Clustering of Unseen Datasets with Self-Supervised Encoders

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SDU

An Empirical Study into Clustering of Unseen Datasets with Self-Supervised Encoders

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http://scottclowe.com/zs-ssl-clustering/

Abstract

Can pretrained models generalize to new datasets without any retraining? We deploy pretrained image models on datasets they were not trained for, and investigate whether their embeddings form meaningful clusters. Our suite of benchmarking experiments use encoders pretrained solely on ImageNet-1k with either supervised or self-supervised training techniques, deployed on image datasets that were not seen during training, and clustered with conventional clustering algorithms. This evaluation provides new insights into the embeddings of self-supervised models, which prioritize different features to supervised models. Supervised encoders typically offer more utility than SSL encoders within the training domain, and vice-versa far outside of it, however, fine-tuned encoders demonstrate the opposite trend. Clustering provides a way to evaluate the utility of self-supervised learned representations orthogonal to existing methods such as kNN. Additionally, we find the silhouette score when measured in a UMAP-reduced space is highly correlated with clustering performance, and can therefore be used as a proxy for clustering performance on data with no ground truth labels. Our code implementation is available at https://github.com/scottclowe/zs-ssl-clustering/.

1 Introduction

Self-supervised learning (SSL) has attracted great interest in recent years across almost every machine learning sub-field, due to the promise of being able to harness large quantities of unlabelled data and obtaining generic feature embeddings useful for a variety of downstream tasks (Balestriero et al., 2023). This has, for example, led to the development of impressive large language models (Brown et al., 2020) and computer vision systems trained on 1 billion images (Goyal et al., 2021). However, while the embeddings from an SSL-trained encoder can perform well on downstream tasks after fine-tuning the network, there has been less investigation into the utility of the embeddings without fine-tuning. Prior work (Vaze et al., 2022; Zhou and Zhang, 2022) suggests SSL feature encoders generate embeddings suitable for clustering, but nonetheless adjust the feature encoders through fine-tuning. Yet, widespread interest in the application of large pretrained models on custom datasets, combined with prohibitive cost of compute, make this question important and increasingly urgent.

We find that to date there has been no investigation into whether SSL-trained feature encoders can serve as a foundation for clustering, yielding informative groupings of embeddings on real-world datasets that were totally unseen to the encoder during its training. Vaze et al. (2023) showed that features from SSL encoders are typically biased toward shape features and not color, texture, or count when clustered using K-Means. However, this was conducted using a synthetic dataset, where very specific object attributes could be disentangled. In contrast, in this work we perform a *zero-shot transfer-learning task*, evaluating the

*Joint first author. †Joint last author.

The Cost of Training Networks

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Model to Reproduce	GPU Type	GPU Power consumption	GPU-hours	PUE	Total power consumption	Carbon emitted (tCO_2eq)
DINOv2-g	A100-40GB	400W	22,016	1.1	9.7 MWh	3.7

DINOv2: Learning Robust Visual Features without Supervision, Oquab et al., 2024

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- → Not sustainable (or feasible) to retrain these models
- → How can such models be efficiently reused?

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→ But what if you don’t want to train anything or don’t have a labeled dataset?

→ Could clustering of features be a viable alternative?

Zero-Shot Clustering

The Main Idea

How well does features from (SSL)-pretrained networks cluster?

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→ We take already trained networks

→ Only fit a classical clustering method on a limited set of ”training” datasets

→ Transfer encoders and fitted clustering method to new datasets – *no adjustments made!*

Encoders

Encoders

→ We only consider networks trained on ImageNet-1K

→ Most commonly used backbones for SSL pretraining (at the time) are: ViT-B and ResNet-50

Encoders

→ Cross-Entropy Supervised

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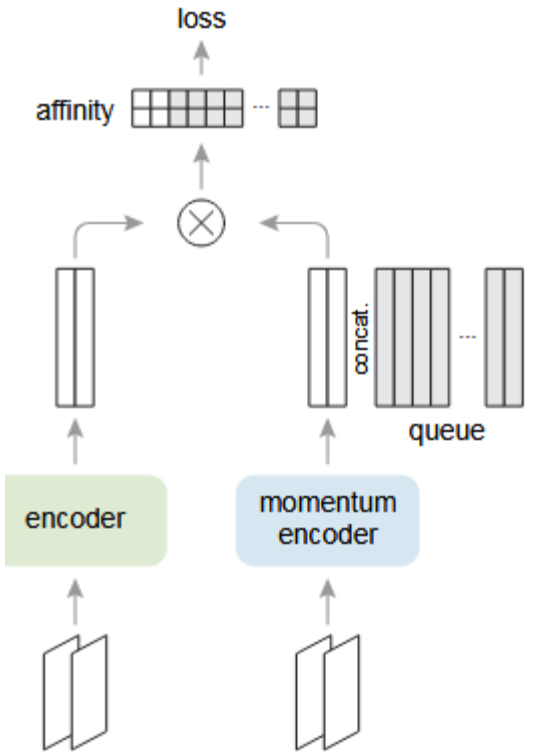
→ Contrastive Learning: MoCo-v3



Improved Baselines with Momentum Contrastive Learning, Chen et al, 2020

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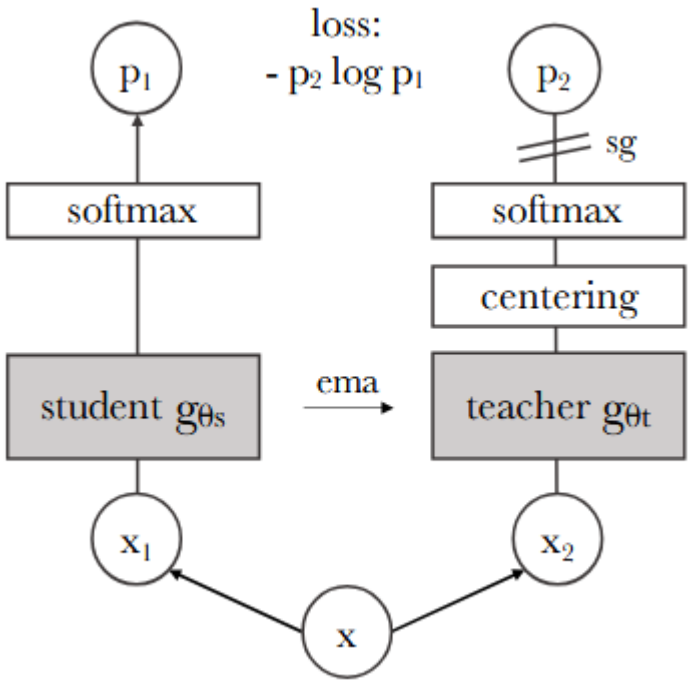
→ Self-Distillation: DINO



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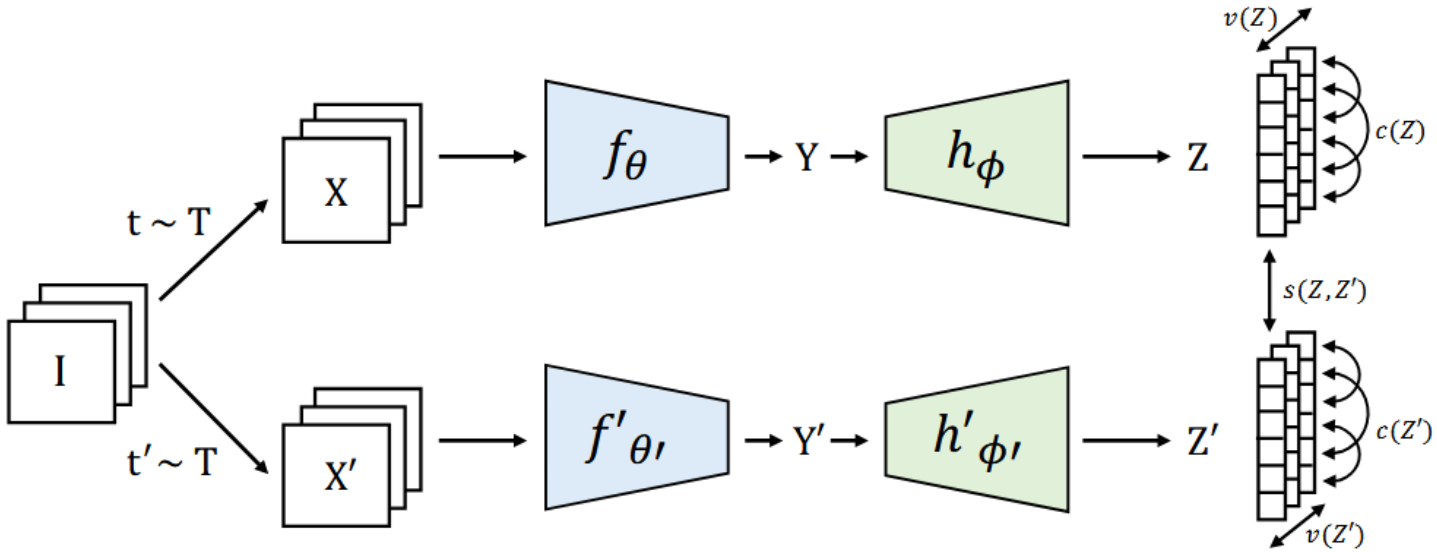

VICReg: Variance-Invariance-Covariance Regularization for Self-Supervised Learning, Bardes et al., 2022

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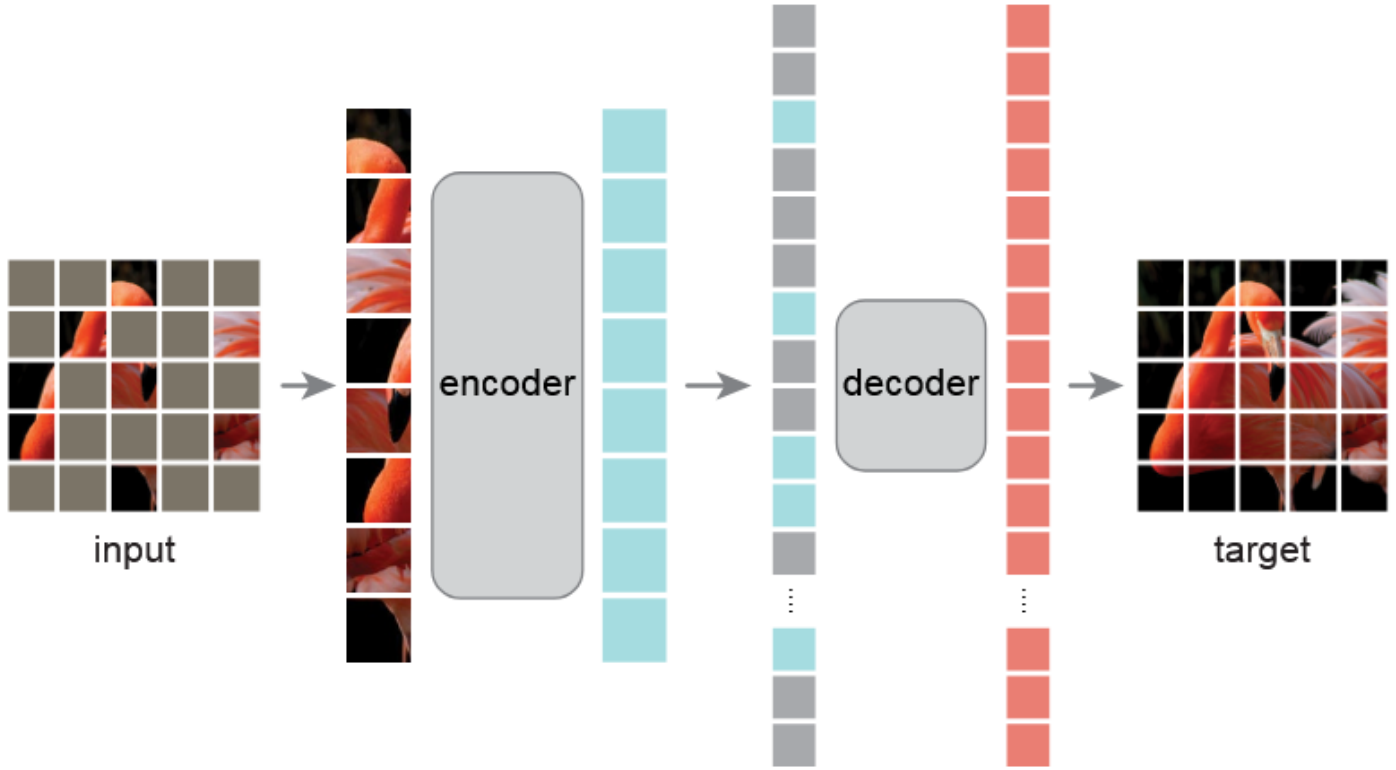
→ Masked Image Modelling: MAE



