

# Why are Convolutional Nets more sample-efficient than Fully-Connected Nets?

Zhiyuan Li, Yi Zhang, Sanjeev Arora

Presented by

Evangelos Chatzipantazis  
vaghat@seas.upenn.edu

University of Pennsylvania  
April 21, 2022

## On Equivariant Learning Algorithms and their sample complexity

## Motivation and Main Result

## Setting up the problem

### The Learning Protocol

## Parametric Models

## Equivariance

### From Design to Analysis

### Equivariant Algorithms

## Lower Bounds on Equivariant Algorithms

### 0. Warm-Up example

### 1. Single function, All Distributions

### 2. Single Distribution

## Conclusions

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- ▶ In principle, for every CNN we can construct an FCNN that can simulate it.
- ▶ But these FCNNs tend to require many more data points to find the correct CNN inside the class.
- ▶ Quantifying it should not rely only on the expressivity of the model, it must be the combination (model, training algorithm).

Observe the quantifiers!

## Theorem (Informal Theorem)

There *exists* a distribution, and a labelling function s.t. *for all* orthogonally equivariant algorithms (including (S)GD on Fully-Connected Nets) we need  $\Omega(d^2)$  examples to learn the labelling function, while *there is* some Convolutional Net that approximates it in  $O(1)$  examples (and with GD).

- ▶ Show that no "(S)GD + FCNet" can learn some (specific) CNN with good generalization.
- ▶ Typical lower bounds that ignore the algorithm do not work. But a lower bound that would take the algorithm into account is hard because of the non-convexity of the problem and the unknown dynamics of (S)GD.
- ▶ They unify all Fully-Connected Nets under the concept of orthogonal equivariance. Independently of height, width. With optional weight decay, batchnorm, momentum. Then they prove that orthogonally equivariant algorithms are bad learners.

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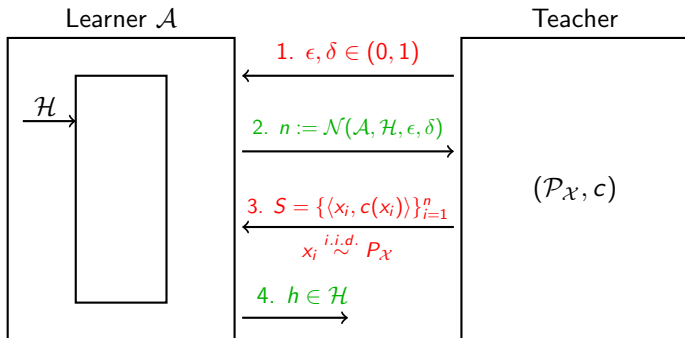
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- ▶ Binary classification i.e.,  $\mathcal{Y} = \{-1, 1\}$ . Data domain:  $\mathcal{X} = \mathbb{R}^d$  and  $P_{\mathcal{X}}$  be a distribution over  $\mathcal{X}$ .
- ▶ We denote a hypothesis by  $h : \mathcal{X} \rightarrow \mathcal{Y}$  and the hypothesis space by  $\mathcal{H} \subseteq \mathcal{Y}^{\mathcal{X}}$ .
- ▶ Joint distribution  $P$  supported on  $\mathcal{X} \times \mathcal{Y} = \mathbb{R}^d \times \{-1, 1\}$ . In this setting  $P_{Y|X}$  is a deterministic function,  $h^* : \mathbb{R}^d \rightarrow \{-1, 1\}$ , i.e.,  $P = P_{\mathcal{X}} \diamond h^*$ .
- ▶ A **problem**  $\mathcal{P} = \mathcal{P}_{\mathcal{X}} \diamond \mathcal{H} = \{P_{\mathcal{X}} \diamond h | P_{\mathcal{X}} \in \mathcal{P}_{\mathcal{X}}, h \in \mathcal{H}\}$  is a set on joint distributions.
- ▶ A learning algorithm  $\mathcal{A}$  is a map  $\mathcal{A} : \bigcup_{n=0}^{\infty} (\mathcal{X} \times \mathcal{Y})^n \rightarrow \mathcal{H}$ . In other words, given a sample  $S = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$  it produces a hypothesis  $\mathcal{A}(S) \in \mathcal{H}$ . If  $\mathcal{A}$  is randomized then it outputs a distribution over hypotheses.
- ▶ 0-1 error of a hypothesis  $h \in \mathcal{H}$ :  $\text{err}_P(h) := \mathbb{P}_{(x,y) \sim P}[h(x) \neq y]$



