

Agreement-on-the-Line: Predicting the Performance of Neural Networks under Distribution Shift

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Problem

In practice, machines often need to perform well on distributions that are different from what it has been trained on.

Estimating **out-of-distribution (OOD)** performance is hard because labeled data is expensive.

However, unlabeled data is easier to obtain...

Problem

Say we are given

- a collection of models $\mathcal{H} = \{h_1, h_2, \dots, h_n\}$ trained on in-distribution (ID) data $X_{train}, y_{train} \sim \mathcal{D}_{ID}$
- labeled ID validation data and unlabeled OOD test data
 $X_{val}, y_{val} \sim \mathcal{D}_{ID}$ and $X_{test} \sim \mathcal{D}_{OOD}$

Can we predict OOD performance of models in \mathcal{H} with only **unlabeled data?**

Characterizing the Shift

Corollary 1. (Garg, et al. 2022)

Absent assumptions on the classifier f , no method of estimating accuracy will work in all scenarios, i.e., for different nature of distribution shifts.

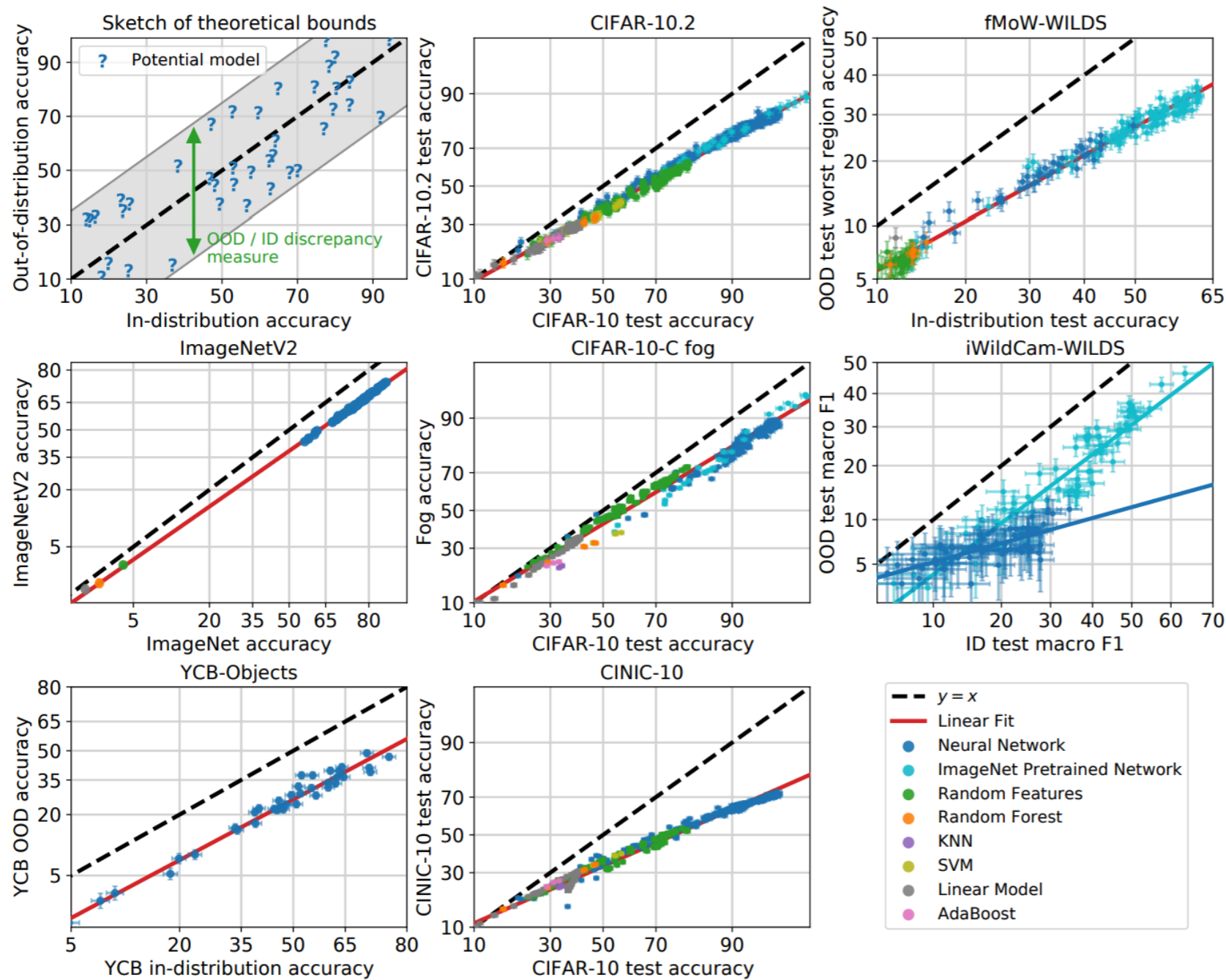
Simple proof:

If the classifier has no assumptions, accuracy is only identifiable IFF $p_t(y | x)$ is uniquely identified given $p_s(x, y)$ and $p_t(x)$.

