Mitigating Simplicity Bias in Neural Networks

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Based on joint works with

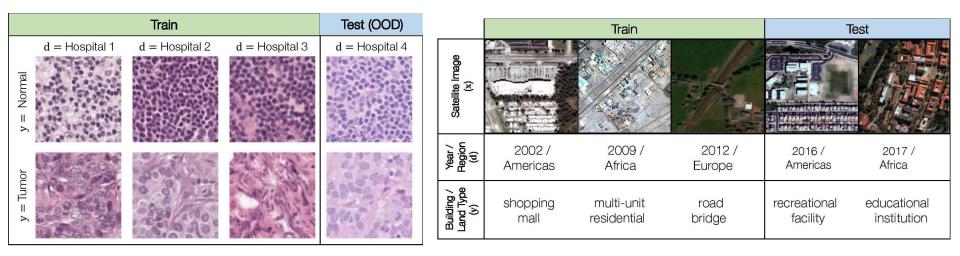
Anshul Nasery, Sravanti Addepalli, Harshay Shah, Kaustav Tamuly, Aditi Raghunathan, R. Venkatesh Babu and Prateek Jain



Outline

- Distribution Shifts
- Simplicity Bias
- Two key observations
 - Feature Replication Hypothesis
 - Non-robust features
- Algorithmic ideas
 - Feature Reconstruction Regularizer
 - Adversarial Fine-tuning
- Evaluation
- Conclusion

Distribution shift between train and test data



Camelyon17 - WILDS

fMoW - WILDS

WILDS: A Benchmark of in-the-Wild Distribution Shifts by Koh et al., 2020



Accuracy loss due to distribution shifts

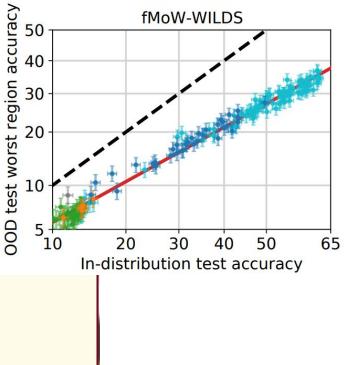
- Loss of accuracy for various models due to distribution shift between train and test data [1].
- In some cases, can change from highly accurate to close to random.

<u>This talk</u>

- 1. Why are neural networks (NNs) brittle?
- 2. How do we make them robust?

New conceptual and algorithmic insights.

[1] Accuracy on the Line: On the Strong Correlation Between Out-of-Distribution and In-Distribution Generalization, Miller et al., ICML 2021





Thought Experiment

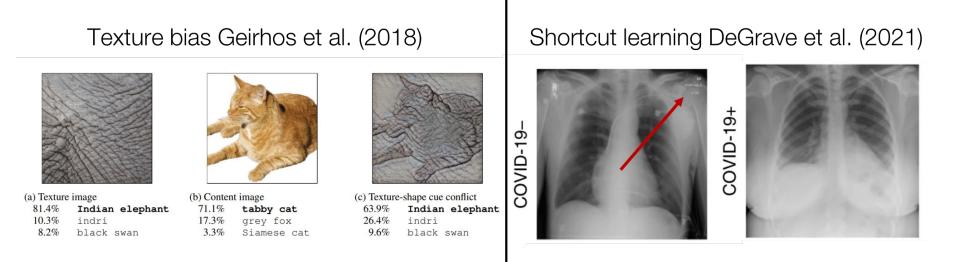
How do we distinguish swans and bears?





- Several features available: color, background, shape, organs etc.
- Humans look at these holistically. What does an NN learn?

Neural Networks Learn Only Some Features



Why do NNs learn only some features?

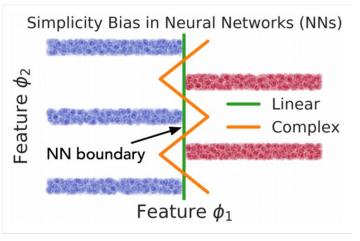
Which features do NNs learn?