- ▶ Teacher: deterministic, infallible. Requests accuracy  $\epsilon$ , confidence  $\delta$ .
- ▶ Realizable setting:  $c \in \mathcal{H}$  (learner has the capacity to learn)
- ▶ We say the algorithm  $\mathcal{A}$   $(\epsilon, \delta)$ -learns  $\mathcal{H}$  if for all  $P_{\mathcal{X}}, c \in \mathcal{H}$ :

$$\mathbb{P}_{S \sim P_{\mathcal{X}}^n} [\text{err}_{P_{\mathcal{X}} \diamond c}(\mathcal{A}(S)) < \epsilon] \geq 1 - \delta$$

- ▶ If  $\mathcal{A}$  is randomized the probability is over its randomization too.
- ▶ Sample complexity  $\mathcal{N}(\mathcal{A}, \mathcal{H}, \epsilon, \delta)$ : smallest  $n \in \mathbb{N}$  s.t.  $\mathcal{A}$   $(\epsilon, \delta)$ -learns  $\mathcal{H}$ .
- ▶ One (computer scientist) could argue that this is not an algorithm!  
Time-complexity requirements are missing. The learner might not even be computable.



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## Theorem (Blumer et al. 1989)

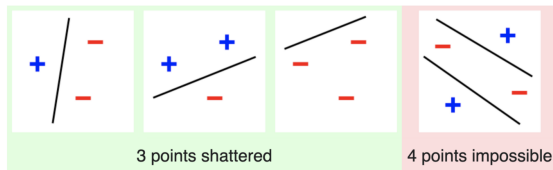
*If  $\mathcal{A}$  is consistent (the output hypothesis agrees with the sample) and ranges in  $\mathcal{H}$ , then for any  $\epsilon, \delta \in (0, 1)$*

$$\mathcal{N}(\mathcal{A}, \mathcal{H}, \epsilon, \delta) = O\left(\frac{1}{\epsilon}(\text{VCdim}(\mathcal{H}) \ln \frac{1}{\epsilon} + \ln \frac{1}{\delta})\right)$$

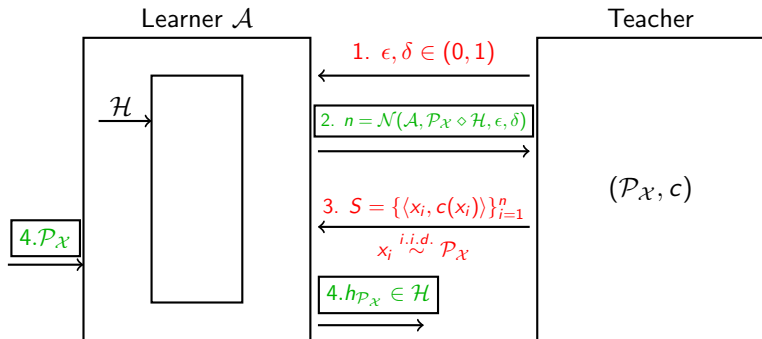
*For any  $\mathcal{A}$  and any  $\epsilon, \delta \in (0, 1)$*

$$\mathcal{N}(\mathcal{A}, \mathcal{H}, \epsilon, \delta) = \Omega\left(\frac{1}{\epsilon}(\text{VCdim}(\mathcal{H}) + \ln \frac{1}{\delta})\right)$$

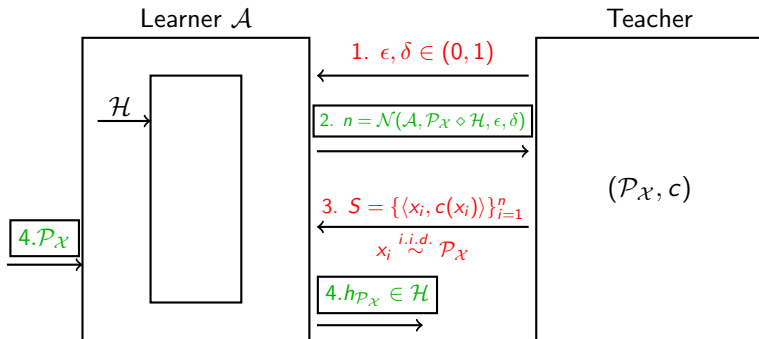
- ▶ Intricate connection between PAC-learnability and VC- dimension.
- ▶ *Growth function*  $\Pi_{\mathcal{H}}(n) := \sup_{x_1, \dots, x_n \in \mathcal{X}} |\{(h(x_1), \dots, h(x_n)) | h \in \mathcal{H}\}|$
- ▶  $\text{VCdim}(\mathcal{H}) := \max\{n | \Pi_{\mathcal{H}} = 2^n\}$
- ▶ VCdim of 2D linear functions is 3.