Characterizing the Shift

1. What are reasonable assumptions we can make about the **distribution shift** and the **behavior of the classifier**?
2. Is there an easy way to “**check**” whether these assumptions hold?

Accuracy on the Line (Miller, et al. 2021)



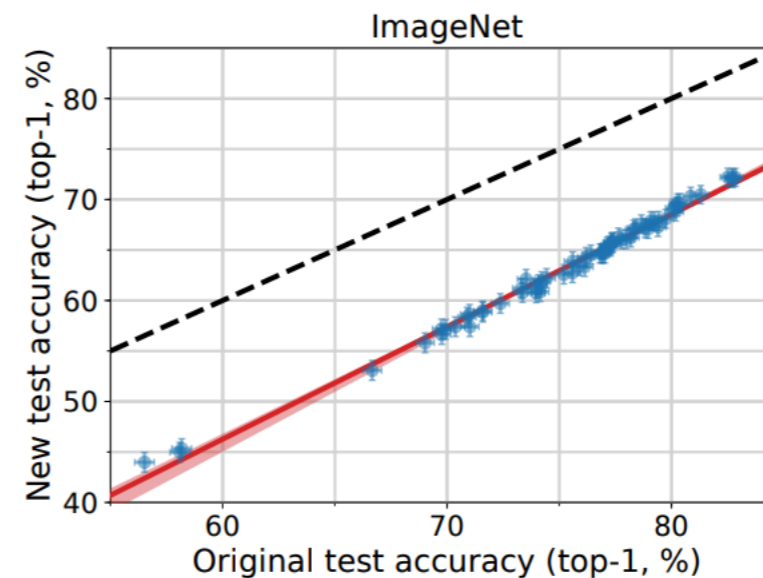
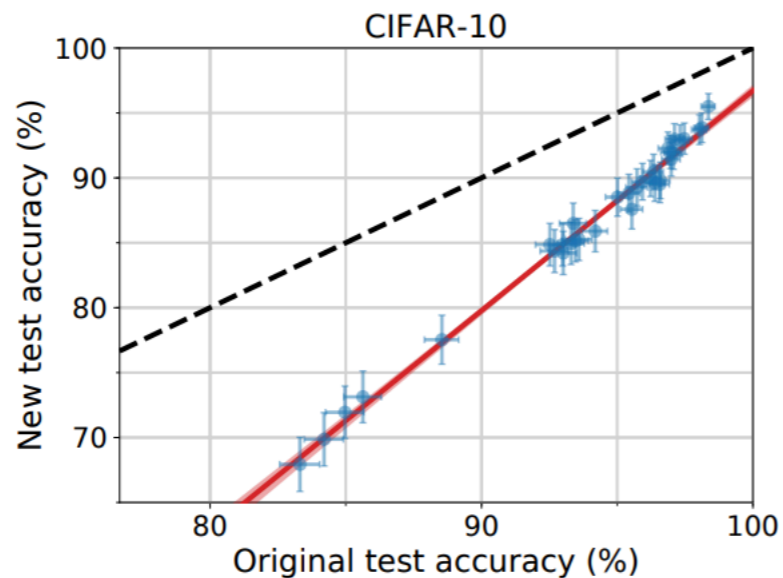
In popular OOD benchmarks, **ID** and **OOD test accuracy** are **strongly linearly correlated**

*They first scale the accuracies by probit transform $\Phi^{-1}(\cdot)$

Accuracy on the Line (Miller, et al. 2021): OOD Benchmarks

Dataset reproduction

- CIFAR10.1, ImageNetV2 [Recht, et al. 2019]
- CIFAR10.2 [Lu, et al. 2020]