Masked Autoencoders Are Scalable Vision Learner, He et al., 2021

Clustering Methods

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→ Graph theoretical: **Affinity Propagation** (AP) & **Spectral**

→ Density-based: **HDBSCAN**

Dimensionality Reduction

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→ Principle Component Analysis (PCA)

→ Uniform Manifold Approximation and Projection (UMAP)

→ Pairwise Controlled Manifold Approximation Projection (PaCMAP)

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Entropy of Clusters

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→ However, NMI is not corrected for chance. Simply increasing number of clusters can increase NMI

→ Use Adjusted Mutual Information (AMI) instead

$$\mathrm{AMI}(U, V) = \frac{\mathrm{MI}(U, V) - \mathbb{E}[\mathrm{MI}(U, V)]}{\mathrm{mean}(\mathrm{H}(U) + \mathrm{H}(V)) - \mathbb{E}[\mathrm{MI}(U, V)]}$$

Hyperparameter Search

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→ HPs selectected over three ImageNet-based datasets

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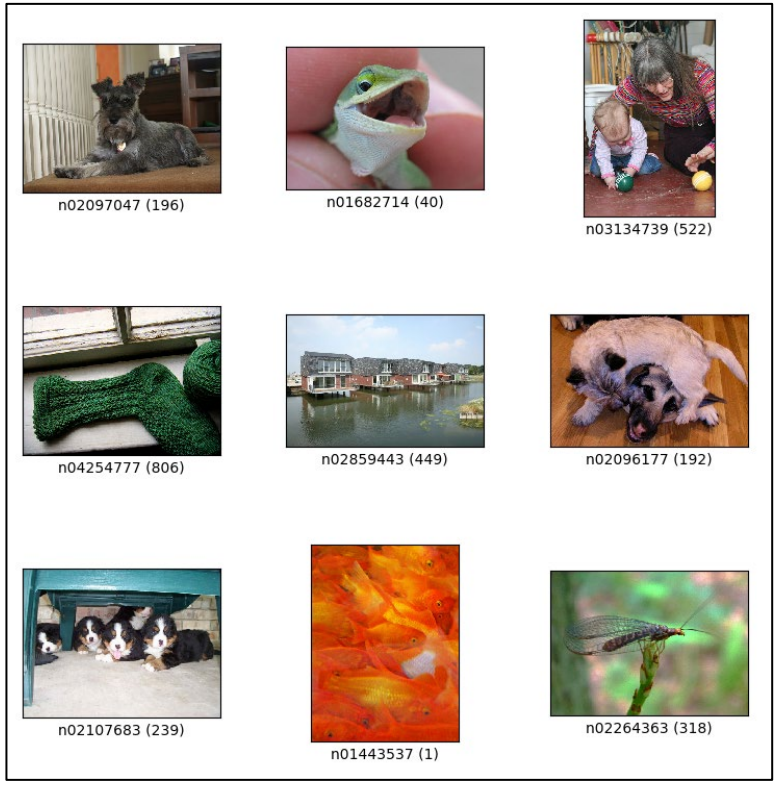
ImageNet-1K



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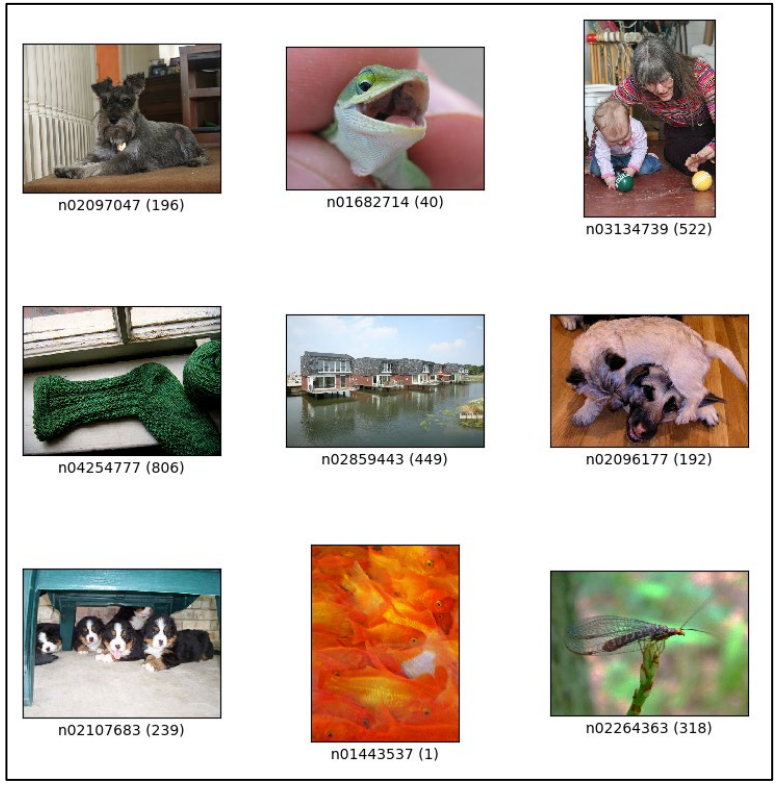
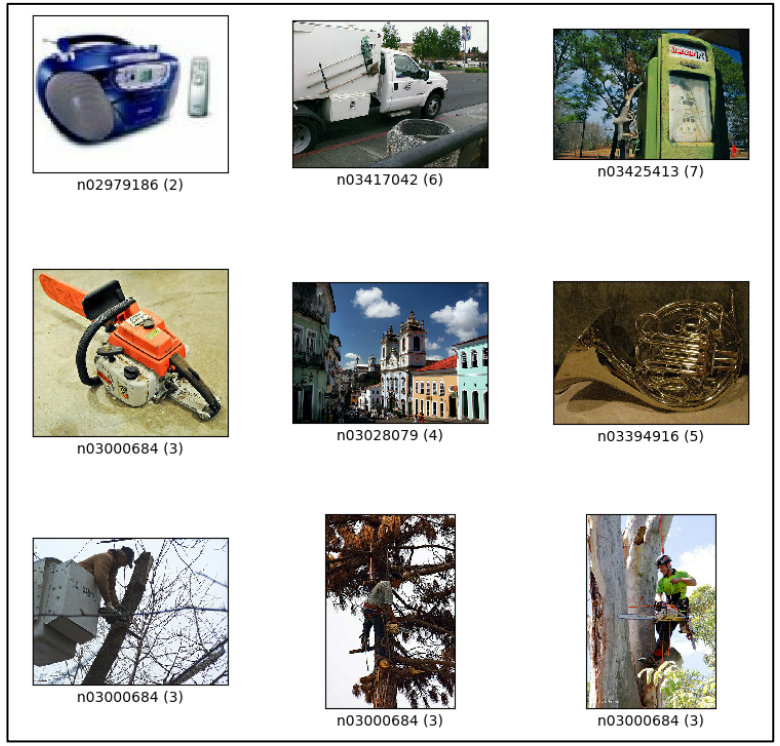


Imagenette



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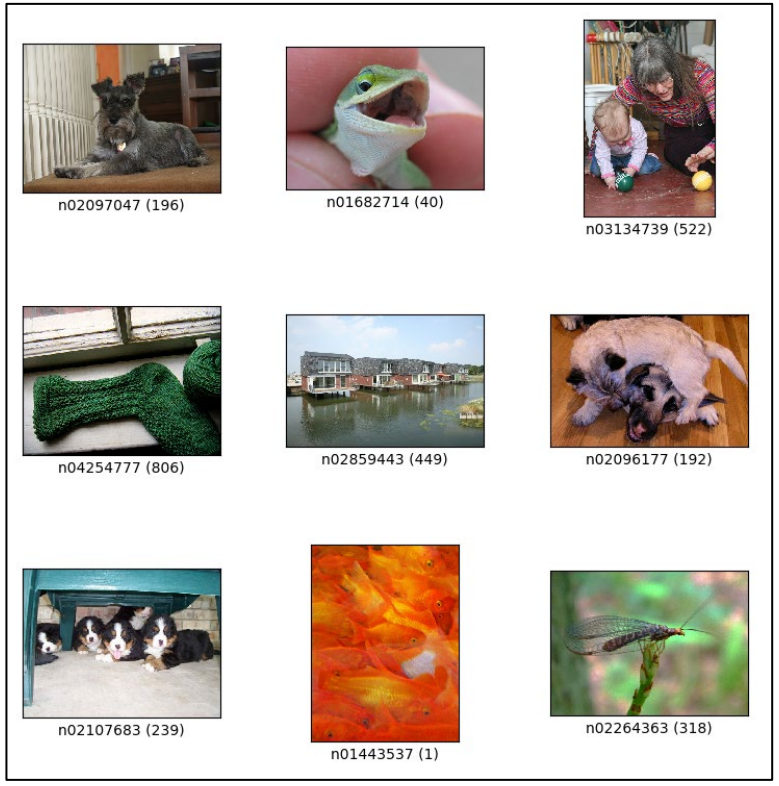

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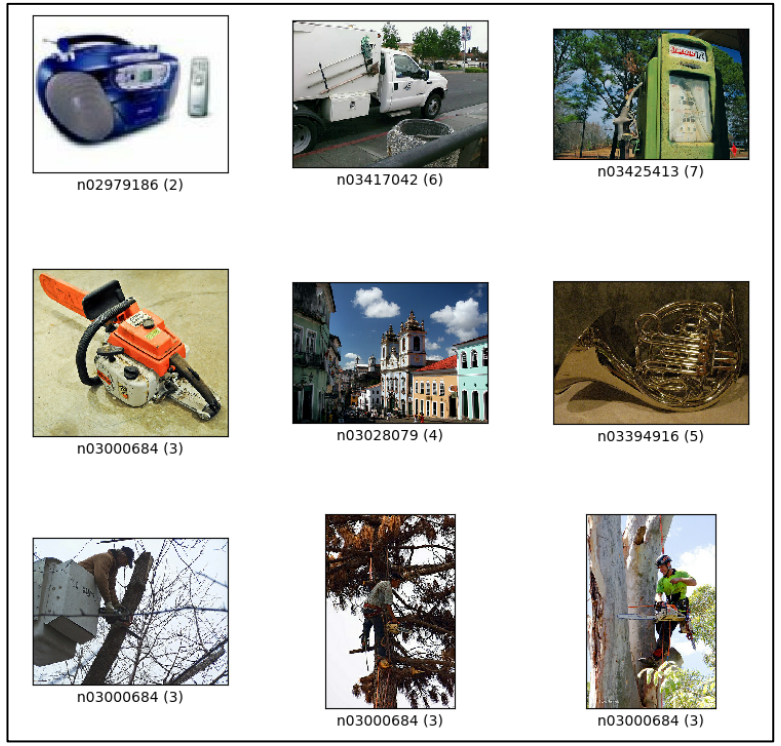