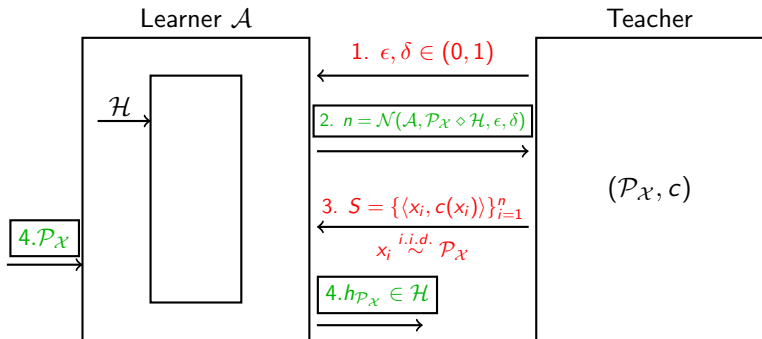
- ▶ VCdim:
  - ▶ Given  $\mathcal{H}$ , select a configuration of  $d$  points from  $\mathcal{X}$ .
  - ▶ An adversary that also knows  $\mathcal{H}$  will label them.
  - ▶ You need to select an  $h \in \mathcal{H}$  that classifies them correctly.
  - ▶ If you can do it,  $\text{VCdim} \geq d$ , else  $\text{VCdim} < d$ .
- ▶ Let  $\text{VCdim}(\mathcal{H}) = d$ . For  $n < d$ ,  $\Pi_{\mathcal{H}}(n) = 2^n$ . For  $n \geq d$ ,  $\Pi_{\mathcal{H}}(n) \leq \left(\frac{en}{d}\right)^d$



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- For example, if  $\mathcal{P}_{\mathcal{X}}$  is discrete then every class  $\mathcal{H}$  is learnable w.r.t.  $\mathcal{P}_{\mathcal{X}}$  (in realizable setting). How? Forget the  $\epsilon$ -tail!



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- For example, if  $\mathcal{P}_{\mathcal{X}}$  is discrete then every class  $\mathcal{H}$  is learnable w.r.t.  $\mathcal{P}_{\mathcal{X}}$  (in realizable setting). How? Forget the  $\epsilon$ -tail!
- Find the  $k$  most frequent points, where  $k$  is s.t.  $C = \{x_i\}_{i=1}^k$  s.t.  $\sum_{i=1}^k \mathcal{P}_{\mathcal{X}}(x_i) > 1 - \epsilon$ . Suppose the  $k$ -th is the least probable in  $C$ . Ask  $n \geq \ln(k/\delta)/\mathcal{P}_{\mathcal{X}}(x_k)$  samples. Each element of  $C$  appears in the samples at least once w.p. at least  $1 - \delta$ . Output any hypothesis **consistent** with the sample.

- ▶ This framework opens up the possibility to discuss **learning a problem  $\mathcal{P}$**  instead of just **learning a class  $\mathcal{H}$** .
- ▶ Especially for lower bounds on the sample complexity because one needs to account for those algorithms that "hard-code"  $\mathcal{P}$ .
- ▶ Given a problem  $\mathcal{P}$  and an algorithm  $\mathcal{A}$ , we can define the  **$(\epsilon, \delta)$ -sample complexity  $\mathcal{N}(\mathcal{A}, \mathcal{P}, \epsilon, \delta)$**  as the smallest  $n \in \mathbb{N}$  s.t.  $\forall P \in \mathcal{P}$  w.p. at least  $1 - \delta$  over the randomness of  $S = \{x_i, y_i\}_{i=1}^n$  and the algorithm,  $\text{err}_P(\mathcal{A}(S)) \leq \epsilon$ .

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- ▶ Also, we define the  **$\epsilon$ -expected sample complexity  $\mathcal{N}^*(\mathcal{A}, \mathcal{P}, \epsilon)$**  as the smallest  $n \in \mathbb{N}$  s.t.  $\forall P \in \mathcal{P}$ ,  $\mathbb{E}_{S \sim P^n}[\text{err}_P(\mathcal{A}(S))] \leq \epsilon$

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- ▶  $\mathcal{N}^*(\mathcal{A}, \mathcal{P}, \epsilon + \delta) \leq \mathcal{N}(\mathcal{A}, \mathcal{P}, \epsilon, \delta) \leq \mathcal{N}^*(\mathcal{A}, \mathcal{P}, \epsilon\delta), \forall \epsilon, \delta \in [0, 1]$



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### Theorem (Benedek and Itai 1991)

For any algorithm  $\mathcal{A}$  that  $(\epsilon, \delta)$ -learns  $\mathcal{H}$  with  $n$  i.i.d. samples from a fixed distribution  $\mathcal{P}_{\mathcal{X}}$  it must hold:

$$\mathcal{N}(\mathcal{A}, \mathcal{P}_{\mathcal{X}}, \epsilon, \delta) \geq \log[(1 - \delta)D(\mathcal{H}, \rho_{\mathcal{X}}, 2\epsilon)]$$

$D(\mathcal{H}, \rho_{\mathcal{X}}, \epsilon)$   $\epsilon$ -packing number i.e., the largest number of  $\epsilon$ -far hypotheses  $h \in \mathcal{H}$ . Distance is measured by  $\rho_{\mathcal{X}}(h, h') := \mathbb{P}_{X \sim \rho_{\mathcal{X}}}[h(X) \neq h'(X)]$ .

