}_i, y_i = c) \propto \exp(r \cdot |\text{proj}_1(\mathbf{x}_i)|)$, $r > 0$.



Select the labeled set to violate the i.i.d. assumption.





- ★ ERM corresponds to supervised learning on the labeled set
- ★ $PL_{\theta=0.8}$ uses a fixed threshold $\theta = 0.8$ (Lee, 2013)
- ★ $CSTA_{\Delta=0.4}$ takes $\Delta\%$ most confident (Cascante-Bonilla et al., 2020)
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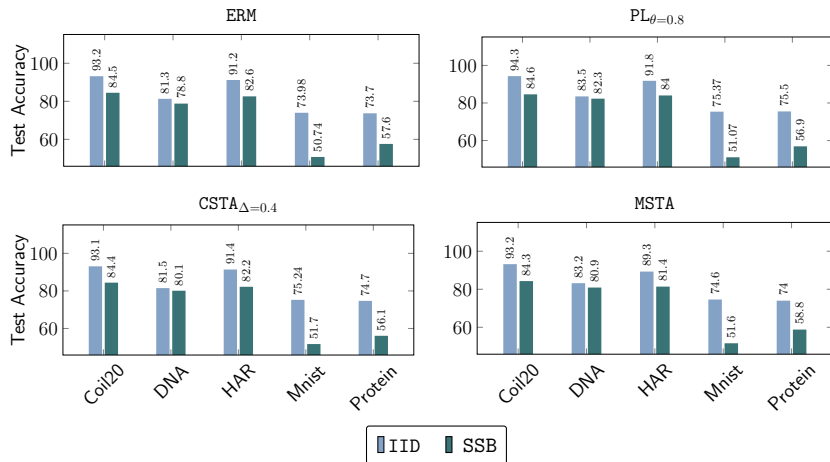


Figure: Test accuracies of the different baselines on 5 datasets. Full results to be found [here](#).



LOO over-optimistic w.r.t. generalization performance (Figure 1).

- Leave one labeled point out;
- Train on the remaining $n_\ell - 1$;
- Test on the one left out;
- Repeat for each labeled point.

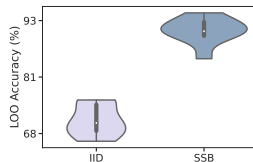


Figure: LOO on Mnist.

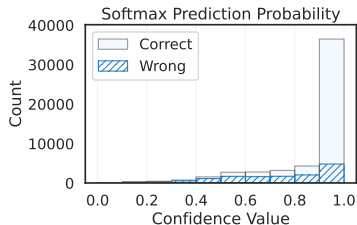


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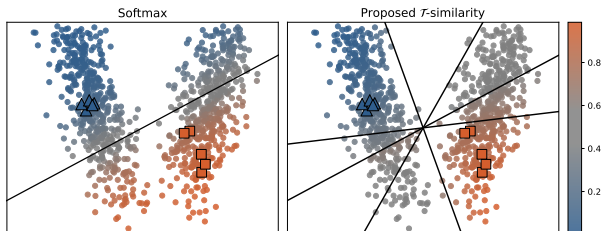


softmax-based confidence measure is unreliable in SSL + SSB.

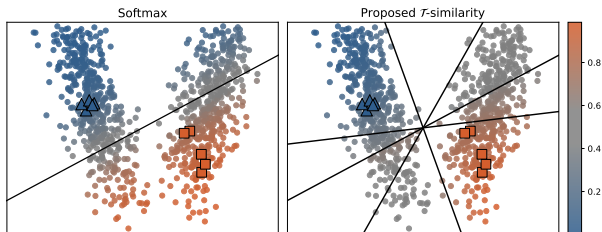
- NNs are overconfident;
- softmax predictions biased towards the labeled set.



→ We propose a novel confidence measure for NNs.