Imagewoof

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→ All clustering methods (except Spectral) performs best with UMAP
→ Reducing to 5-200 dimensions leads to equal performance

Datasets

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Type	Dataset	Reference	# Sample	# Class	ρ	Description
In-Domain	ImageNet-1k	Russakovsky et al. (2015)	50 000	1 000	1.00	Diverse general objects
	ImageNet-v2	Recht et al. (2019)	10 000	1 000	1.00	Diverse general objects
	CIFAR-10	Krizhevsky (2009)	10 000	10	1.00	Diverse general objects
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Domain-shift	ImageNet-9 FG-only	Xiao et al. (2020)	4 050	9	1.00	Isolated foregrounds
	ImageNet-9 MixRand	Xiao et al. (2020)	4 050	9	1.00	Remixed fore/background
	ImageNet-R	Hendrycks et al. (2021a)	30 000	200	8.43	Art/sculptures of objects
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Fine-grained	FGVC Aircraft	Maji et al. (2013)	3 333	100	1.03	Aircraft variants
	Stanford Cars	Krause et al. (2013)	8 041	196	2.83	Car variants
	Oxford Flowers	Nilsback and Zisserman (2008)	6 149	102	11.90	Flower variants
	NABirds	Van Horn et al. (2015)	24 633	555	6.67	Bird species
	BIOSCAN-1M	Gharaee et al. (2023)	24 799	2 688	782.50	Insect species
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Far-OOD	CelebA	Liu et al. (2015)	19 962	1 000	32.00	Human faces (identity)
	UTKFace	Zhang et al. (2017)	5 925	101	549.00	Human faces (age)
	BreakHis	Spanhol et al. (2016)	3 164	32	8.60	Tumor tissue microscopy
	DTD	Cimpoi et al. (2014)	1 880	47	1.00	Texture descriptions
	EuroSAT	Helber et al. (2019)	4 050	10	1.50	Satellite RGB images
	MNIST	LeCun et al. (1998)	10 000	10	1.27	Handwritten digits
	Fashion MNIST	Xiao et al. (2017)	10 000	10	1.00	Clothing articles
	SVHN	Netzer et al. (2011)	26 032	10	3.20	House numbers

Results

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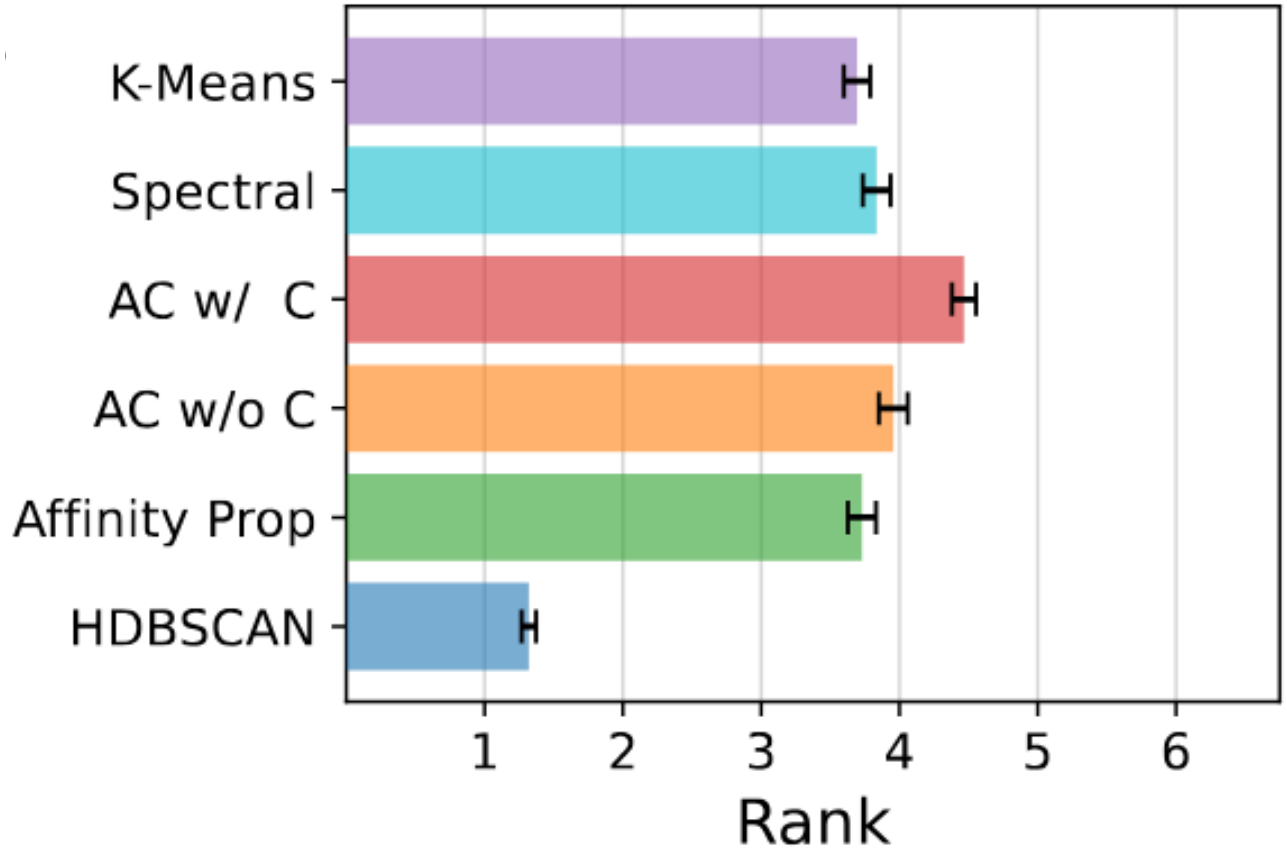

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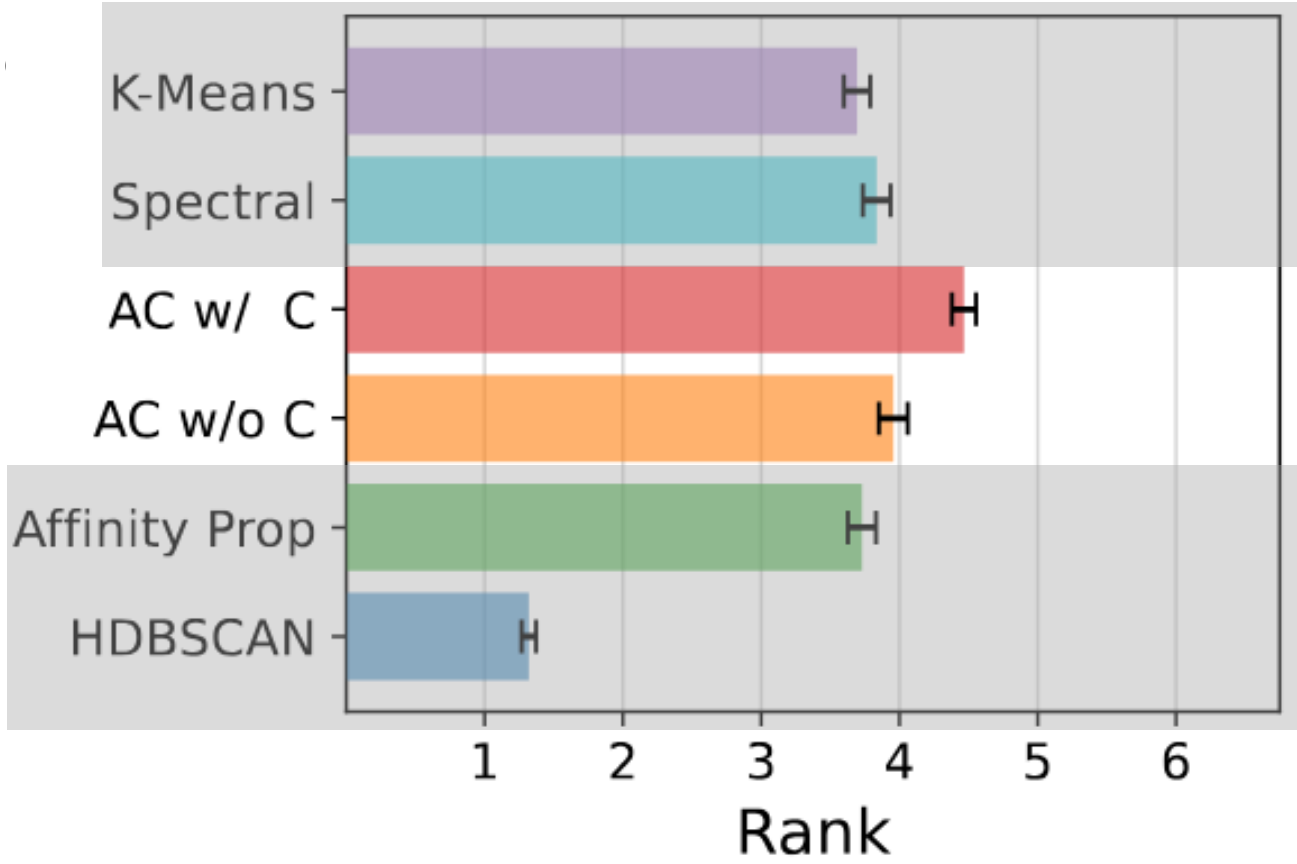

