MaNo: Exploiting Matrix Norm for Unsupervised Accuracy Estimation

Ambroise Odonnat
Noah's Ark Lab, Inria
Université Rennes 2, CNRS, IRISA

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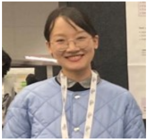
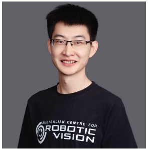
Co-authors

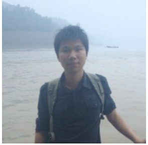


Renchunzi Xie
NTU

Vasilii Feofanov
Noah's Ark Lab



Weijian Deng
ANU



Jianfeng Zhang
Noah's Ark Lab

Bo An
NTU

Outline

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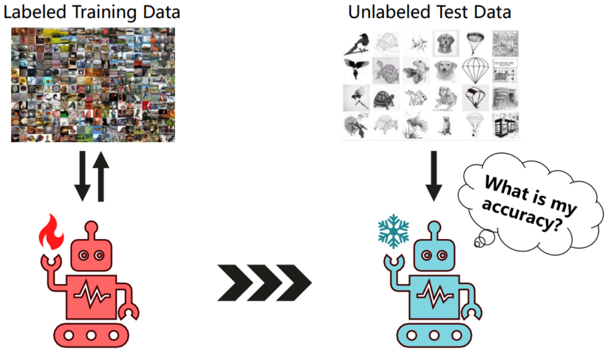
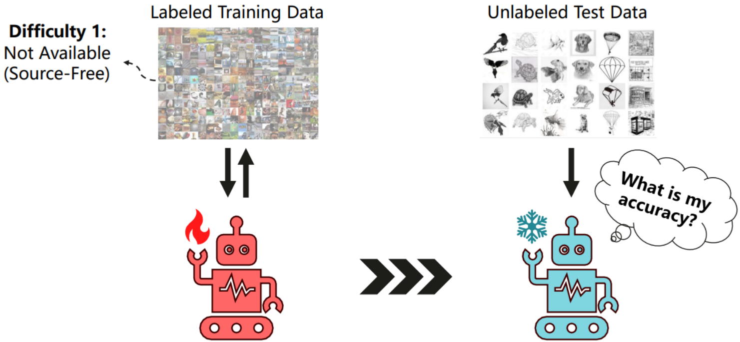
Goal: Predict accuracy of pre-trained model f on test set $\mathcal{D}_{\text{test}}$.



Unsupervised Accuracy Estimation

Goal: Predict accuracy of pre-trained model f on test set $\mathcal{D}_{\text{test}}$.



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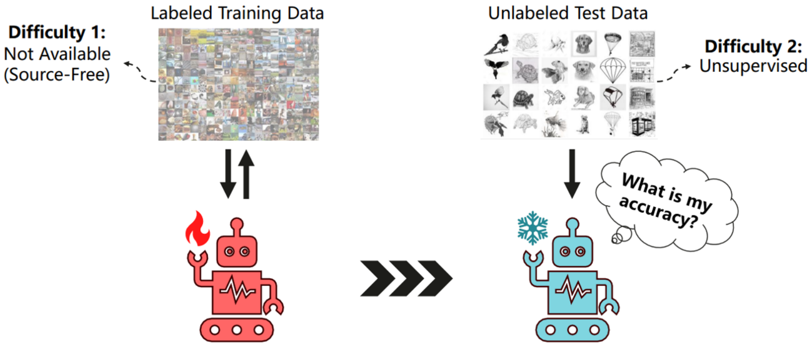
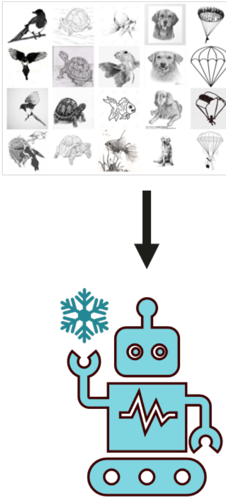


→ **Challenging task often occurring in real-world scenarios.**

Logits-based Methods

Unlabeled Test Data



Logits-based Methods

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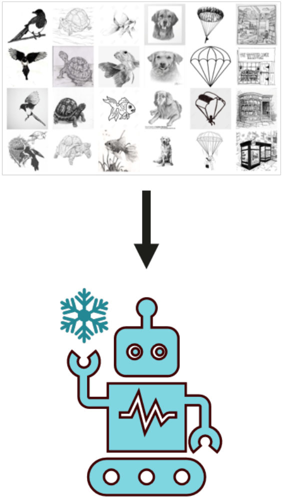