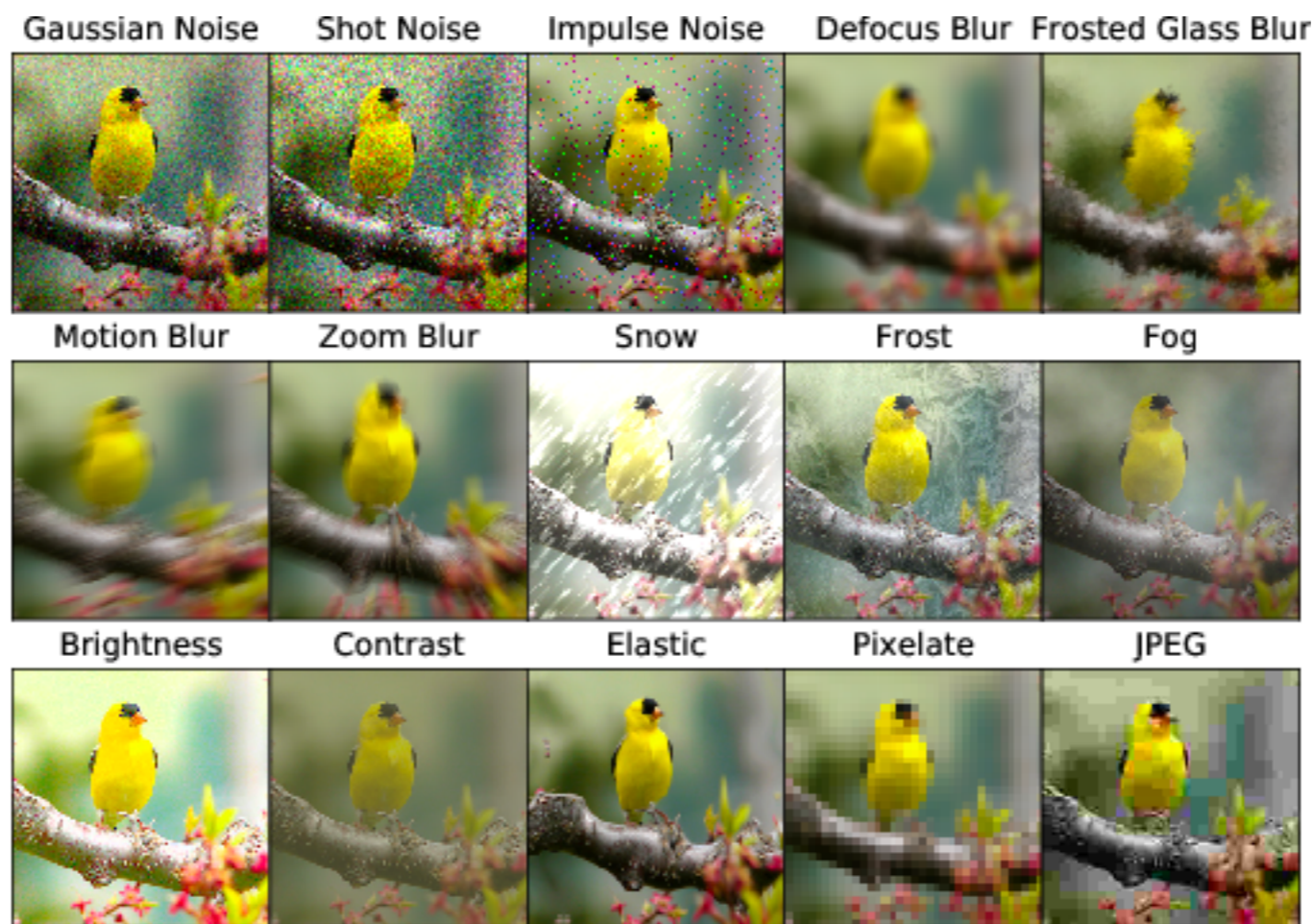


--- Ideal reproducibility ● Model accuracy — Linear fit

Accuracy on the Line (Miller, et al. 2021): OOD Benchmarks

Synthetic corruptions






- CIFAR10C [Hendrycks and Dietterich, 2019]



Accuracy on the Line (Miller, et al. 2021): OOD Benchmarks

Real world shifts (Environmental changes, human activity)

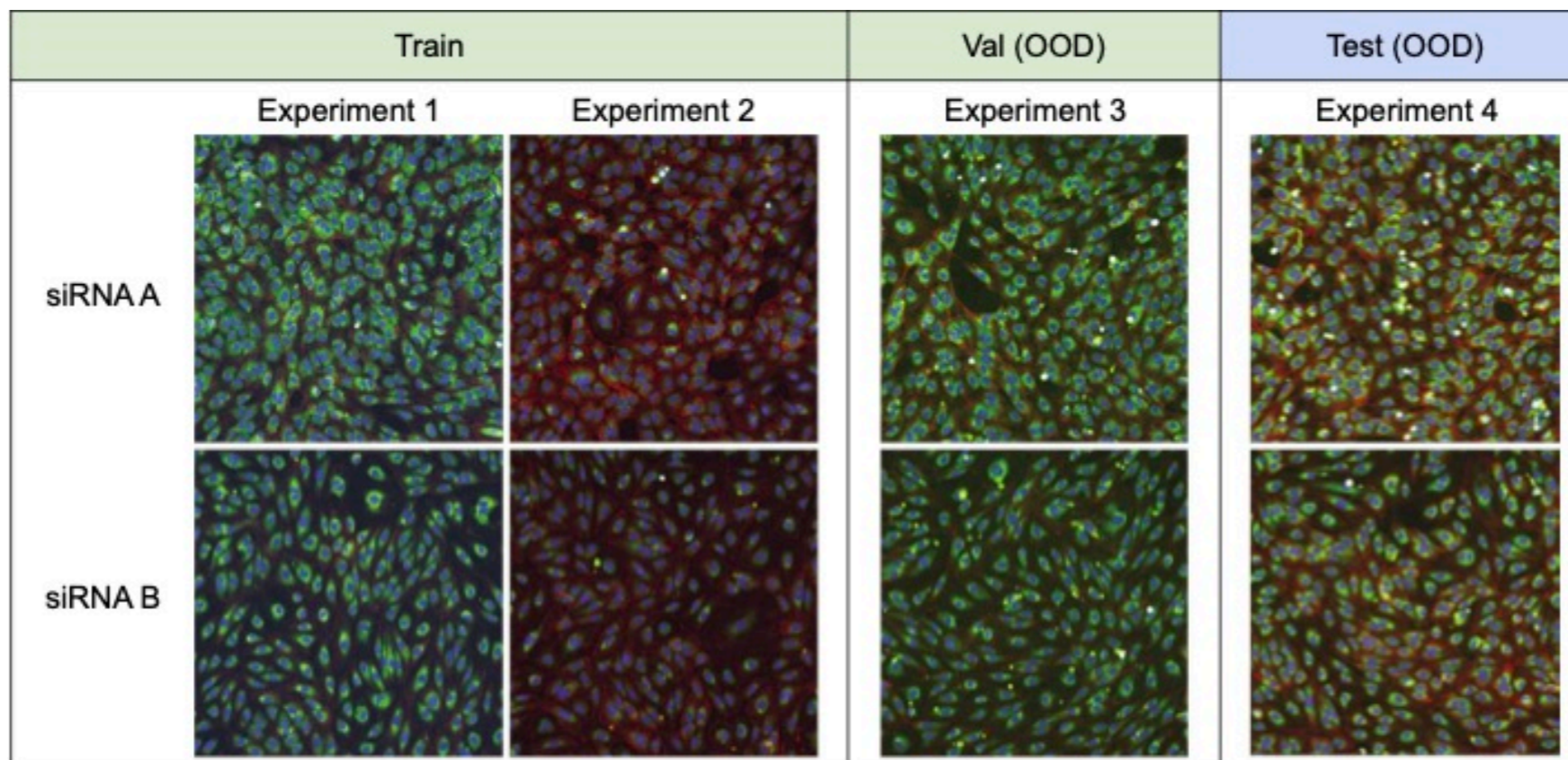
- **fMoW-wilds**
- RxRx1-wilds
- Camelyon17-wilds
- iWildCam-wilds