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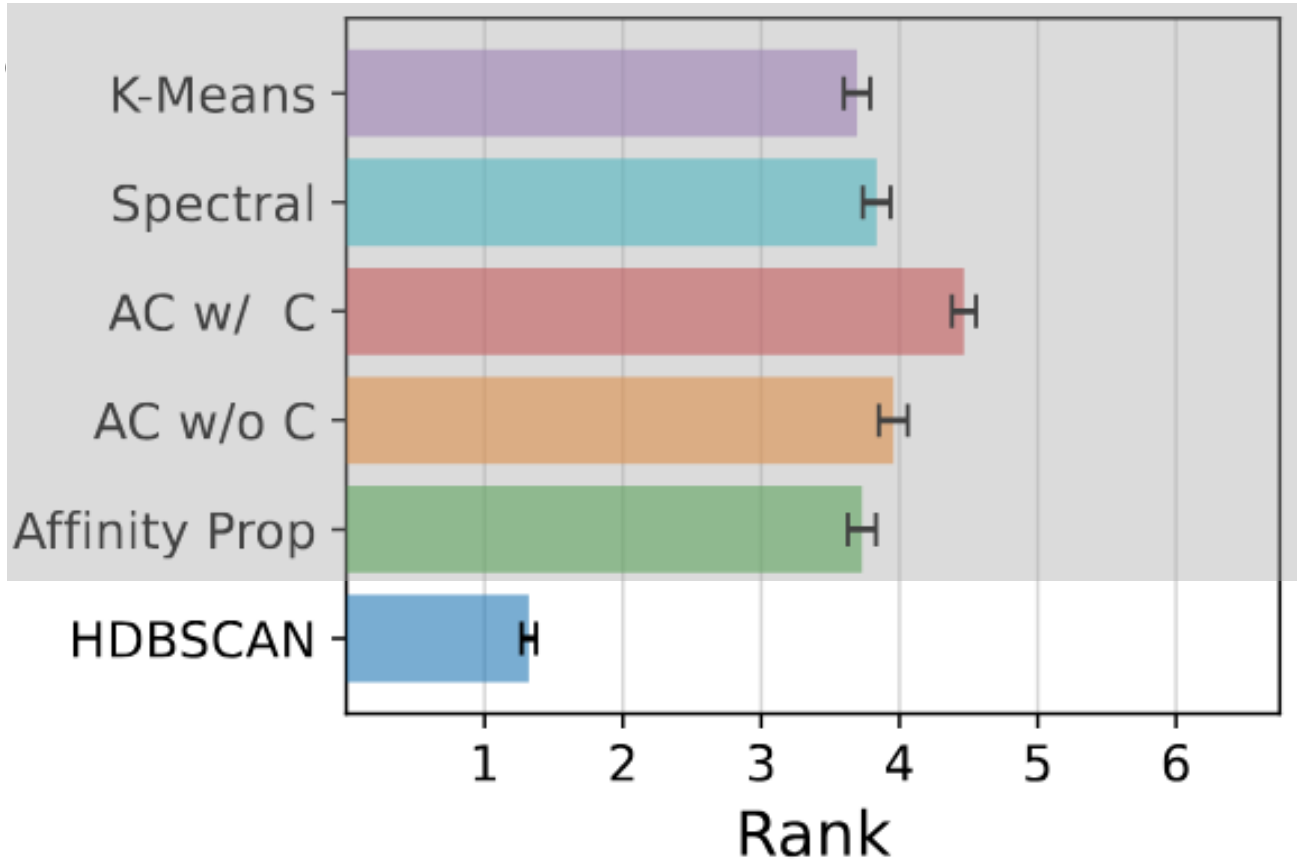

Comparing Supervised & SSL Pretrained Encoders

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→ We compare the effect of SSL pretraining to fully-supervised Cross Entropy models

→ Measuered as difference in AMI scores (Δ AMI)

SSL Pretrained Encoders

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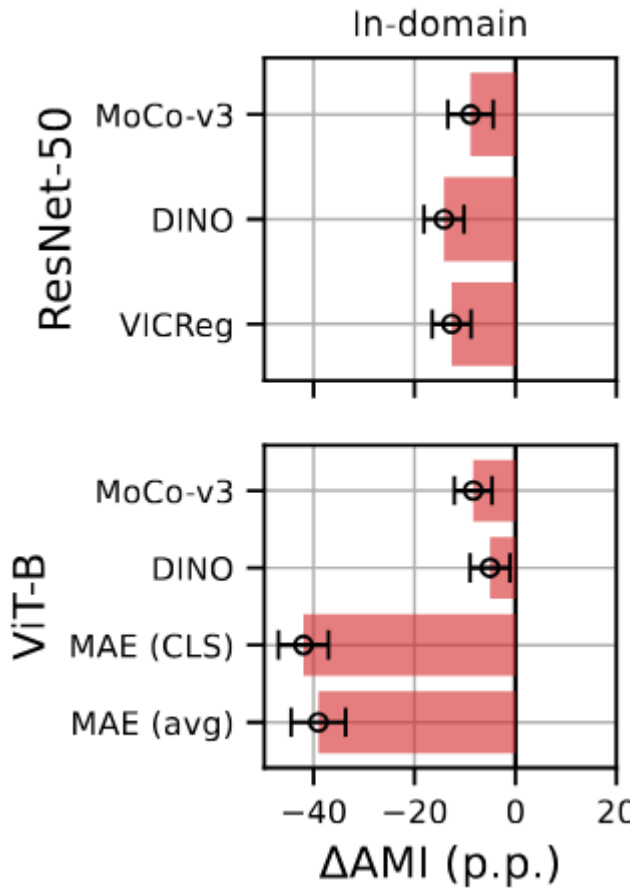

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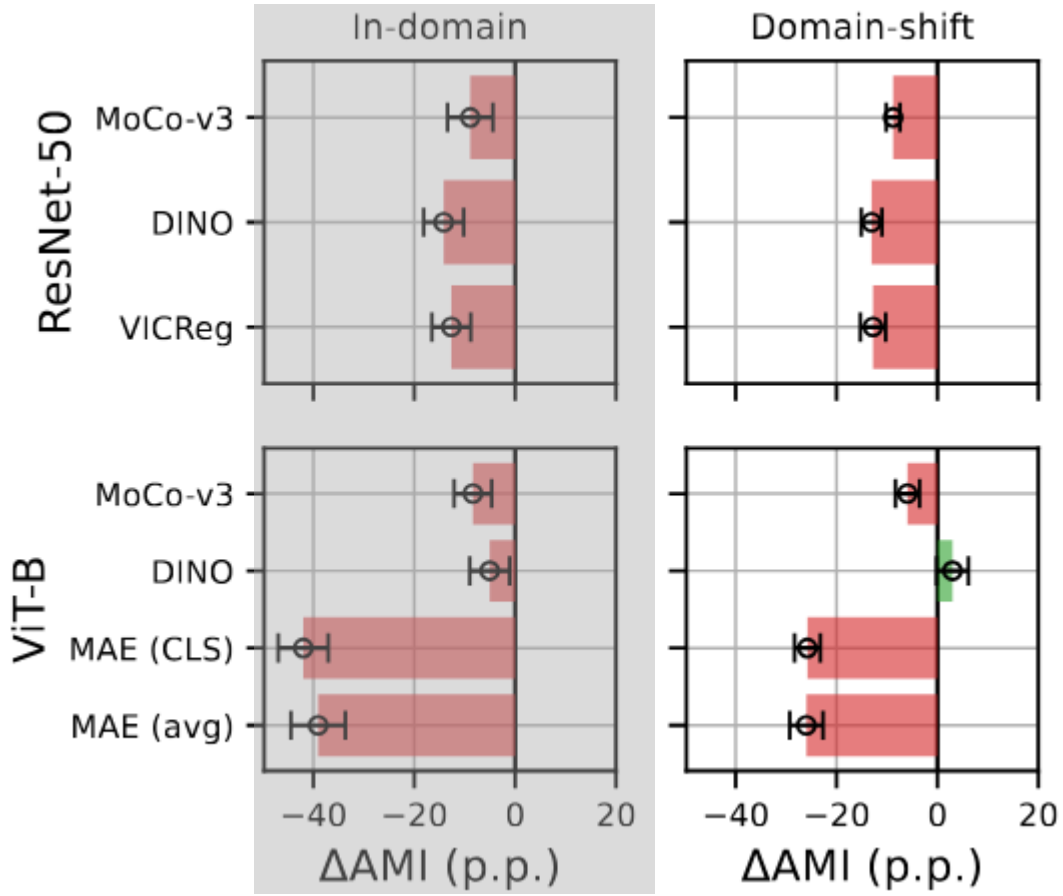

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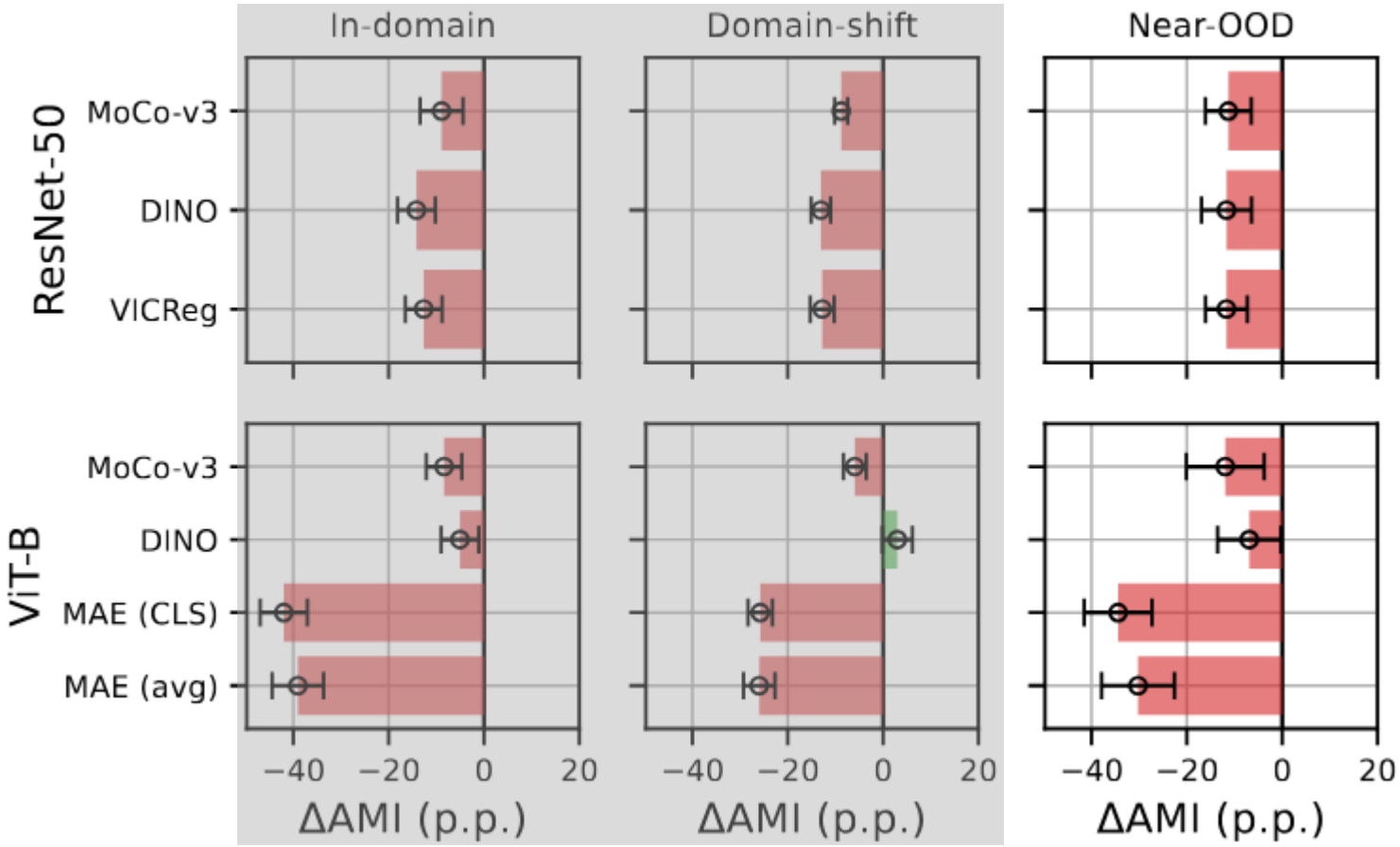