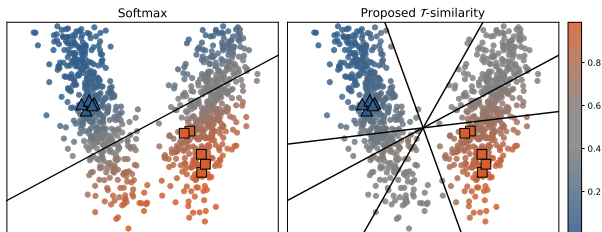
$$\min_{\mathcal{T}} \frac{1}{M} \sum_{h \in \mathcal{T}} \underbrace{\left(\frac{1}{n_{\ell}} \sum_{(\mathbf{x}, y) \in \mathbf{X}_{\ell} \times \mathbf{Y}_{\ell}} \ell(h(\mathbf{x}), y) \right)}_{\text{supervised loss}} + \underbrace{\frac{\gamma}{n_u M(M-1)} \sum_{h \neq \tilde{h} \in \mathcal{T}} \sum_{\mathbf{x} \in \mathbf{X}_u} h(\mathbf{x})^{\top} \tilde{h}(\mathbf{x})}_{\text{agreement loss}}$$



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We jointly train the ensemble to

- ① Fit very well the labeled data
- ② Disagree as much as possible on unlabeled data



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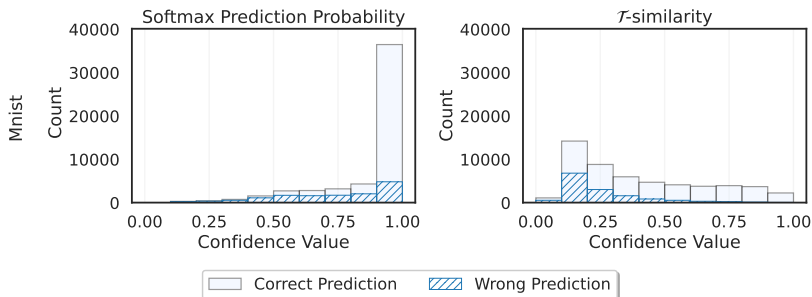
- ① Fit very well the labeled data
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- ★ We define the \mathcal{T} -similarity as:

$$s_{\mathcal{T}}(\mathbf{x}) = \frac{1}{M(M-1)} \sum_{h \neq \tilde{h} \in \mathcal{T}} h(\mathbf{x})^{\top} \tilde{h}(\mathbf{x}).$$

- ★ For any \mathbf{x} , we have $0 \leq s_{\mathcal{T}}(\mathbf{x}) \leq 1$.





- 1 Projection layers are learned through a classification head;
- 2 Confidence estimator is ensemble of $M = 5$ linear heads that don't affect representation.

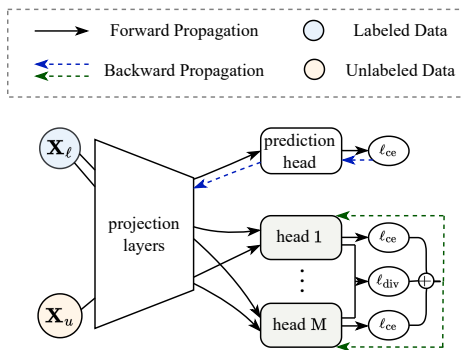


Figure: Architecture of the model.



- Fixed representation of dimension d , binary linear classification
- Linear ensemble $\mathbf{W} = \{\mathbf{w}_m \in \mathbb{R}^d | 1 \leq m \leq M\}$
- Prediction of ω_m on \mathbf{x} is $\text{sign}(\omega_m^\top \mathbf{x})$

$$\begin{aligned}
 \underset{\mathbf{W} \in \mathbb{R}^{d \times M}}{\text{argmin}} \mathcal{L}(\mathbf{W}) := & \underbrace{\frac{1}{M n_\ell} \sum_{m=1}^M \sum_{i=1}^{n_\ell} \left(y_i - \omega_m^\top \mathbf{x}_i \right)^2}_{\text{label fidelity term}} + \underbrace{\frac{1}{M} \sum_{m=1}^M \lambda_m \|\omega_m\|^2}_{\text{regularization}} \\
 & + \underbrace{\frac{\gamma}{n_u M (M-1)} \sum_{m \neq k} \sum_{i=n_\ell+1}^{n_\ell+n_u} \omega_m^\top \mathbf{x}_i \omega_k^\top \mathbf{x}_i}_{\text{agreement term}},
 \end{aligned}
 \tag{P}$$

where γ controls the influence of the diversity on the learning.