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Simplicity Bias (SB) [STRJN, NeurIPS 2020]

NNs learn *simplest* features useful for classification

- Margin = Closest distance to decision boundary
- Orange classifier has larger margin compared to green classifier.
- NNs have the capacity to learn Orange classifier.
- In practice however, NNs learn the green classifier.

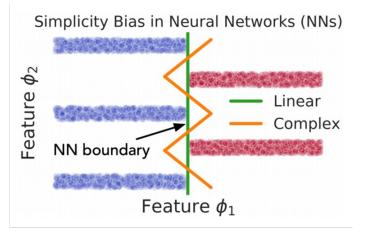


NNs Provably Exhibit Simplicity Bias

$$f(x) = \sum_{j=1}^{\kappa} ReLU(\langle w_j, x \rangle), \qquad x \in \mathbb{R}^d$$

- Initialization: $w_j \sim N(0, \frac{1}{dk}I)$
- Number of samples: $\Omega(d^2)$
- Number of nodes: $\tilde{O}(d^2)$
 - Covers overparameterised setting

Weight of "linear feature": $O(\frac{1}{\sqrt{k}})$

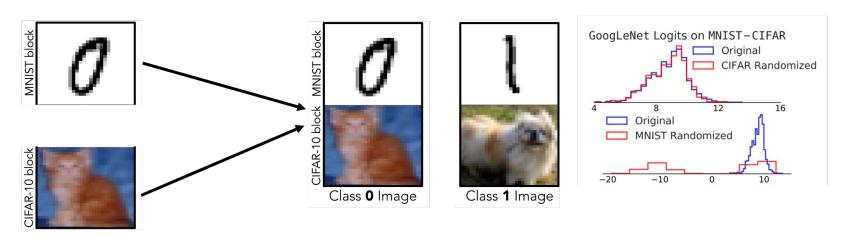




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Towards Real Datasets

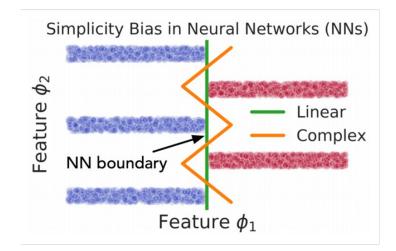
MNIST-CIFAR dataset and randomization tests MNIST: 0/1 digit classification CIFAR: cat/dog classification



- CIFAR randomized: Randomize the CIFAR part of the image
- Logits do not change ⇒ Prediction **does not depend at all** on CIFAR part

Consequences of SB

SB leads to brittleness to distribution shifts and adversarial examples



(Simple features \neq True features) \Rightarrow Accuracy loss with distribution shifts



Adversarial examples and robustness

- Small, invisible to the eye, perturbations can drastically change model predictions.
- Termed adversarial examples.
- SB smaller margin poor adversarial robustness



b) "Dog" perturbed noise x127 "Toilet tissue"



Bio-inspired Robustness: A Review, by Machiraju et al., 2021



Fixing SB through adversarial training

• Given data points $(x_1, y_1), \dots, (x_n, y_n)$ and a predictor function $f_{\theta}(x)$

(e.g., neural network), the standard empirical risk minimization (ERM)

objective is given by:
$$\hat{\theta}_{std} = \operatorname{argmin}_{\theta} \frac{1}{n} \sum_{i=1}^{n} (y_i - f_{\theta}(x_i))^2$$

• Adversarial training: $\hat{\theta}_{adv} = \operatorname{argmin}_{\theta} \frac{1}{n} \sum_{i=1}^{n} \max_{\tilde{x}_i: \|\tilde{x}_i - x_i\| \le \epsilon} (y_i - f_{\theta}(\tilde{x}_i))^2$

3.	CIFAR10-Randomized Accuracy		
	Standard SGD	ℓ_∞ Adv. Training	
	0.493 ± 0.005	0.493 ± 0.001	
	0.494 ± 0.005	0.501 ± 0.003	
	0.501 ± 0.001	0.499 ± 0.002	

• Doesn't fix SB.

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Fixing SB through ensembles

- Ensembles refer to training of multiple models with different subsets of data, random initializations etc.
- Helps when there are multiple features of *similar* complexity.
 - Different models learn different features.
- However, when different features have widely different complexities, all models learn the same feature.