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Let  $\mathcal{W}$  be a parameter space (in our cases Euclidean space). A parametric model is an operator  $\mathcal{M} : \mathcal{W} \rightarrow \mathcal{Y}^{\mathcal{X}}$  i.e., given  $W \in \mathcal{W}$ ,  $\mathcal{M}[W] : \mathcal{X} \rightarrow \mathcal{Y}$ .

## Fully-Connected (FC) Neural Networks: $\mathbb{R}^d \rightarrow \mathbb{R}$

FC-NN[ $\mathbf{W}$ ]( $\mathbf{x}$ ) =  $W^L \sigma(W^{L-1} \dots \sigma(W_2 \sigma(W_1 \mathbf{x} + b_1) + b_2) + b_{L-1}) + b_L$ ,  
 where  $\mathbf{W} = (\{W_i, b_i\}_{i=1}^L)$ ,  $W_i \in \mathbb{R}^{d_{i-1} \times d_i}$ ,  $b_i \in \mathbb{R}^{d_i}$ ,  $d_0 = d$ ,  $d_L = 1$ .  
 Here  $\sigma : \mathbb{R} \rightarrow \mathbb{R}$  activation, (abusing notation)  $[\sigma(x)]_i = \sigma(x_i)$

## Convolutional Neural Network: $\mathbb{R}^d \rightarrow \mathbb{R}$

$$CNN[\mathbf{W}](\mathbf{x}) = \sum_{i=1}^r a_i \sigma([\mathbf{w} * \mathbf{x}]_{d'(r-1)+1:d'r}) + b,$$

where  $\mathbf{W} = (\mathbf{w}, \mathbf{a}, b) \in \mathbb{R}^k \times \mathbb{R}^r \times \mathbb{R}$ ,  $d = d' r$ .  $*$  :  $\mathbb{R}^k \times \mathbb{R}^d \rightarrow \mathbb{R}^d$   
 convolution, defined as  $[\mathbf{w} * \mathbf{x}]_i = \sum_{j=1}^k w_j x_{[i-j-1 \bmod d]+1}$  and  $\sigma : \mathbb{R}^{d'} \rightarrow \mathbb{R}$  is a composition of (strided) pooling and element-wise non-linearity.

- ▶ In principle, any CNN can be simulated by a large enough FCNN.
- ▶ There might even exist algorithms that, given a finite sample, can always find this CNN among the FCNNs.
- ▶ But (stochastic) gradient descent on FCNNs with gaussian initialization and optional weight decay, momentum, batch norm cannot do that for all CNNs.
- ▶ The authors prove that there is a CNN such that in the worst case, this algorithm requires samples that scale quadratically with the dimension of the features to achieve that.
- ▶ They find an explicit joint distribution on which some CNN is more-sample efficient than every FCNet.

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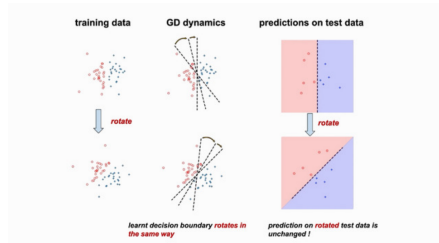
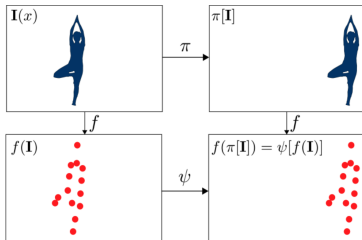
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- Usually task unknown, but symmetries (**group**) known. We exploit that by building parametric models that respect those symmetries (**equivariance**).