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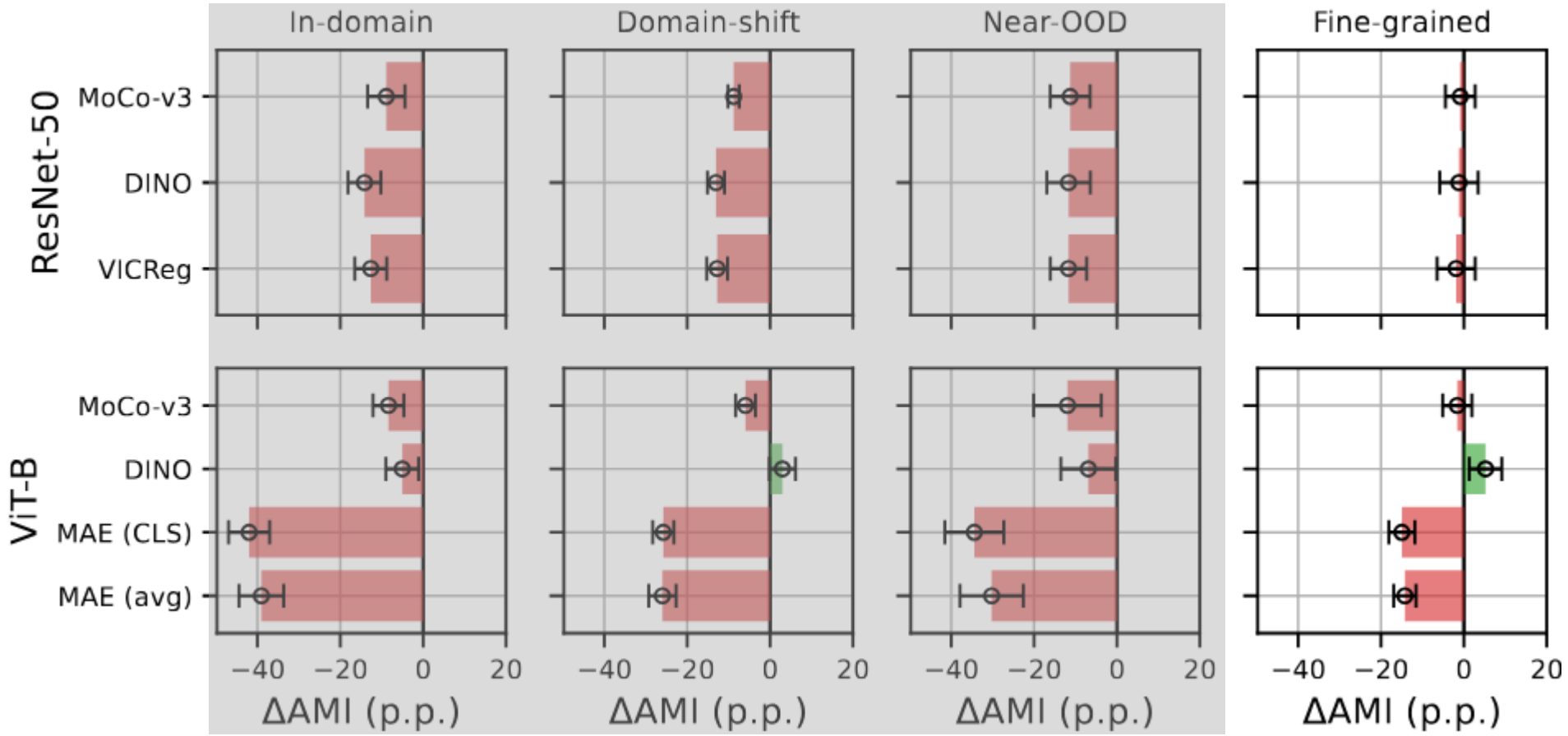

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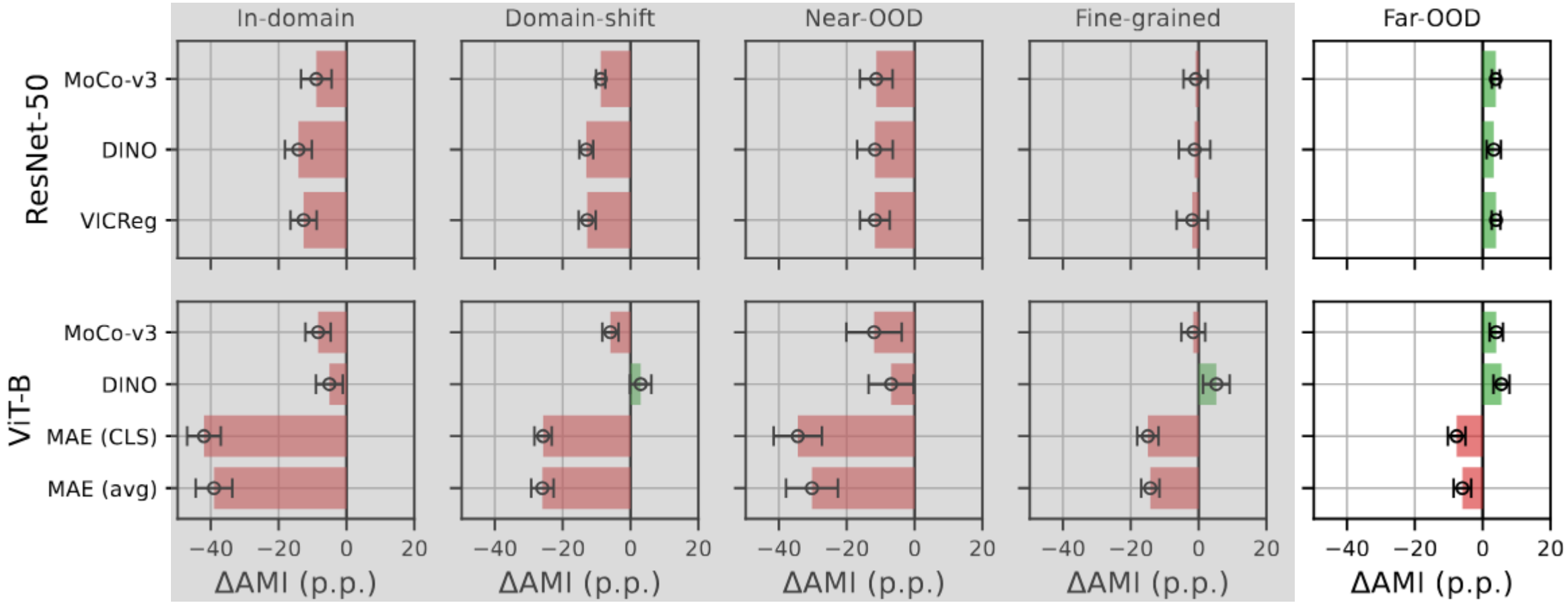
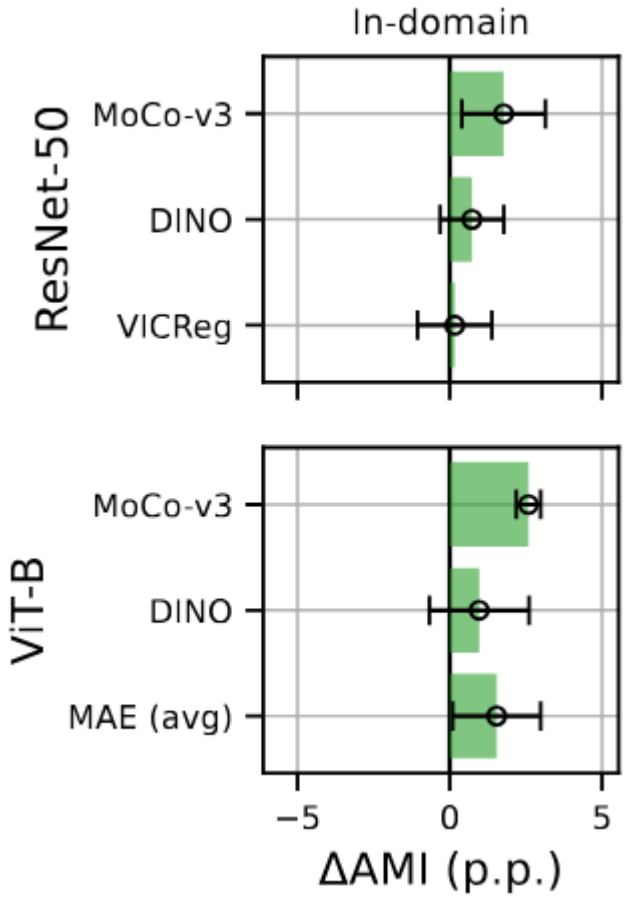


SSL Fine-tuned Encoders

SSL Fine-tuned Encoders



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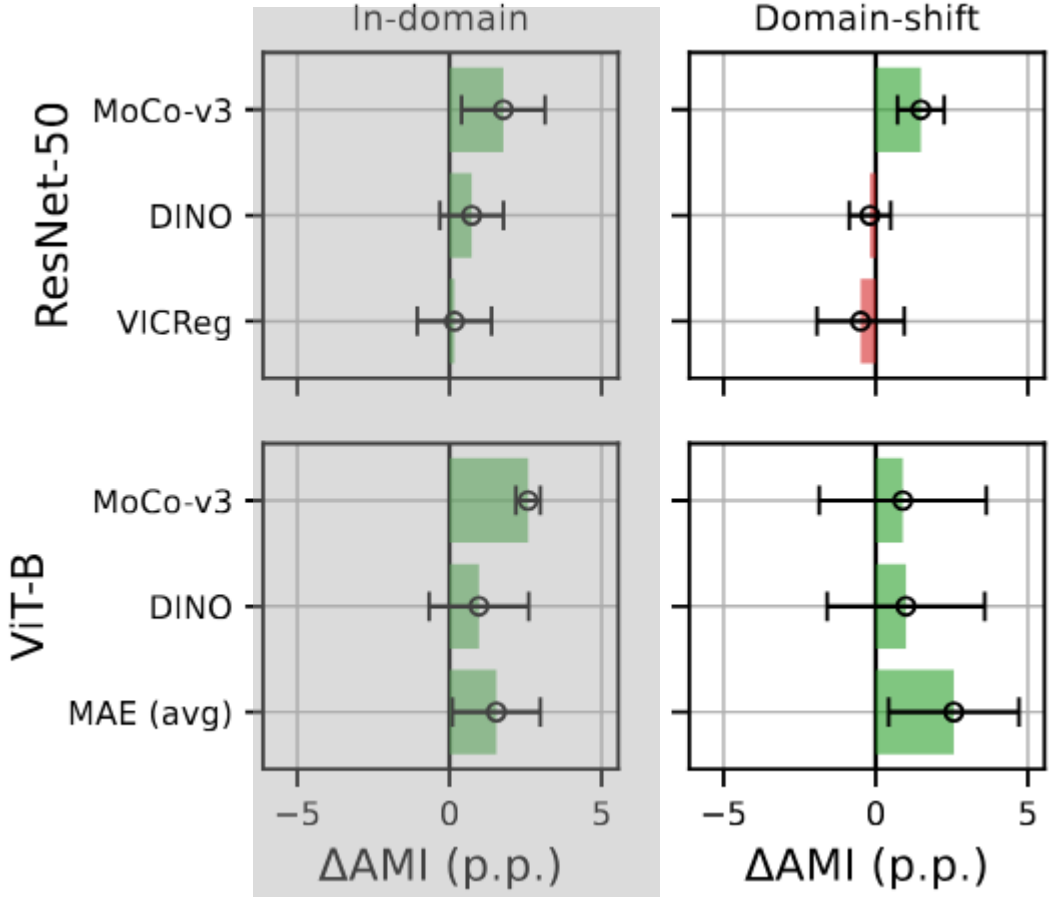