	Train			Test	
Satellite Image (x)					
Year / Region (d)	2002 / Americas	2009 / Africa	2012 / Europe	2016 / Americas	2017 / Africa
Building / Land Type (y)	shopping mall	multi-unit residential	road bridge	recreational facility	educational institution

Accuracy on the Line (Miller, et al. 2021): OOD Benchmarks

Real world shifts (Environmental changes, human activity)

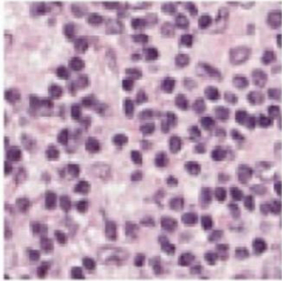
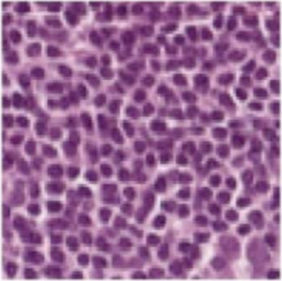
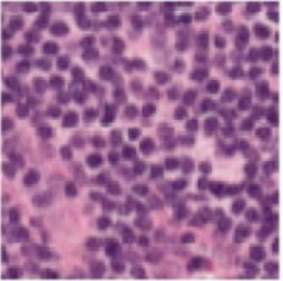
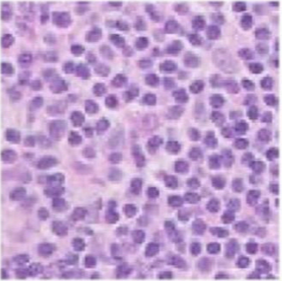
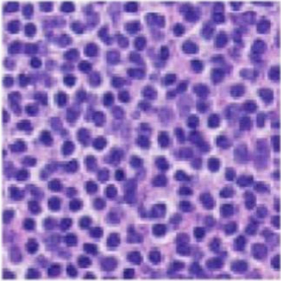
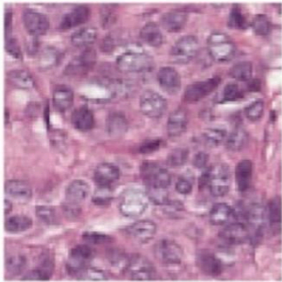
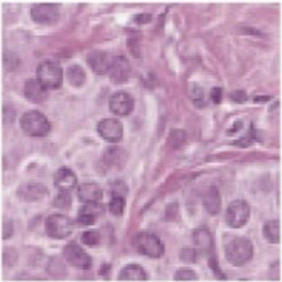
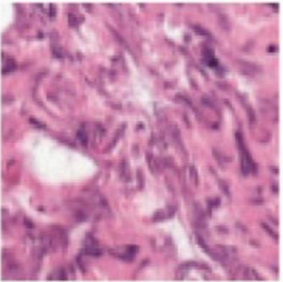
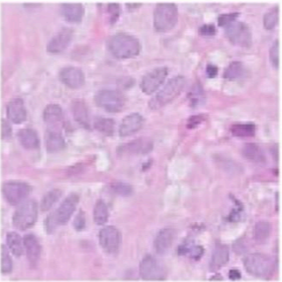
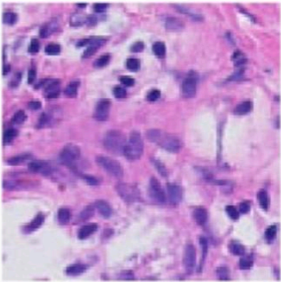
- fMoW-wilds
- **RxRx1-wilds**
- Camelyon17-wilds
- iWildCam-wilds