## Definition (Equivariance)

Consider a group  $\mathcal{G}$  acting on  $\mathcal{X}$  via " $\cdot$ " and on  $\mathcal{X}'$  via " $*$ ". We call a map  $f : \mathcal{X} \rightarrow \mathcal{X}'$   **$\mathcal{G}$ -equivariant** (w.r.t. these group actions) if it satisfies:

$$f(g \cdot x) = g * f(x), \forall g \in \mathcal{G}, x \in \mathcal{X}.$$

- ▶ The algorithm is a function that, given a sample  $S = \{x_i, y_i\}_{i=1}^n$ , produces a hypothesis  $h \in \mathcal{H}$ .
- ▶ If we define the actions:
  - ▶  $g.S = \{(g(x_i), y_i)\}_{i=1}^n$
  - ▶  $g * h = h \circ g^{-1}$

Then the definition above specializes to:

## Definition (Equivariant algorithm)

A learning algorithm  $\mathcal{A}$  is  $\mathcal{G}_{\mathcal{X}}$ -equivariant iff for any dataset  $\{(x_i, y_i)\}_{i=1}^n$  and  $\forall g \in \mathcal{G}_{\mathcal{X}}, x \in \mathcal{X}$

$$\mathcal{A}(\{(g(x_i), y_i)\}_{i=1}^n)(g(x)) \stackrel{d}{=} \mathcal{A}(\{x_i, y_i\}_{i=1}^n)(x)$$

- ▶ If  $\mathcal{A}$  outputs  $h$  on data  $S$  and outputs  $h \circ g^{-1}$  on data  $g.S$ , it is equivariant.

- ▶ (S)GD on FCNNs is (rotational)  $\mathcal{O}(d)$ -equivariant.
- ▶ (S)GD on a network with its first layer fully-connected is (rotational)  $\mathcal{O}(d)$ -equivariant even if the rest of the layers are e.g. convolutional.

$$\text{FC-NN}[\mathbf{W}](\mathbf{x}) = W_L \sigma(W_{L-1} \cdots \sigma(W_2 \sigma(W_1 \mathbf{x} + b_1) + b_2) + b_{L-1}) + b_L.$$

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## Algorithm 6 Gradient Descent for FC-NN (FC networks)

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**Input:** Initial parameter distribution  $P_{init}$ , total iterations  $T$ , training dataset  $\{\mathbf{x}_i, y_i\}_{i=1}^n$ , loss function  $\ell$

Sample  $\mathbf{W}^{(0)} \sim P_{init}$ .

**for**  $t = 0$  to  $T - 1$  **do**

$$\mathbf{W}^{(t+1)} = \mathbf{W}^{(t)} - \eta \sum_{i=1}^n \nabla \ell(\text{FC-NN}(\mathbf{W}^{(t)})(\mathbf{x}_i), y_i)$$

**return**  $h = \text{sign} [\text{FC-NN}[\mathbf{W}^{(T)}]]$ .

---

**Goal:**  $\text{FC-NN}[\widetilde{\mathbf{W}}^{(t)}](R\mathbf{x}) = \text{FC-NN}[\mathbf{W}^{(t)}](\mathbf{x})$ , where  $\widetilde{\mathbf{W}}$  trained on  $R\mathbf{x}_i$  and  $\mathbf{W}$  trained on  $\mathbf{x}_i$ .

**Claim:**  $\widetilde{W}_1^{(0)} = W_1^{(0)} R^{-1}, \widetilde{\mathbf{W}}_{-1}^{(0)} = \mathbf{W}_{-1}^{(0)} \implies \widetilde{W}_1^{(t)} = W_1^{(t)} R^{-1}, \widetilde{\mathbf{W}}_{-1}^{(t)} = \mathbf{W}_{-1}^{(t)}, \forall t$ .

**Induction:** If  $\widetilde{\mathbf{W}} = (\widetilde{W}_1, \widetilde{\mathbf{W}}_{-1}) = (W_1 R^{-1}, \mathbf{W}_{-1})$ , then  $\forall R \in \mathcal{O}(d)$ ,

$$\nabla_{\widetilde{W}_1} \ell(\text{FC-NN}(\widetilde{\mathbf{W}})(R\mathbf{x}_i), y_i) = \nabla_{W_1} \ell(\text{FC-NN}(\mathbf{W})(\mathbf{x}_i), y_i) R^{-1} \quad (\text{chain rule})$$

$$\nabla_{\widetilde{\mathbf{W}}_{-1}} \ell(\text{FC-NN}(\widetilde{\mathbf{W}})(R\mathbf{x}_i), y_i) = \nabla_{\mathbf{W}_{-1}} \ell(\text{FC-NN}(\mathbf{W})(\mathbf{x}_i), y_i) \quad (\widetilde{W}_1 R\mathbf{x}_i = W_1 \mathbf{x}_i)$$

- ▶ Is (S)GD on CNNs  $\mathcal{O}(d)$ -equivariant? Not in general! No proof.
- ▶ Intuitively before a rotation  $\mathbf{x} \rightarrow R\mathbf{x}$  was absorbed by  $W_1 \rightarrow W_1 R^{-1}$ . If we stack the convolutional weights on a matrix  $W_1$ , then  $W_1 R^{-1}$  will not be implementable by a convolution.