- Labeled set $(\mathbf{X}_\ell, \mathbf{y}_\ell) = (\mathbf{x}_i, y_i)_{i=1}^{n_\ell}$
- Unlabeled set $\mathbf{X}_u = (\mathbf{x}_i)_{i=n_\ell+1}^{n_\ell+n_u}$
- Assumption:

$$\forall m \in \llbracket 1, M \rrbracket, \lambda_m > \frac{\gamma(M+1)}{n_u(M-1)} \lambda_{\max}(\mathbf{X}_u^\top \mathbf{X}_u) \quad (\mathbf{A})$$

Theorem (O., Feofanov, Redko)

*Under Assumption **A**, \mathcal{L} is strictly convex and coercive on $\mathbb{R}^{d \times M}$. Hence, the optimization problem **(P)** admits a unique solution \mathbf{W}^* that verifies*

$$\nabla \mathcal{L}(\mathbf{W}^*) = 0. \quad (1)$$



$$\ell_{\text{div}}(\mathbf{W}, \mathbf{X}_u) = -\frac{1}{n_u M(M-1)} \sum_{m \neq k} \boldsymbol{\omega}_m^\top \mathbf{X}_u^\top \mathbf{X}_u \boldsymbol{\omega}_k.$$

Theorem (O., Feofanov, Redko)

$$\begin{aligned} \gamma \ell_{\text{div}}(\mathbf{W}^*, \mathbf{X}_u) &\geq \frac{1}{2n_\ell M} \sum_{m=1}^M \|\mathbf{y}_\ell - \mathbf{X}_\ell \boldsymbol{\omega}_m^*\|_2^2 \\ &\quad + \frac{1}{2M} \sum_{m=1}^M (\boldsymbol{\omega}_m^*)^\top \left(\lambda_m \mathbf{I}_d + \frac{\mathbf{X}_\ell^\top \mathbf{X}_\ell}{n_\ell} \right) \boldsymbol{\omega}_m^*. \end{aligned}$$

- 1 Trade-off between supervised performance and margin term
- 2 Assuming orthogonality, the predictors $\boldsymbol{\omega}_m$ span the M directions of largest variance of the labeled data.



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Theorem (O., Feofanov, Redko)

$$\gamma \ell_{\text{div}}(\mathbf{W}^*, \mathbf{X}_u) \geq \frac{1}{2M} \left(\lambda + \frac{1}{n_\ell} \lambda_{\min}(\mathbf{X}_\ell^\top \mathbf{X}_\ell) \right) \|\mathbf{W}^*\|_{\text{F}}^2.$$

- 1 Direction of smallest variance is also important for diversity
- 2 Theorem shows the importance of representation learning



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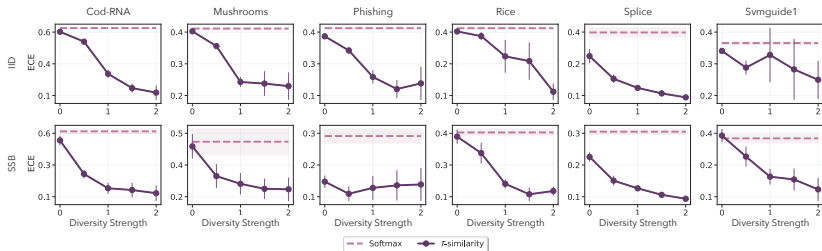