Accuracy on the Line (Miller, et al. 2021): OOD Benchmarks

Real world shifts (Environmental changes, human activity)







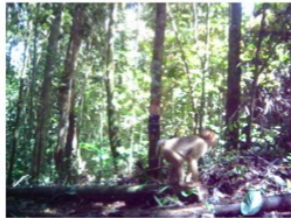
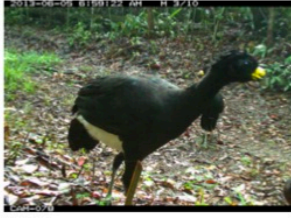


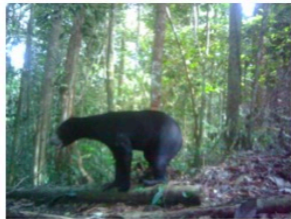
- fMoW-wilds
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- **Camelyon17-wilds**
- iWildCam-wilds

	Train			Val (OOD)	Test (OOD)
	d = Hospital 1	d = Hospital 2	d = Hospital 3	d = Hospital 4	d = Hospital 5
y = Normal					
y = Tumor					

Accuracy on the Line (Miller, et al. 2021): OOD Benchmarks

Real world shifts (Environmental changes, human activity)

- fMoW-wilds
- RxRx1-wilds
- Camelyon17-wilds
- iWildCam-wilds

Train			Test (OOD)
$d = \text{Location 1}$	$d = \text{Location 2}$	$d = \text{Location 245}$	$d = \text{Location 246}$
			
Vulturine Guineafowl	African Bush Elephant	...	unknown
			
Cow	Cow	Southern Pig-Tailed Macaque	Great Curassow
Test (ID)			
$d = \text{Location 1}$	$d = \text{Location 2}$	$d = \text{Location 245}$	
			
Giraffe	Impala	Sun Bear	

Models

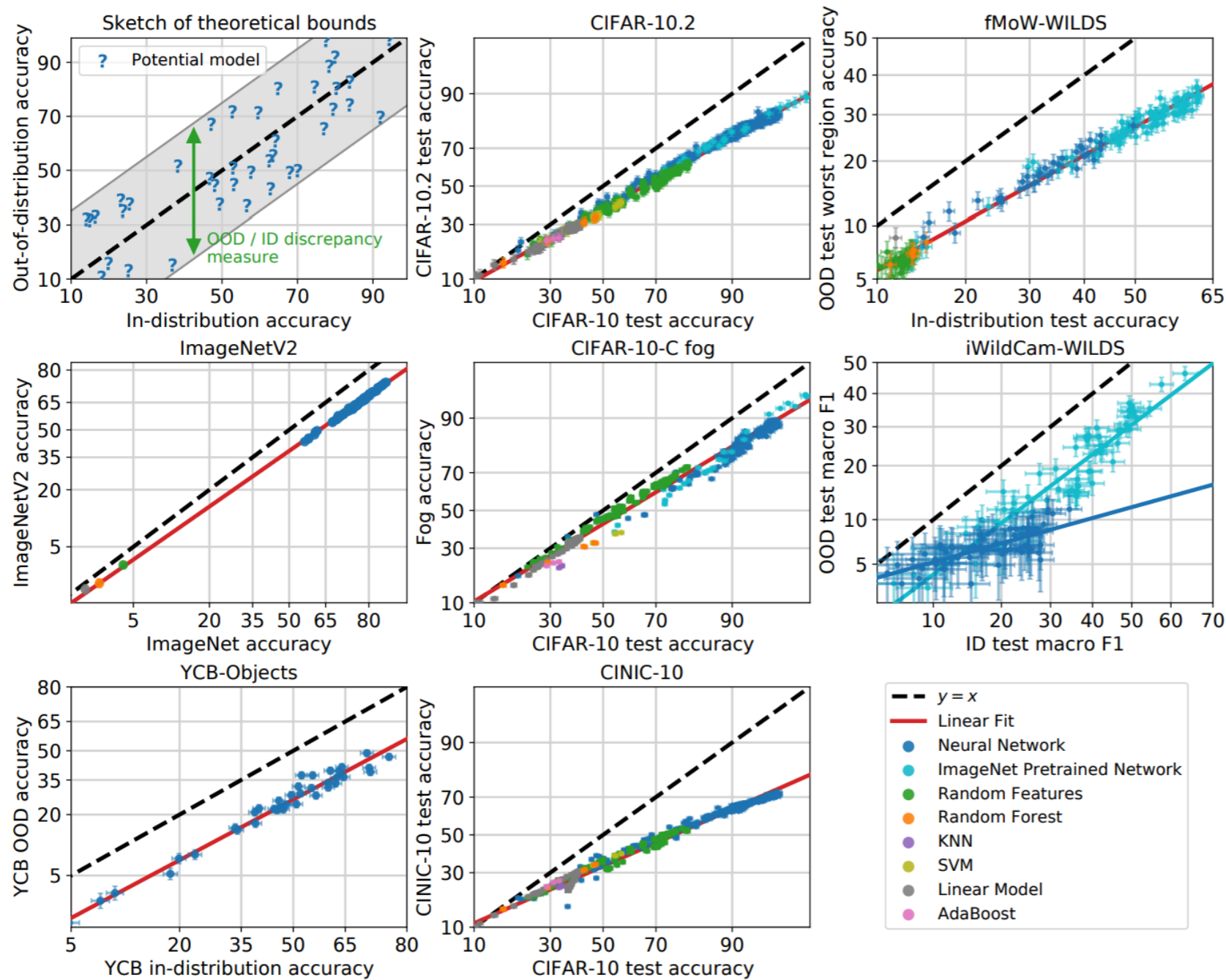
Our model collection \mathcal{H} consists of **CNNs** and **Vision Transformers** trained using different