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## Algorithm 1 Iterative algorithm $\mathcal{A}$

---

**Input:** Initial parameter distribution  $P_{init}$  supported in  $\mathcal{W} = \mathbb{R}^m$ , total iterations  $T$ , training dataset  $\{\mathbf{x}_i, y_i\}_{i=1}^n$ , parametric model  $\mathcal{M} : \mathcal{W} \rightarrow \mathcal{Y}^{\mathcal{X}}$ , (possibly random) iterative update rule  $F(\mathbf{W}, \mathcal{M}, \{\mathbf{x}_i, y_i\}_{i=1}^n)$

**Output:** Hypothesis  $h : \mathcal{X} \rightarrow \mathcal{Y}$ .

Sample  $\mathbf{W}^{(0)} \sim P_{init}$ .

**for**  $t = 0$  to  $T - 1$  **do**

$\mathbf{W}^{(t+1)} = F(\mathbf{W}^{(t)}, \mathcal{M}, \{\mathbf{x}_i, y_i\}_{i=1}^n)$ .

**return**  $h = \text{sign} [\mathcal{M}[\mathbf{W}^{(T)}]]$ .

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### Theorem

The iterative algorithm  $\mathcal{A}$  is  $\mathcal{G}_{\mathcal{X}}$ -equivariant if the following conditions are met:

- ① There's a group  $\mathcal{G}_{\mathcal{W}}$  acting on  $\mathcal{W}$  and a group isomorphism  $\tau : \mathcal{G}_{\mathcal{X}} \rightarrow \mathcal{G}_{\mathcal{W}}$ , such that  $\mathcal{M}[\tau(g)(\mathbf{W})](g(\mathbf{x})) = \mathcal{M}[\mathbf{W}](\mathbf{x})$ ,  $\forall \mathbf{x} \in \mathcal{X}, \mathbf{W} \in \mathcal{W}, g \in \mathcal{G}$ .
- ② The initialization  $P_{init}$  is invariant under group  $\mathcal{G}_{\mathcal{W}}$ , i.e.  $\forall g \in \mathcal{G}_{\mathcal{W}}, P_{init} = P_{init} \circ g^{-1}$ .
- ③ Update rule  $F$  is invariant under any joint group action  $(g, \tau(g))$ ,  $\forall g \in \mathcal{G}$ . In other words,  $[\tau(g)](F(\mathbf{W}, \mathcal{M}, \{\mathbf{x}_i, y_i\}_{i=1}^n)) = F([\tau(g)](\mathbf{W}), \mathcal{M}, \{g(\mathbf{x}_i), y_i\}_{i=1}^n)$ .

### Remark

(1) is the minimum expressiveness requirement, (2) is the induction basis and (3) is the for induction

For non-iterative algorithms, the authors also show that:

- ▶ Kernel Regression:

$$\text{REG}_K(\{x_i, y_i\}_{i=1}^n)(x) := 1[K(x, X_n) \cdot K(X_n, X_n)^\dagger y \geq 0]$$

is  $\mathcal{G}_X$ -equivariant if the kernel  $K(x, y)$  is invariant i.e.,  
 $K(gx, gy) = K(x, y), \forall x, y \in \mathcal{X}, g \in \mathcal{G}_X$ .

- ▶ Empirical Risk Minimization:

$$\text{ERM}_{\mathcal{H}}(\{x_i, y_i\}_{i=1}^n) := \arg \min_{h \in \mathcal{H}} \sum_{i=1}^n 1[h(x_i) \neq y_i]$$

is  $\mathcal{G}_X$ -equivariant if the minimum is unique and  $\mathcal{H} = \mathcal{H} \circ \mathcal{G}_X$ .

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## Conclusions

## References

- ▶  $\mathcal{X} = \mathbb{R}^d$ ,  $P$  is uniform on the set  $\{(\mathbf{e}_i y, y) | i \in [d], y = \pm 1\}$
- ▶ Observe that the sign of the one-hot encoded vectors determine their label.
- ▶ A simple average pooling would learn this task.
- ▶ If  $\mathcal{A}$  is orthogonal equivariant then  $\forall R \in \mathcal{O}(d)$ ,

$$\mathcal{A}(\{R\mathbf{x}_i, y_i\}_{i=1}^n)(R\mathbf{x}) = \mathcal{A}(\{\mathbf{x}_i, y_i\}_{i=1}^n)(\mathbf{x})$$

- ▶ Let  $S = \{\mathbf{x}_i, y_i\}_{i=1}^n$  be a sample from  $P$ .
- ▶ There is a function  $f_S$  s.t.  $\mathcal{A}(S)(\mathbf{x}) = f_S(\mathbf{x}^T \mathbf{x}_1, \dots, \mathbf{x}^T \mathbf{x}_n)$
- ▶ When  $n \leq d/2$ , with probability at least  $1/2$ ,  $\mathcal{A}(S)(\mathbf{x}) = f_S(0, 0, \dots, 0)$ . That's because any unseen point would produce only zero inner products.
- ▶ Thus  $\mathcal{A}$  outputs the wrong answer with probability at least  $1/4$ .