Figure: Increasing the diversity improves the classifier's calibration



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Dataset	ERM	PL $\theta=0.8$		CSTA $\Delta=0.4$		MSTA	
		softmax	\mathcal{T} -similarity	softmax	\mathcal{T} -similarity	softmax	\mathcal{T} -similarity
Cod-RNA	74.51 \pm 8.86	74.75 \pm 8.14	80.06 \pm 3.55	73.39 \pm 7.36	78.39 \pm 4.66	75.28 \pm 8.79	76.88 \pm 7.67
COIL-20	84.54 \pm 2.19	84.69 \pm 3.56	84.57 \pm 2.85	84.38 \pm 3.05	84.57 \pm 3.16	84.32 \pm 2.34	84.07 \pm 2.85
Digits	75.68 \pm 4.59	80.47 \pm 3.8	78.2 \pm 3.34	78.4 \pm 3.28	79.14 \pm 3.5	78.02 \pm 5.15	79.8 \pm 5.92
DNA	78.82 \pm 2.31	80.29 \pm 2.24	79.06 \pm 2.31	80.12 \pm 2.08	80.76 \pm 2.24	80.89 \pm 2.64	84.09 \pm 1.7
DryBean	64.6 \pm 3.89	65.6 \pm 4.18	61.55 \pm 4.91	64.91 \pm 3.72	64.6 \pm 3.53	66.24 \pm 4.31	67.0 \pm 3.96
HAR	82.57 \pm 1.96	82.87 \pm 3.02	83.12 \pm 2.27	82.19 \pm 2.61	83.53 \pm 3.77	81.35 \pm 2.54	81.16 \pm 1.63
Mnist	50.74 \pm 2.25	51.08 \pm 2.55	52.69 \pm 2.42	51.7 \pm 3.52	54.26 \pm 1.82	51.6 \pm 2.58	54.18 \pm 2.34
Mushrooms	69.45 \pm 7.29	59.53 \pm 10.46	71.36 \pm 6.63	62.98 \pm 7.25	77.55 \pm 7.65	72.16 \pm 7.59	76.16 \pm 13.04
Phishing	67.42 \pm 3.55	66.08 \pm 5.66	77.41 \pm 3.93	66.88 \pm 5.64	76.17 \pm 8.58	69.48 \pm 4.37	75.83 \pm 7.52
Protein	57.57 \pm 6.33	57.45 \pm 6.36	57.61 \pm 6.23	56.09 \pm 5.61	57.74 \pm 7.8	58.81 \pm 6.54	59.88 \pm 6.29
Rice	79.19 \pm 5.12	80.54 \pm 4.31	81.1 \pm 4.28	79.88 \pm 4.48	81.56 \pm 3.61	80.35 \pm 4.89	82.63 \pm 5.63
Splice	66.13 \pm 4.47	67.14 \pm 2.62	67.45 \pm 2.53	67.28 \pm 2.07	68.05 \pm 2.17	66.08 \pm 4.98	66.32 \pm 4.73
Svmguide1	70.89 \pm 10.98	70.35 \pm 11.74	81.07 \pm 5.39	69.84 \pm 11.06	74.46 \pm 7.23	71.04 \pm 11.11	73.13 \pm 8.82

★ \mathcal{T} -similarity is better overall;



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- ★ \mathcal{T} -similarity is better overall;
- ★ **Mushrooms** and **Phishing** \rightarrow from degradation to improvement;