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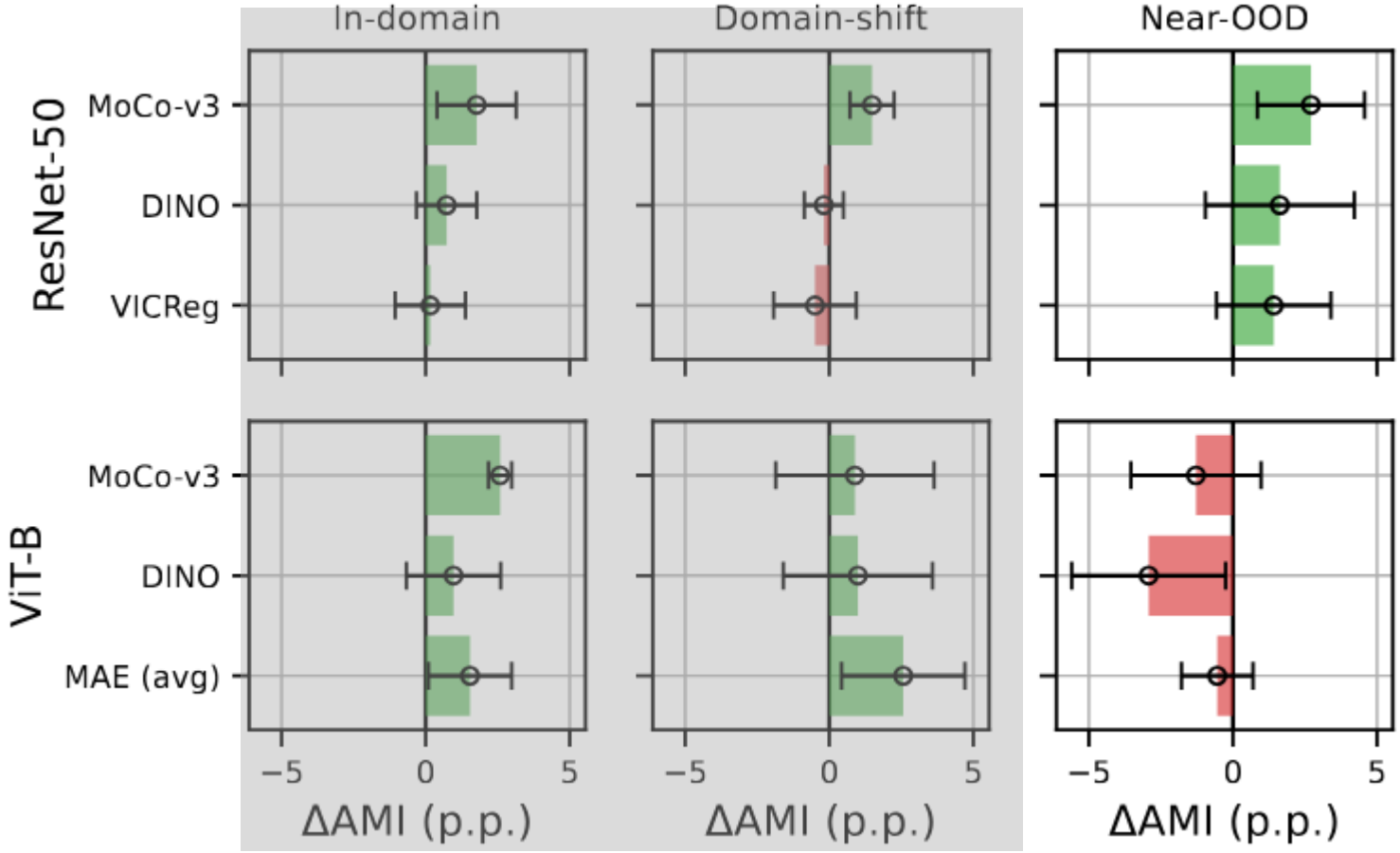

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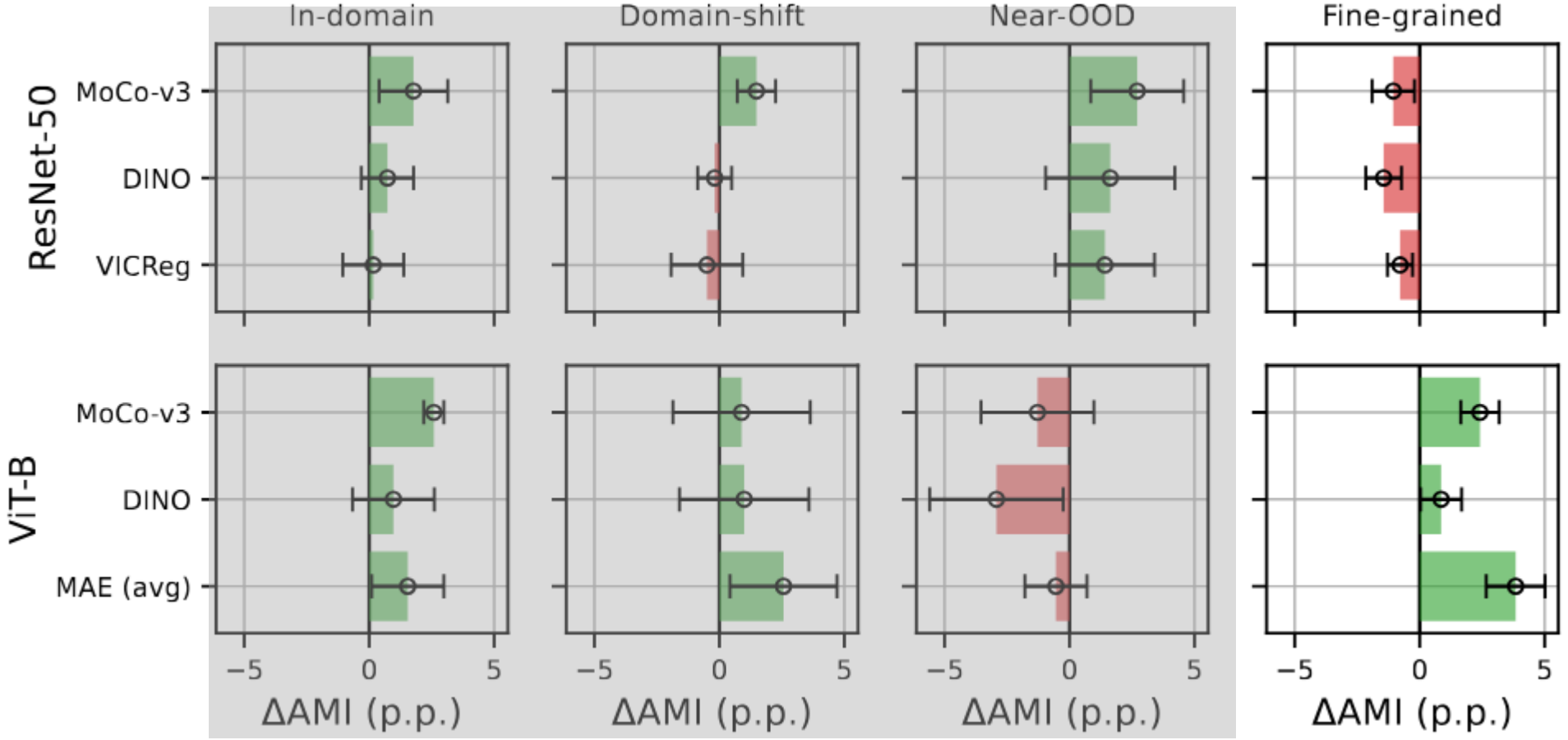

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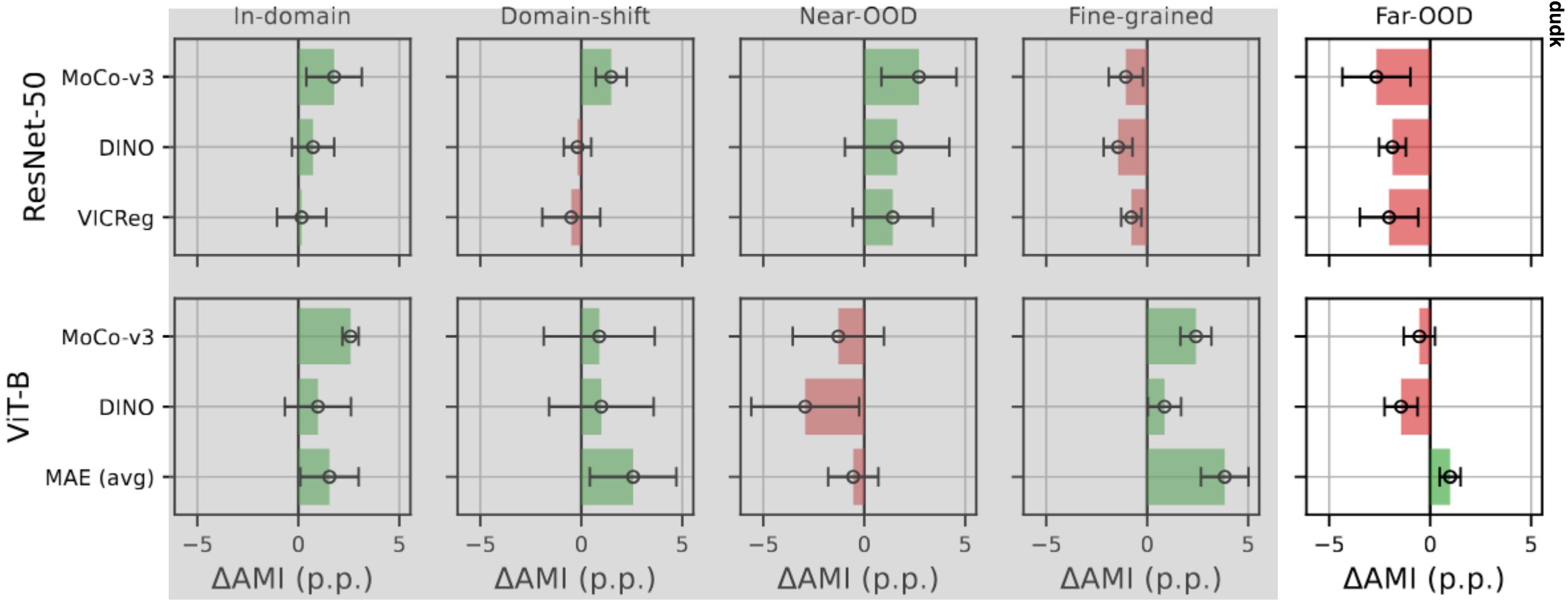

Taxonomic Hierarchies

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→ How well does the clusters match the taxonomic hierarchies?