## Notation:

- ▶  $g : \mathcal{X} \rightarrow \mathcal{X}$  is a 1-1 transformation. We can define  $gP_{\mathcal{X}} = P_{\mathcal{X}} \circ g^{-1}$  so that  $X \sim P_{\mathcal{X}} \iff gX \sim gP_{\mathcal{X}} = P_{\mathcal{X}} \circ g^{-1}$
- ▶  $gP = P \circ g^{-1}$  similarly as  $X \sim P_{\mathcal{X}} \iff (gX, Y) \sim P \circ g^{-1}$  where  $P = P_{\mathcal{X}} \diamond h$ . In other words,  $(P_{\mathcal{X}} \diamond h) \circ g = (P_{\mathcal{X}} \circ g) \diamond (h \circ g)$

## Observation:

- ▶ Clearly, for any  $\mathcal{G}_{\mathcal{X}}$ -equivariant algorithm we have:

$$\mathcal{N}^*(\mathcal{A}, \mathcal{P}, \epsilon) = \mathcal{N}^*(\mathcal{A}, \mathcal{P} \circ g, \epsilon), \forall g \in \mathcal{G}_{\mathcal{X}}.$$

or

$$\mathcal{N}^*(\mathcal{A}, \mathcal{P}, \epsilon) = \mathcal{N}^*(\mathcal{A}, \mathcal{P} \circ \mathcal{G}_{\mathcal{X}}, \epsilon)$$

Theorem (Reducing Learning using Equivariant Algorithms to Learning an augmented class)

1. Let  $\mathbb{A}$  be the set of all algorithms and  $\mathbb{A}_{\mathcal{G}_{\mathcal{X}}}$  be the set of all  $\mathcal{G}_{\mathcal{X}}$ -equivariant algorithms. Then,

$$\inf_{\mathcal{A} \in \mathbb{A}_{\mathcal{G}_{\mathcal{X}}}} \mathcal{N}^*(\mathcal{A}, \mathcal{P}, \epsilon) \geq \inf_{\mathcal{A} \in \mathbb{A}} \mathcal{N}^*(\mathcal{A}, \mathcal{P} \circ \mathcal{G}_{\mathcal{X}}, \epsilon) \quad (1)$$

2. Let the set  $\mathcal{P}_{\mathcal{X}}$  be invariant under  $\mathcal{G}_{\mathcal{X}}$ , i.e.,  $\mathcal{P}_{\mathcal{X}} \circ \mathcal{G}_{\mathcal{X}} = \mathcal{P}_{\mathcal{X}}$ . Then,

$$\inf_{\mathcal{A} \in \mathbb{A}_{\mathcal{G}_{\mathcal{X}}}} \mathcal{N}^*(\mathcal{A}, \mathcal{P}_{\mathcal{X}} \diamond \mathcal{H}, \epsilon) \geq \inf_{\mathcal{A} \in \mathbb{A}} \mathcal{N}^*(\mathcal{A}, \mathcal{P}_{\mathcal{X}} \diamond (\mathcal{H} \circ \mathcal{G}_{\mathcal{X}}), \epsilon) \quad (2)$$

The equalities in both are attained when  $\mathcal{G}_{\mathcal{X}}$  is a compact group.

- **Take home message:** Learning under algorithmic equivariance is at least as hard as learning an augmented function class.

Suppose we need to learn a single labelling function  $h^*$ :

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- ▶ But this is not orthogonal equivariant! If you just rotate the data points it observed (not the distribution or the labels):  $\{g(x_i), y_i\}_{i=1}^n$  it will still output  $h^*$ , not  $h^* \circ g^{-1}$ !