1. hyperparameter
2. training set size
3. training duration

Architecture	Number of models
Adversarial Inception v3 [46]	1
AlexNet [45]	1
BEiT [2]	1
BoTNet [68]	1
CaiT [74]	1
CoaT [78]	2
ConViT [20]	3
ConvNeXT [50]	1
CrossViT [8]	9
DenseNet [37]	3
DLA [79]	10
EfficientNet [72]	1
HaloNet [75]	1
NFNet [7]	1
ResNet [33]	10
ResNeXT [77]	1
Inception v3 [71]	1
VGG [67]	1

Architecture	Number of models
DenseNet121 [37]	21
DenseNet169 [37]	8
EfficientNetB0 [72]	13
ResNet18 [33]	13
ResNet50 [33]	18
ResNet101 [33]	7
PreActResNet18 [32]	63
PreActResNet34 [32]	9
PreActResNet50 [32]	11
PreActResNet101 [32]	4
ResNeXT 2 × 64d [77]	12
ResNeXT 32 × 4d [77]	8
ResNeXT 4 × 64d [77]	1
RegNet X200 [62]	11
RegNet X400 [62]	13
RegNet Y400 [62]	5
VGG11 [67]	16
VGG13 [67]	13
VGG16 [67]	13
VGG19 [67]	12
ShuffleNetV2 [53]	56
ShuffleNetG2 [81]	13
ShuffleNetG3 [81]	8
AlexNet [45]	2
MobileNet [65]	12
MobileNetV2 [65]	13
PNASNet-A [48]	13
PNASNet-B [48]	13
PNASNet-5-Large [48]	3
SqueezeNet [39]	3
SENet18 [42]	13
GoogLeNet [70]	20
DPN26 [11]	8
DPN92 [11]	2
MyrtleNet [Repo]	1
Xception [12]	3

Accuracy on the Line (Miller, et al. 2021)



There is a **structure** to the way distributions commonly shift

...but this fact does not solve the problem of **needing OOD labels for accuracy.**

Agreement

Measure the rate at which predictions of two hypotheses agree

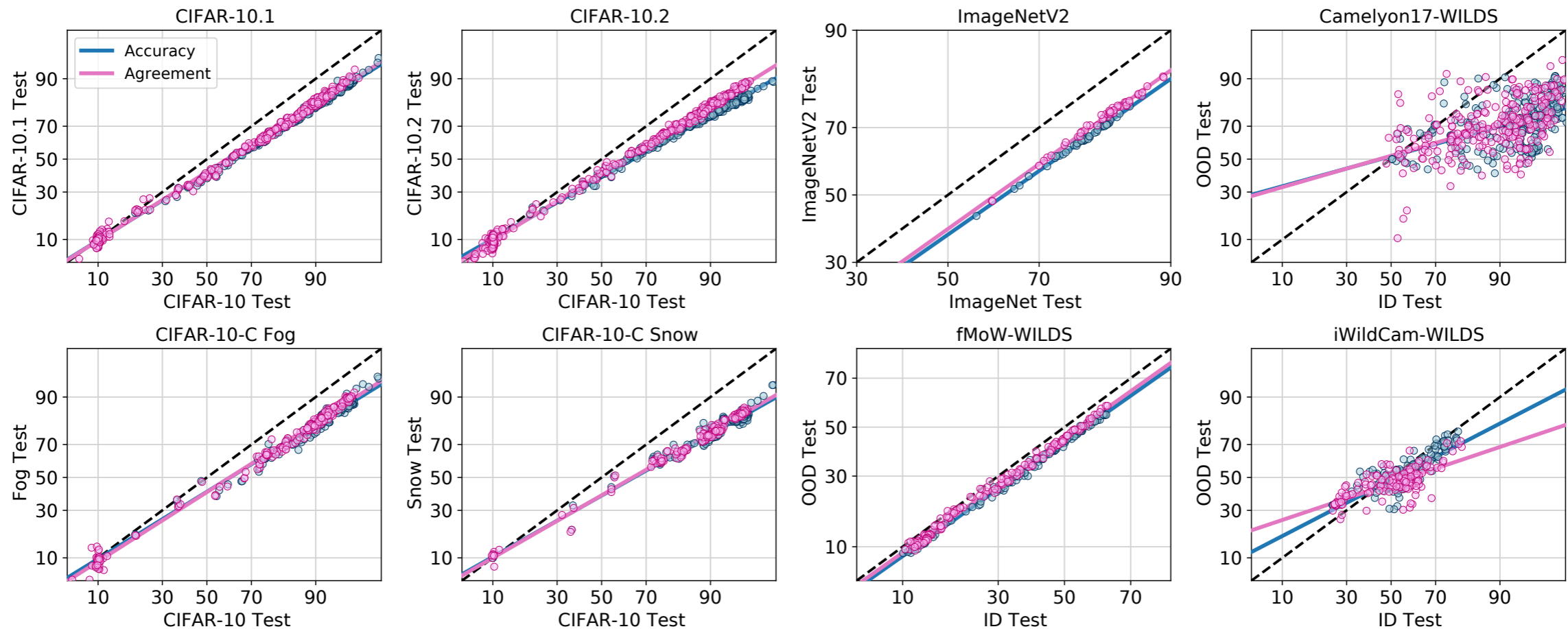
Test Input $(x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_9, x_{10})$