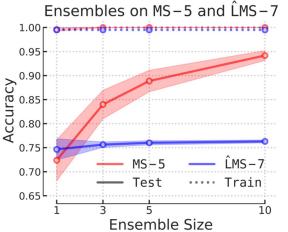
Noisy Linear Coordinate

~

First 7-Slab

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 $MC = \Gamma$



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To fix SB,

need to understand its precise manifestation ...



Test-bed dataset: ColoredMNIST





Task: Classify (mostly red) 0 vs (mostly yellow) 1

VS

High correlation between color and digit (label).

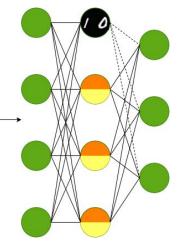


Key insight I: Feature replication (ICLR 2023)

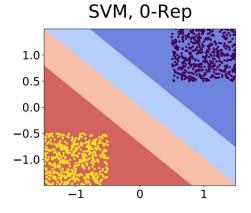
- Some features (e.g., color) are replicated multiple times in the feature space compared to other features (e.g., digit shape).
- Final linear classifier relies more on such replicated features.
- 3 layer CNN with 32 penultimate features has more color features than shape features.
- Output is more dependent on color features than shape features.

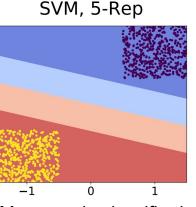
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Type of feature	Number	Output correlation
Color	26	0.81
Shape	4	0.61



Max-Margin Classifier under Feature Replication

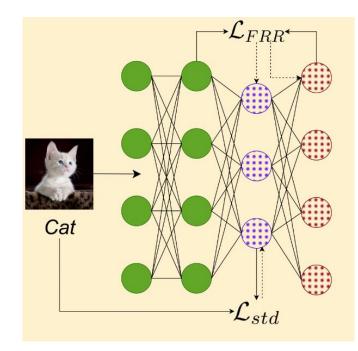




Max margin classifier in replicated feature space - $w = \left[\frac{2}{d}, \cdots, \frac{2}{d}\right]$

- SGD trained networks converge to the max-margin solution.
- When features are replicated, max-margin classifier gives more weight to the replicated feature.
- Becomes worse with increasing dimensions!

Feature Reconstruction Regularizer (FRR)



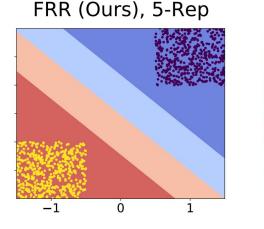
- Reconstruct features from logits
- Minimize the reconstruction loss
- Mathematical formulation -

 $\mathcal{L}_{\text{FRR}}(x,\theta,W,\phi) = ||f_{\theta}(x) - \mathcal{T}_{\phi}(W^T f_{\theta}(x))||_p$

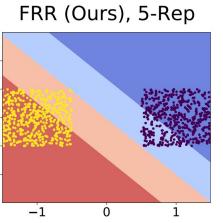
• Ensures that logits contain

information about *all* features.

FRR under Feature Replication



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- FRR gives equal weightage to replicated and unreplicated features
- Requires-
 - Relatively diverse

representations

 Some conditional variance between core and spurious features.

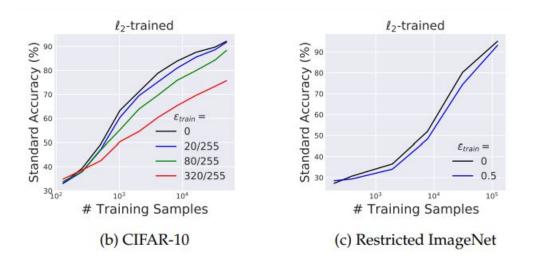
Key insight II: Replicated features are often non-robust

- Replicated features (e.g. color) learned and used by models are often brittle to small adversarial perturbations.
- We train two models on data with perfect shape and color correlation respectively, and compute their accuracy on adversarially perturbed images.
- The performance of a model dependent on color features sees a huge drop.