✓ Model's outputs: logits

$$\text{logits: } \mathbf{q}_i = (\mathbf{w}_1^\top \phi(\mathbf{x}_i), \ldots, \mathbf{w}_K^\top \phi(\mathbf{x}_i)),$$

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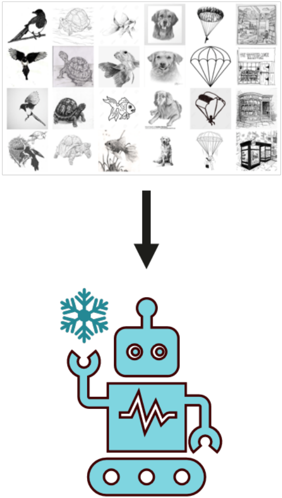

- ✓ Model's outputs: logits
- ✓ Different range → normalize

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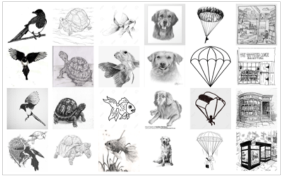

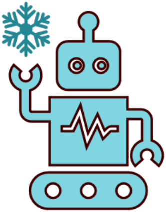

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- ✓ Fill prediction matrix $\mathbf{Q}$

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Logits-based Methods

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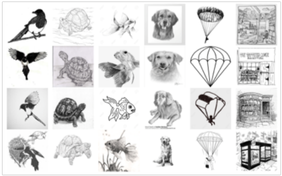

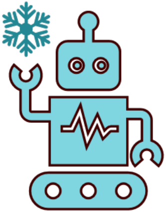

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- ✓ Different range $\rightarrow$ normalize
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- ✓ Compute estimation score

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Research Questions

Question 1: *What explains the correlation between logits and generalization performance?*

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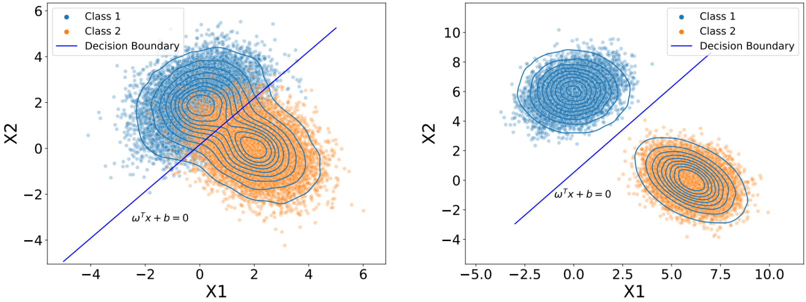
Question 2: *How to alleviate the overconfidence issues of logits-based methods?*

Outline

Low-Density Separation Assumption

LDS assumption: classifier makes mistakes in high-density regions.



(a) High-density region (b) Low-density region.

$\rightarrow$ **Misclassified samples are closer to decision boundaries.**

Logits Reflect Distances to Decision Boundaries

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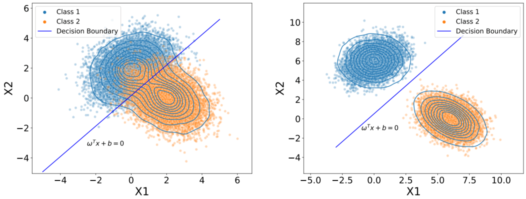

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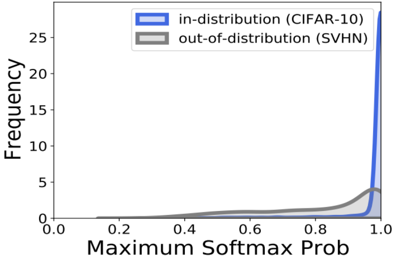
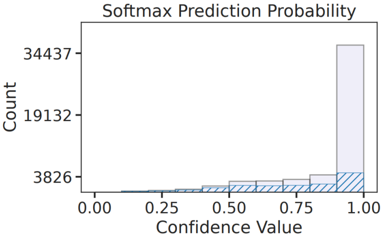
Logits capture the generalization performance.