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$$\mathrm{AMI}(\mathrm{Y}_{\mathrm{True}}, \mathrm{Y}_{\mathrm{Pred}}) = \frac{\mathrm{MI}(\mathrm{Y}_{\mathrm{True}}, \mathrm{Y}_{\mathrm{Pred}}) - \mathbb{E}[\mathrm{MI}(\mathrm{Y}_{\mathrm{True}}, \mathrm{Y}_{\mathrm{Pred}})]}{\mathrm{mean}\big(\mathrm{H}(Y_{\mathrm{True}}) + \mathrm{H}(Y_{\mathrm{Pred}})\big) - \mathbb{E}[\mathrm{MI}(\mathrm{Y}_{\mathrm{True}}, \mathrm{Y}_{\mathrm{Pred}})}$$

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→ Now describes the percentage of entropy in the label that is explained by observing the prediction

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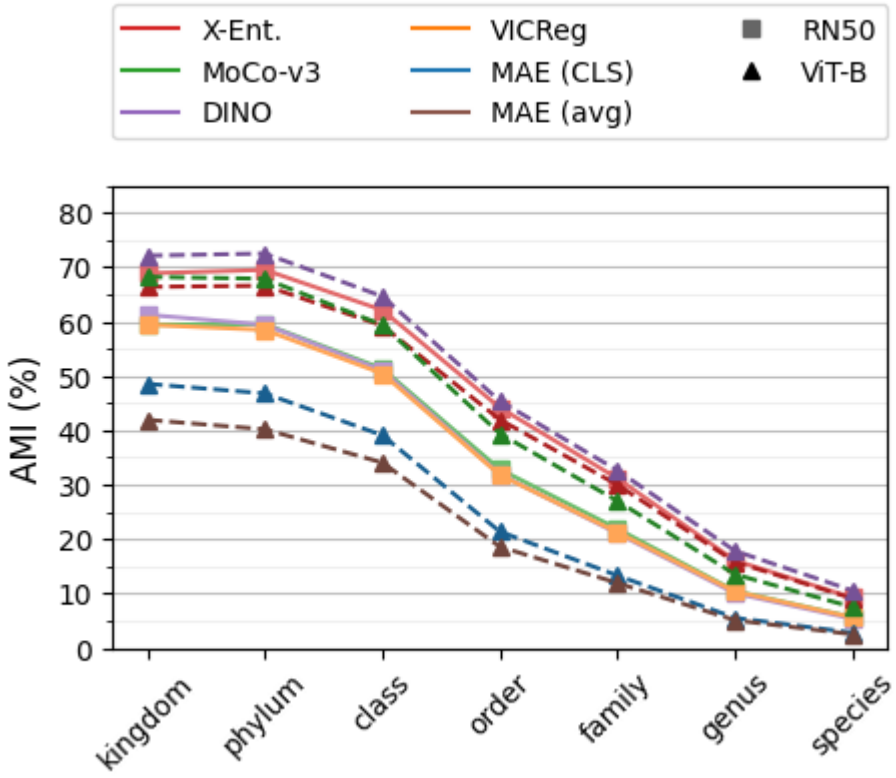
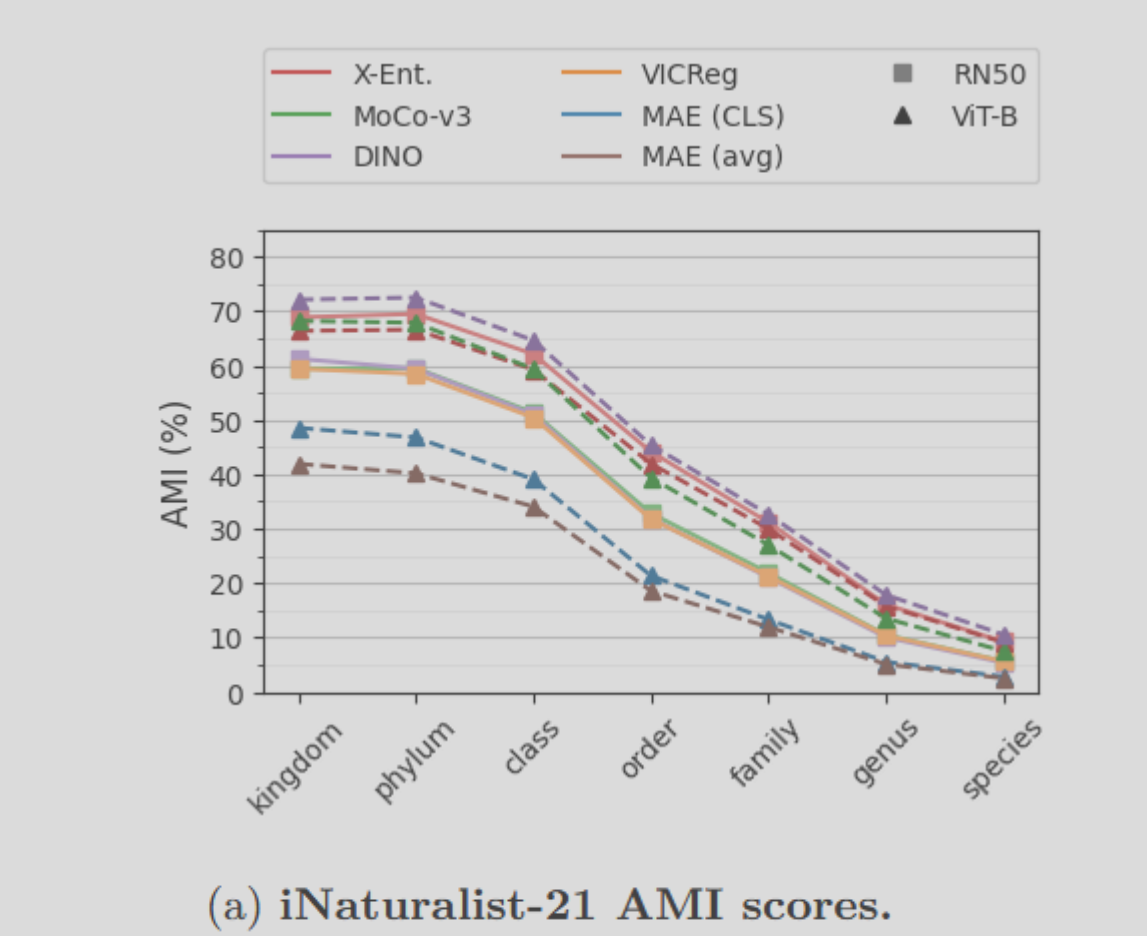
Taxonomic Hierarchies



(a) **iNaturalist-21 AMI scores.**

Taxonomic Hierarchies



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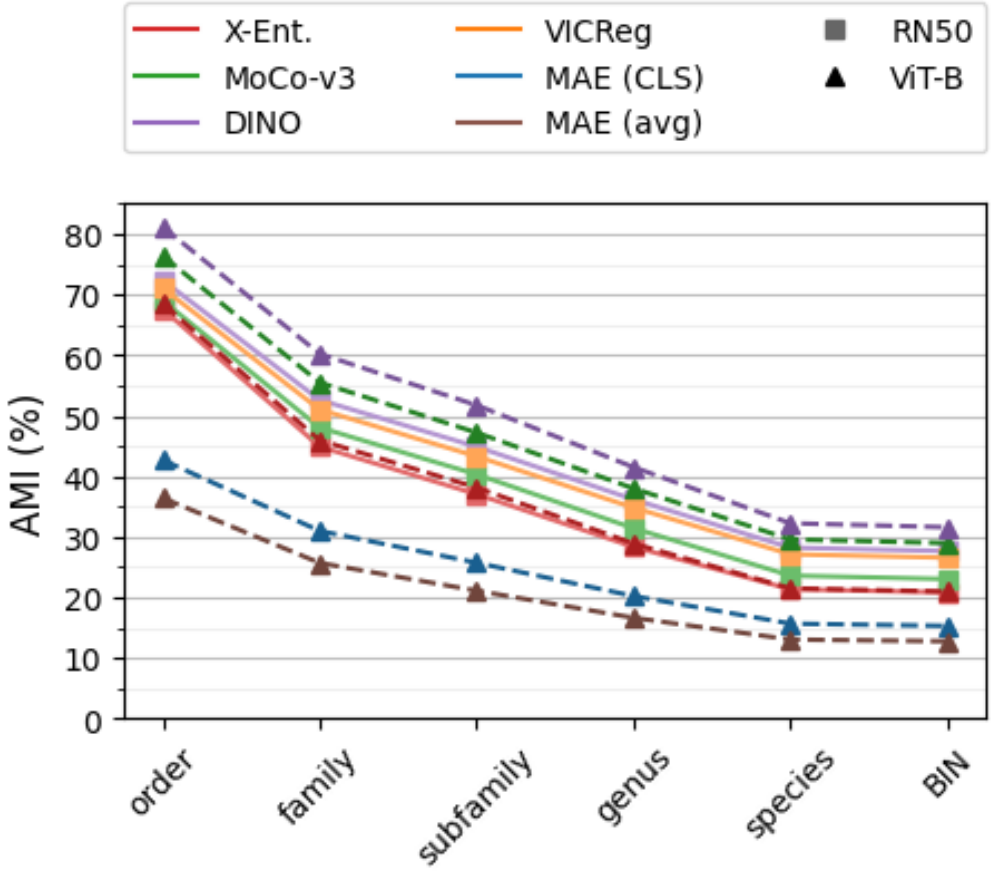

(b) BIOSCAN-1M AMI scores.

Taxonomic Hierarchies – BIOSCAN-5M

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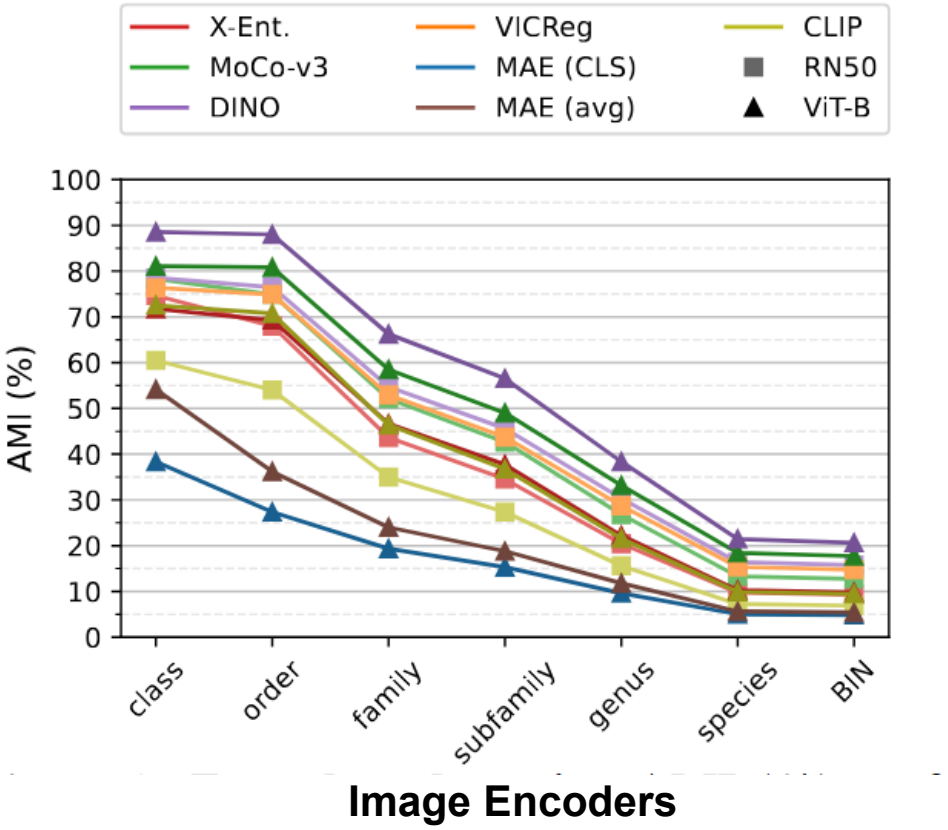