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Feature used by model	Test Accuracy	Adv. accuracy with perturbation=0.1
Color	99%	53%
Shape	99%	85%

Can we use adversarial training?



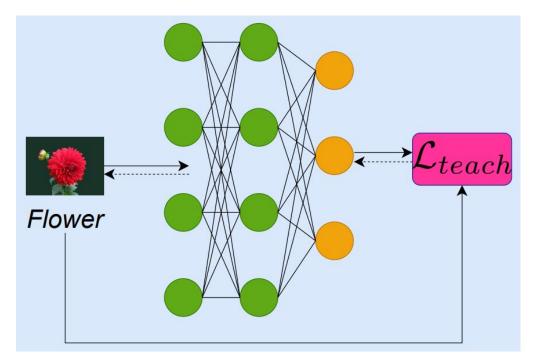
Prior work [1] has shown that adversarial robustness is negatively correlated with clean accuracy.

Experiments earlier showed that adversarial training doesn't fix SB.

[1] Towards Deep Learning Models Resistant to Adversarial Attacks by Madry et al



Adversarial fine-tuning: The sweet spot



We freeze the backbone of an ERM trained network and fine-tune the final linear layer using adversarial training.



Aside: Distillation

- First train a large model and use its predictions to train a smaller model.
 - Observed to give better performance on standard accuracy and is widely used.

$$\hat{\theta}_{\text{big}} = \operatorname{argmin}_{\theta} \frac{1}{n} \sum_{i=1}^{n} (y_i - f_{\theta}(x_i))^2$$
$$\hat{\theta}_{\text{small}} = \operatorname{argmin}_{\theta} \frac{1}{n} \sum_{i=1}^{n} (f_{\theta_{\text{big}}}(x_i) - f_{\theta}(x_i))^2$$

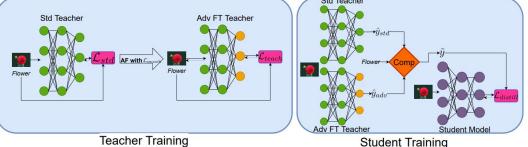
• Can we use this to improve out of distribution robustness?

Distillation for OOD robustness

- Standard distillation doesn't transfer robustness from large model to small model.
- Key Idea: Ensure incorrect logits of teacher are informative with
 - good teachers with adversarial finetuning

Figure 1: DAFT overview. We pre-train a teacher, followed by adversarial fine-tuning using \mathcal{L}_{smooth} (2). We then distill a student from both standard and adversarial teachers. The Comp operator outputs \hat{y}_{adv} if adversarial teacher's prediction is correct, else it outputs \hat{y}_{std} .

- poorer in domain accuracy of teacher mitigated
- A smaller model with DAFT can outperform larger ERM trained models.



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Our results

DomainBed is a large scale benchmark

with multiple domain shift datasets.



We achieve a new state of the art on this benchmark.

Method	Accuracy on DomainBed	Improvement over previous SOTA
ERM	63.3	-
SWAD (Previous SoTA)	66.8	-
DAFT [1]	66.9	0.1
FRR [2]	67.9	1.1
FRR+DAFT	68.4	1.6

[1] Draft on arxiv; [2] Accepted to ICLR 2023.

Conclusion

- Neural networks suffer from extreme simplicity bias (SB).
- SB is a key reason behind poor robustness to distribution shifts.
- Non-robust features and Feature replication: Two empirically grounded hypotheses for OOD brittleness of neural networks.
- Two methods to alleviate these issues-FRR utilizes all learned features, even under feature replication [ICLR 2023]
 - DAFT combines adversarial fine-tuning and distillation to learn robust features
- New SOTA on large scale OOD benchmark.

Future directions of work

- Currently, the era of foundation models trained on large/diverse data.
- Do foundation models suffer from SB? If yes, how does it manifest? How can we make foundation models more robust?
- Can we improve dataset collection to mitigate SB?
- The role of interpretability methods in analyzing and mitigating SB in trained models.
 - Input gradient based explanations work for adversarially trained models but not for standard models [1]

[1] Do input gradients highlight discriminative features? [SJN, Neurips 2021]