Model 1 Predictions	1	2	2	1	2	1	2	1	1	1
Model 2 Predictions	1	1	2	1	2	2	1	1	2	1

Agreement: 60%

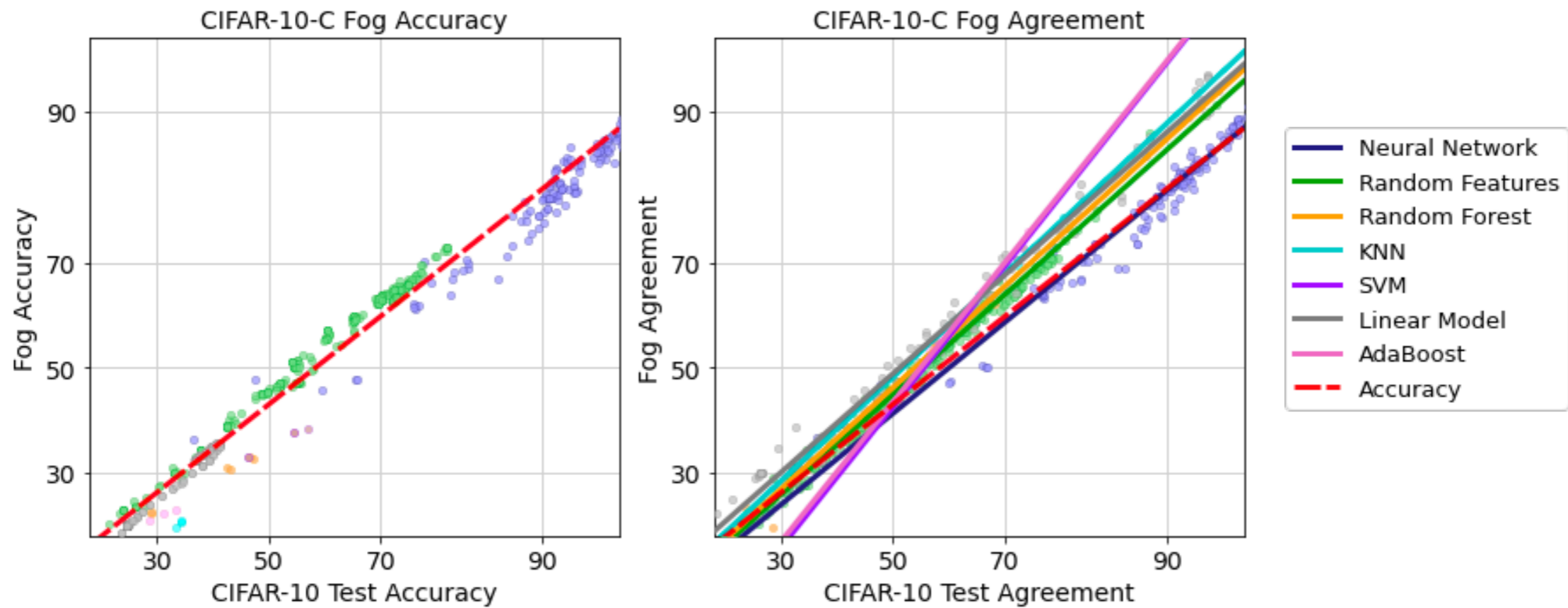
Does not need labels!

Agreement-on-the-Line



- **Strong Correlation** When ID vs OOD **accuracy** is strongly linearly correlated ($\geq 0.95 R^2$ values), ID vs OOD **agreement** is also strongly linearly correlated. Additionally, these linear correlations have almost the **same slope and bias**.
- **Weak Correlation** When ID vs OOD **accuracy** is weakly linearly correlated ($\leq 0.75 R^2$ values), ID and OOD **agreement** is also weakly linearly correlated.