Taxonomic Hierarchies – BIOSCAN-5M

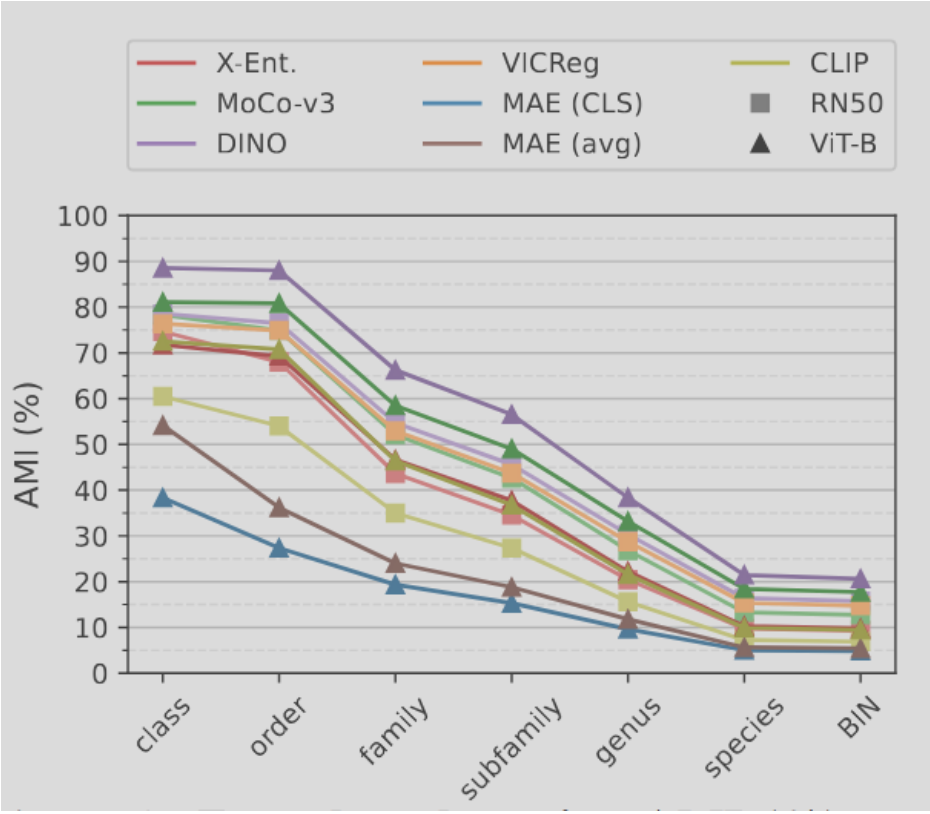
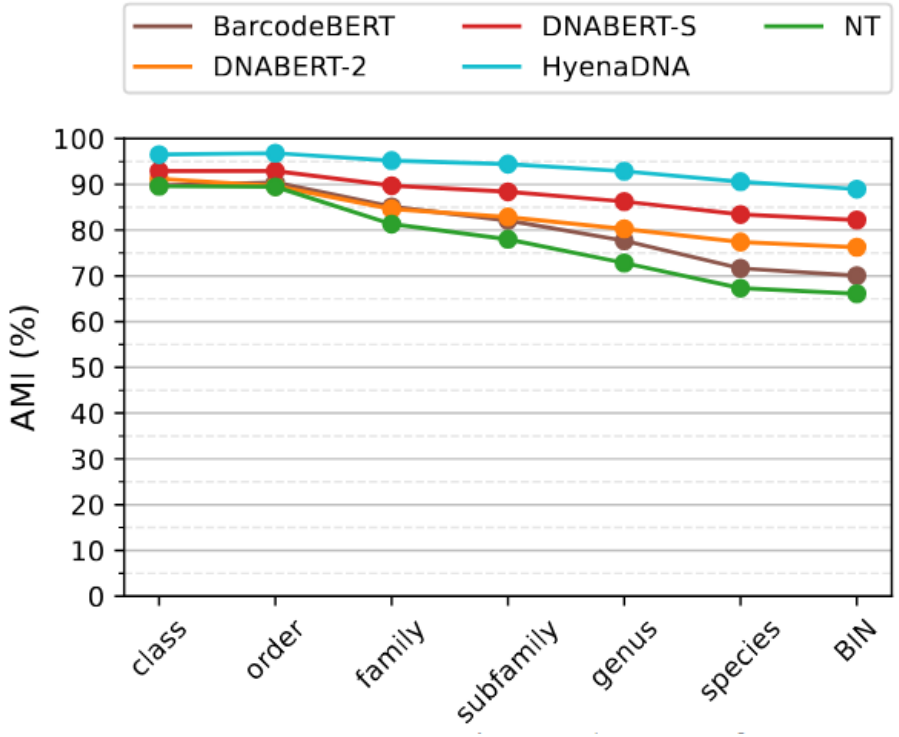


Image Encoders



DNA Encoders

Potential of ZSC Evaluations

How does it compare to probing?

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→ We compare Spearman's Correlation between AMI and kNN accuracy

How does it compare to probing?

Arch.	Clusterer	$k=1$	$k=10$	$k=20$	$k=100$	$k=200$
RN50	K-Means	51	48	48	48	49
	Spectral	54	52	52	53	53
	AC w/ C	49	47	47	47	47
	AC w/o C	45	44	44	44	44
	Affinity Prop.	49	47	47	47	47
	HDBSCAN	51	49	49	49	49
ViT-B	K-Means	37	37	37	39	39
	Spectral	37	38	38	40	40
	AC w/ C	33	34	34	35	36
	AC w/o C	39	40	40	41	41
	Affinity Prop.	36	37	36	38	38
	HDBSCAN	38	39	38	40	40

* Correlation scores multiplied by 100 for readability

How does it compare to probing?

→ AMI and kNN accuracy is only moderately correlated

→ ZSC can therefore be seen as an orthogonal evaluation process to probing

Arch.	Clusterer	$k=1$	$k=10$	$k=20$	$k=100$	$k=200$
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$$S = \frac{1}{N} \sum_{i}^{N} \frac{a_i - b_i}{\max(a_i, b_i)}$$

a_i $-$ *Mean within cluster distance*
b_i $-$ *Mean distance to closest other cluster*

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→ Are the GT-based AMI scores and GT-free Silhouette scores correlated?

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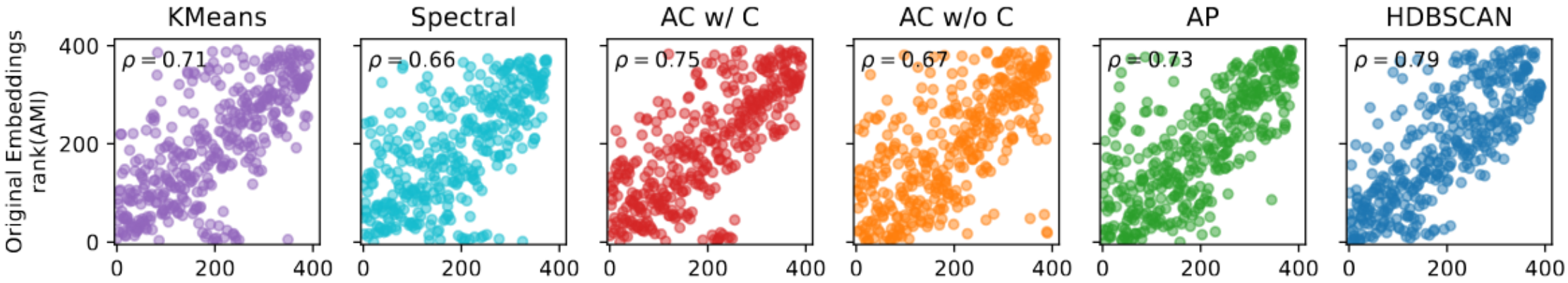

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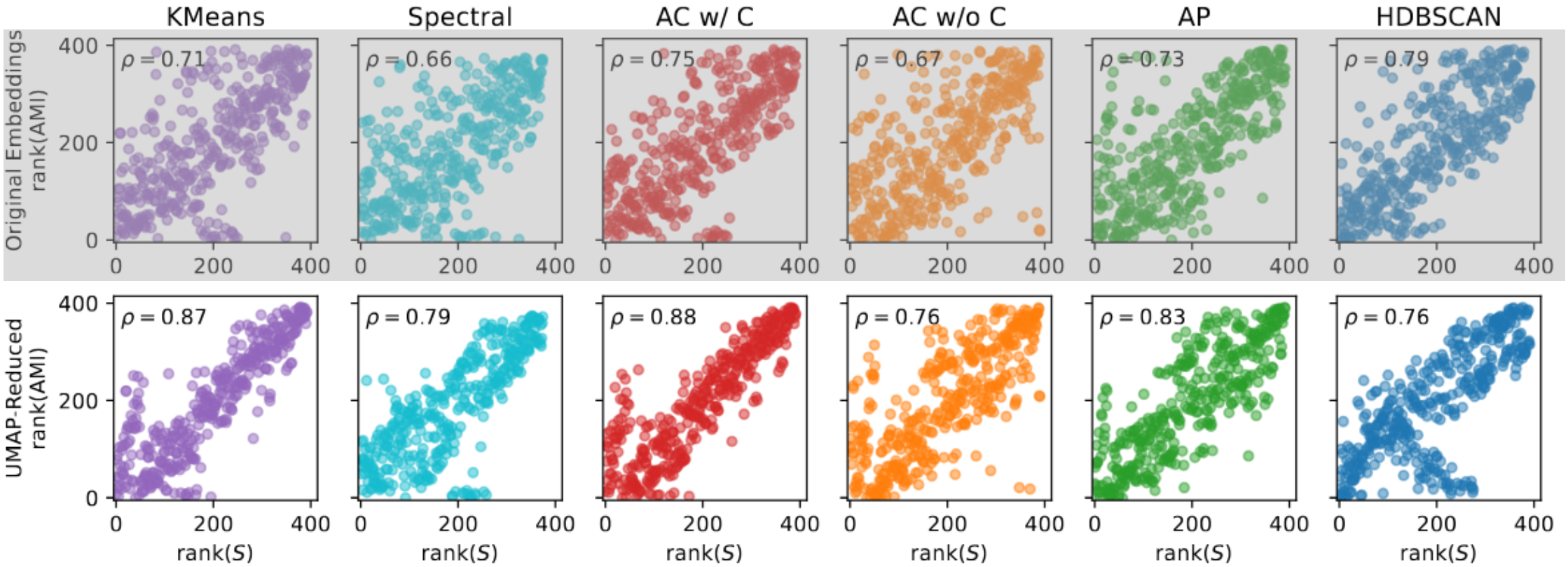

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→ **Yes,** Silhouette and AMI scores are correlated!

→ Allows for proxy-model evalaution on new tasks without any label

→ Much more flexible model selection process compared to

1) kNN probing, which requires stored labeled data points
2) Linear probing, which requires fitting a large linear layer