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Digits	75.68 \pm 4.59	80.47 \pm 3.8	78.2 \pm 3.34	78.4 \pm 3.28	79.14 \pm 3.5	78.02 \pm 5.15	79.8 \pm 5.92
DNA	78.82 \pm 2.31	80.29 \pm 2.24	79.06 \pm 2.31	80.12 \pm 2.08	80.76 \pm 2.24	80.89 \pm 2.64	84.09 \pm 1.7
DryBean	64.6 \pm 3.89	65.6 \pm 4.18	61.55 \pm 4.91	64.91 \pm 3.72	64.6 \pm 3.53	66.24 \pm 4.31	67.0 \pm 3.96
HAR	82.57 \pm 1.96	82.87 \pm 3.02	83.12 \pm 2.27	82.19 \pm 2.61	83.53 \pm 3.77	81.35 \pm 2.54	81.16 \pm 1.63
Mnist	50.74 \pm 2.25	51.08 \pm 2.55	52.69 \pm 2.42	51.7 \pm 3.52	54.26 \pm 1.82	51.6 \pm 2.58	54.18 \pm 2.34
Mushrooms	69.45 \pm 7.29	59.53 \pm 10.46	71.36 \pm 6.63	62.98 \pm 7.25	77.55 \pm 7.65	72.16 \pm 7.59	76.16 \pm 13.04
Phishing	67.42 \pm 3.55	66.08 \pm 5.66	77.41 \pm 3.93	66.88 \pm 5.64	76.17 \pm 8.58	69.48 \pm 4.37	75.83 \pm 7.52
Protein	57.57 \pm 6.33	57.45 \pm 6.36	57.61 \pm 6.23	56.09 \pm 5.61	57.74 \pm 7.8	58.81 \pm 6.54	59.88 \pm 6.29
Rice	79.19 \pm 5.12	80.54 \pm 4.31	81.1 \pm 4.28	79.88 \pm 4.48	81.56 \pm 3.61	80.35 \pm 4.89	82.63 \pm 5.63
Splice	66.13 \pm 4.47	67.14 \pm 2.62	67.45 \pm 2.53	67.28 \pm 2.07	68.05 \pm 2.17	66.08 \pm 4.98	66.32 \pm 4.73
Svmguide1	70.89 \pm 10.98	70.35 \pm 11.74	81.07 \pm 5.39	69.84 \pm 11.06	74.46 \pm 7.23	71.04 \pm 11.11	73.13 \pm 8.82

- ★ \mathcal{T} -similarity is better overall;
- ★ **Mushrooms** and **Phishing** \rightarrow from degradation to improvement.
- ★ Results in i.i.d. SSL: no significant improvement nor degradation.



- ① Introduction
- ② Failure of Self-Training
- ③ Learning with the \mathcal{T} -similarity
- ④ Numerical Experiments
- ⑤ Discussion



- ★ Practical and principled framework to study SSL + SSB;
- ★ Calibrated confidence measure;
- ★ \mathcal{T} -similarity good both in i.i.d. SSL and SSL + SSB.

Future work → use \mathcal{T} -similarity for iterative self-training, domain adaptation, or uncertainty modeling.



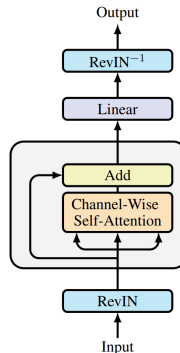
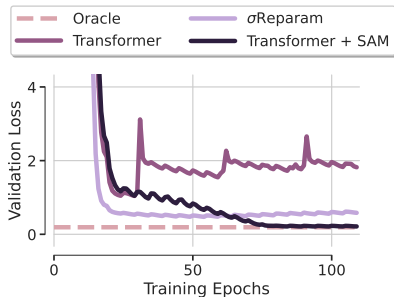
This work has been accepted to AISTATS 2024, Valencia, Spain. You may find the links to the paper and the code below. to know more about my research, see my website: ambroiseodt.github.io and feel free to contact me.

- ★ Paper: <https://arxiv.org/abs/2310.14814>
- ★ Code: <https://github.com/ambroiseodt/tsim>



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SAMformer: Unlocking the Potential of Transformers in Time Series Forecasting - Oral ICML 2024



★ Paper: <https://arxiv.org/pdf/2402.10198>

★ Code: <https://github.com/romilbert/samformer>

Thanks for your attention !



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Dataset	Size	# of lab. examples n_ℓ	Dimension d	# classes C
Cod-RNA	59535	99	8	2
COIL-20	1440	200	1024	20
Digits	1797	99	64	10
DNA	3186	149	180	6
DryBean	13543	104	16	7
HAR	10299	299	561	3
Mnist	70000	100	784	10
Mushrooms	8124	79	112	2
Phishing	11055	99	68	2
Protein	1080	80	77	8
Rice	3810	29	7	2
Splice	3175	39	20	2
Svgmguide1	3089	39	4	2

Table: Characteristics of datasets used in our experiments