The phenomena only occurs for neural networks



OOD Accuracy Estimation

1. Estimate **slope** and **bias** by linear regression of ID vs OOD agreement

$$\Phi^{-1}(\text{Agr}_{\text{OOD}}(h, h')) = a \cdot \Phi^{-1}(\text{Agr}_{\text{ID}}(h, h')) + b$$

2. *If the linear correlation is strong, we know approximately*

$$\Phi^{-1}(\text{Acc}_{\text{OOD}}(h)) = a \cdot \Phi^{-1}(\text{Acc}_{\text{ID}}(h)) + b$$

3. From 1 and 2, note that for any two models $h, h' \in \mathcal{H}$

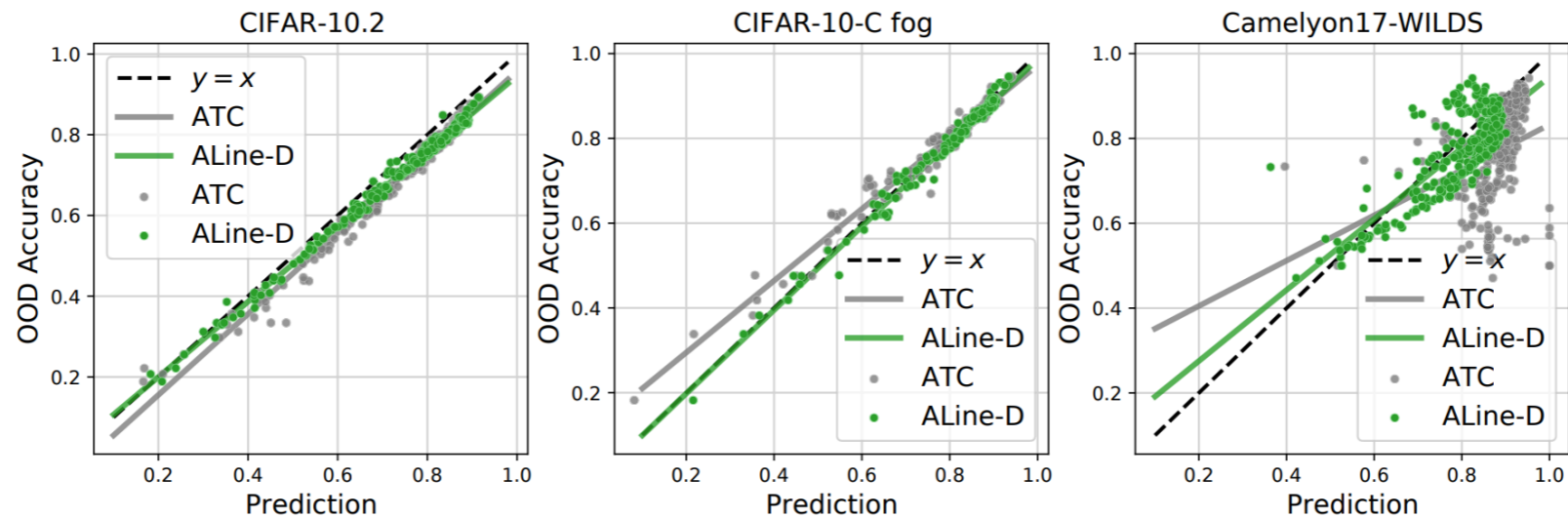
$$\frac{1}{2} \underbrace{\Phi^{-1}(\text{Acc}_{\text{OOD}}(h))}_{\text{unknown}} + \frac{1}{2} \underbrace{\Phi^{-1}(\text{Acc}_{\text{OOD}}(h'))}_{\text{unknown}} = \underbrace{\Phi^{-1}(\text{Agr}_{\text{OOD}}(h, h')) + a \cdot \left(\frac{\Phi^{-1}(\text{Acc}_{\text{ID}}(h)) + \Phi^{-1}(\text{Acc}_{\text{ID}}(h'))}{2} - \Phi^{-1}(\text{Agr}_{\text{ID}}(h, h')) \right)}_{\text{known}}$$

4. Solve system of linear equations for $\Phi^{-1}(\text{Acc}_{\text{OOD}}(h)) \quad \forall h \in \mathcal{H}$

ALine-S: Steps 1-2

ALine-D: Steps 1-4

OOD Accuracy Estimation



Mean Absolute Estimation Error with % as units.

Dataset	ALine-D	ALine-S	ATC [Garg '22]	AC [Hendrycks '17]	DOC [Guillory '17]	Agreement
CIFAR-10.1	1.11	1.17	1.21	4.51	3.87	5.98
CIFAR-10.2	3.93	3.93	4.35	8.23	7.64	5.42
ImageNetV2	2.06	2.08	1.12	66.2	11.50	6.70
CIFAR-10C-Fog	1.45	1.75	1.78	4.47	3.93	3.47
CIFAR-10C-Snow	1.32	1.97	1.31	5.94	5.49	2.57
CIFAR10C-Saturate	0.41	0.77	0.69	2.03	1.51	4.14
fMoW-wilds	1.30	1.44	1.53	2.89	2.60	8.99
RxRx1-wilds	0.27	0.52	2.97	2.46	0.65	8.67
Camelyon17-wilds	5.47	8.31	11.93	13.30	13.57	6.79
iWildCam-wilds	4.95	6.01	12.12	4.46	5.02	7.53

Along One Trajectory

1. Train a single ResNet18 model on CIFAR-10.
2. Every 5 epochs, save the predictions of the model over CIFAR-10 and CIFAR-10.1 Test.
3. Perform ALine-D