Softmax Overconfidence



Wei et al.



Odonnat et al.

→ **Overconfidence and saturation of softmax outputs.**

Prediction Error Accumulation

Logits can be decomposed as follows

$$\underbrace{\mathbf{q}}_{\text{model's logits}} = \underbrace{\mathbf{q}^*}_{\text{ground-truth logits}} + \underbrace{\varepsilon}_{\text{prediction bias}} .$$

Then, the softmax involves computing

$$\exp(\mathbf{q}_{i,k}) = \exp(\mathbf{q}^*_{i,k} + \varepsilon_k) = 1 + (\mathbf{q}^*_{i,k} + \varepsilon_k) + \frac{(\mathbf{q}^*_{i,k} + \varepsilon_k)^2}{2!} + ...$$

Solution: Truncating the Errors

$$\exp(\mathbf{q}_{i,k}) \approx 1 + (\mathbf{q}^*_{i,k} + \varepsilon_k) + \frac{(\mathbf{q}^*_{i,k} + \varepsilon_k)^2}{2!} + ... + \frac{(\mathbf{q}^*_{i,k} + \varepsilon_k)^n}{n!}.$$

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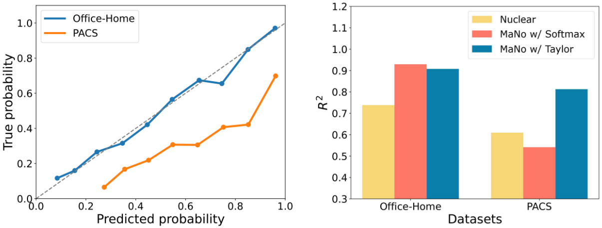

(a) Calibration curves. (b) Type of normalization.

Trade-off information completeness and error accumulation!

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MaNo: A Simple Three-Step Recipe

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- ✓ *Inference:* Recover logits $\mathbf{q}_i = f(\mathbf{x}_i)$,
- ✓ *Criterion:* $\Phi(\mathcal{D}_{\text{test}}) = \mathrm{KL}(\text{uniform}||\text{softmax proba})$

$$\mathbf{1)} \quad v(\mathbf{q}_i) = \begin{cases} 1 + \mathbf{q}_i + \frac{\mathbf{q}_i^2}{2}, & \text{if } \Phi(\mathcal{D}_{\text{test}}) \leq \eta \\ \exp(\mathbf{q}_i), & \text{if } \Phi(\mathcal{D}_{\text{test}}) > \eta \end{cases}$$

$$\mathbf{2)} \quad \sigma(\mathbf{q}_i) = \frac{v(\mathbf{q}_i)}{\sum_{k=1}^K v(\mathbf{q}_i)_k} \in \Delta_K$$

$$\mathbf{3)} \quad \mathcal{S}(f, \mathcal{D}_{\text{test}}) = \frac{1}{\sqrt[p]{NK}} \|\mathbf{Q}\|_p = \left(\frac{1}{NK} \sum_{i=1}^N \sum_{k=1}^K |\sigma(\boldsymbol{q}_i)_k|^p \right)^{\frac{1}{p}}$$

Theorem (Xie, O. et al.)

Given a test set $\mathcal{D}_{\text{test}}$ and a pre-trained model f, the estimation score $\mathcal{S}(f, \mathcal{D}_{\text{test}})$ provided by **MaNo** *is inversely proportional to the model's uncertainty.*

- ✓ Uncertain $\rightarrow$ low accuracy & high entropy $\rightarrow$ low $\mathcal{S}(f, \mathcal{D}_{\text{test}})$,
- ✓ Confident $\rightarrow$ high accuracy & low entropy $\rightarrow$ high $\mathcal{S}(f, \mathcal{D}_{\text{test}})$.

MaNo is positively correlated with the test accuracy.

Outline

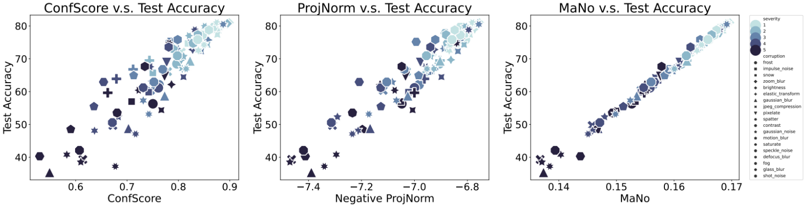
SOTA Results & Efficiency

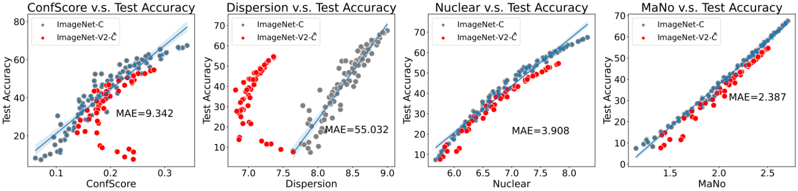
- Comparison with correlation metrics ρ and R^2,
- Comparison across architectures: ResNets, ConvNext, ViT,
- Evaluation on common benchmarks and distribution shifts.

Shift	MaNo -	COT 2024	MDE 2024	Nuclear 2023	Dispersion 2023	ProjNorm 2022
Synthetic	**0.991**	0.988	0.947	0.982	0.960	0.971
Subpopulation	**0.983**	0.962	0.920	0.973	0.909	0.897
Natural	**0.905**	0.871	0.436	0.455	0.410	0.382
Overall improvement		**2%**	**25%**	**6%**	**26%**	**28%**

MaNo outperforms all the baselines while being training-free.

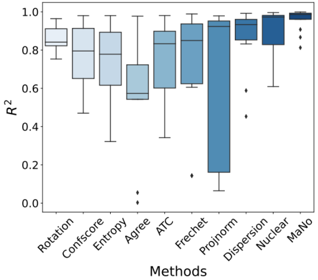
Qualitative Benefit: Linear Correlation

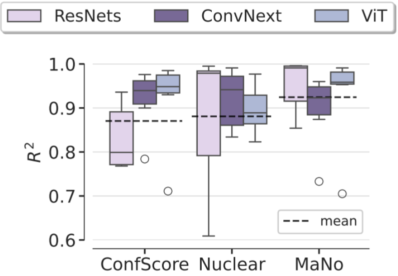




MaNo linearly correlates with the ground-truth performance.

- ✓ Experiments on all distributions shifts,
- ✓ Experiments with various architectures.





MaNo is the best approach to use with SOTA architectures!

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Take Home Message

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- ✓ Predicting accuracy under distribution shifts is challenging.
- ✓ Most methods use logits and fail under miscalibration.
- ✓ **MaNo** $\rightarrow$ theoretically grounded estimation approach.
- ✓ Benefits: **SOTA, efficient, architecture agnostic, robust**.

To Know More

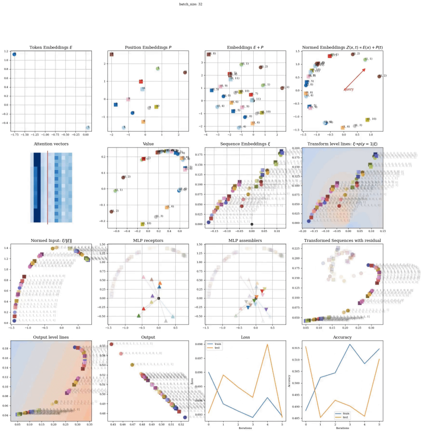
This work has been accepted at NeurIPS 2024.

Paper: https://arxiv.org/pdf/2405.18979
Code: https://github.com/Renchunzi-Xie/MaNo

To know more about my research, check out my website!

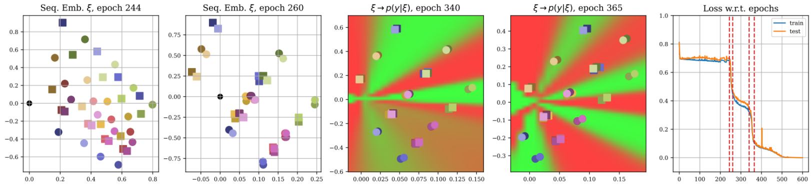
ambroiseodt.github.io

Clustering Head: A Visual Case Study of the Training Dynamics in Transformers



Self-Promotion

Using our visual sandbox, we identify **clustering heads**, circuits that learn the invariance of the sparse addition modular task and study their training dynamics.



Paper: https://arxiv.org/pdf/2410.24050
Code: https://github.com/facebookresearch/pal

Thank you for your attention!