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- ▶ If  $\mathcal{A} \in \mathbb{A}_{\mathcal{G}_X}$  then by definition  $\mathcal{A}$  has the same performance on  $P := P_X \diamond \{h^*\}$  and the rotated  $P \circ g^{-1} := (P_X \circ g^{-1}) \diamond (h^* \circ g^{-1})$ .
- ▶ Because now the learner  $\mathcal{A}$  observes:
  - ▶ the rotated data points with the same probability, i.e.,  $X \rightarrow gX$ ,
  - ▶ At the same time, the label stays fixed i.e.  
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- ▶ Dually  $\mathcal{A} \in \mathbb{A}_{\mathcal{G}_{\mathcal{X}}}$ :  
 $(\epsilon, \delta)$ -learn  $h^*$  on  $\mathcal{P}_{\mathcal{X}} \circ g \implies (\epsilon, \delta)$ -learn  $h^* \circ g^{-1}$  on  $\mathcal{P}_{\mathcal{X}}$ .
- ▶ And thus,  $\mathcal{N}^*(\mathcal{A}, \mathcal{P}, \epsilon) = \mathcal{N}^*(\mathcal{A}, \mathcal{P} \circ g^{-1}, \epsilon)$ , for all  $g \in \mathcal{G}_{\mathcal{X}}$ . That's an invariant **for all orthogonal equivariant learning algorithms**.

- We can consider two important learning settings where the set  $\mathcal{P}_{\mathcal{X}}$  satisfies  $\mathcal{P}_{\mathcal{X}} \circ \mathcal{G}_{\mathcal{X}} = \mathcal{P}_{\mathcal{X}}$ .
  1. All distributions on  $\mathcal{X}$ . Then if  $\mathcal{A} \in \mathbb{A}_{\mathcal{G}_{\mathcal{X}}}$  it learns not only  $h^*$  over all distributions but **all  $h^* \circ \mathcal{G}_{\mathcal{X}}$  over all distributions**. But this is the standard PAC setting and learning is at least as hard for  $\mathcal{A}$  as the best algorithm on  $h^* \circ \mathcal{G}_{\mathcal{X}}$ . Show:  $\text{VCdim}(h^* \circ \mathcal{G}_{\mathcal{X}}) = \Omega(d^2)$ .

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  2.  $\mathcal{P}_{\mathcal{X}} = \{\mathcal{N}(0, I_d)\}$ . Now learning over all rotated copies of the joint is learning **all  $h^* \circ \mathcal{G}_{\mathcal{X}}$  on the gaussian**. Now a bound on VCdim will not suffice and we need to bound the sample complexity in another way. We are not in the standard PAC learning setting. We are in Benedek-Itai's world!

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    - a In this setting, the lower bound on the sample complexity holds **even for the algorithm that knows  $\mathcal{P}_{\mathcal{X}}$**  (but this algorithm still has to learn all concepts  $h^* \circ \mathcal{G}_{\mathcal{X}}$ ).
    - b Use Benedek-Itai bound:  $\mathcal{N}(\mathcal{A}, \mathcal{P}_{\mathcal{X}}, \epsilon, \delta) \geq \log[(1 - \delta)D(\mathcal{H}, \rho_{\mathcal{X}}, 2\epsilon)]$ . Show that  $D(\mathcal{H}, \rho_{\mathcal{X}}, \epsilon_0) = \Omega(d^2)$
    - c Why is the second case stronger conceptually than the first? Because it shows that **ALL orthogonal equivariant algorithms fail in the same single problem (joint distribution)**.

- ▶ The generalization of equivariant algorithms was first studied by [Ng 2004]. The lower bounds there are similar to the first case (but weaker) and cover only the first setting.



- ▶ The generalization of equivariant algorithms was first studied by [Ng 2004]. The lower bounds there are similar to the first case (but weaker) and cover only the first setting.
- ▶ This paper also extends the lower bounds to permutation equivariant algorithms (FCNets+ Adam/Adagrad) as well as  $l_2$ -regression.

Symmetry	Sign Flip	Permutation	Orthogonal	Linear
Matrix Group	Diagonal, $ M_{ii}  = 1$	Permutation	Orthogonal	Invertible
Algorithms	AdaGrad, Adam	AdaGrad, Adam	SGD Momentum	Newton's method
Initialization	Symmetric distribution	i.i.d.	i.i.d. Gaussian	All zero
Regularization	$\ell_p$ norm	$\ell_p$ norm	$\ell_2$ norm	None

**Figure:** Examples of gradient-based equivariant training algorithms for FC Networks. The initialization requirement is only for the first layer of the network.

**Consider:**  $\mathcal{X} = \mathbb{R}^{2d}$  and  $h^*(x) = \text{sign}[\sum_{i=1}^d x_i^2 - \sum_{i=d+1}^{2d} x_i^2]$ .

As we discussed, this setup reduces to standard PAC-learning over the augmented class  $\{h^* \circ g | g \in \mathcal{O}(d)\}$ . Lower bounding the VC-dimension of this class by  $\Omega(d^2)$  and using Blumer's lower bound results in:

## Theorem (Single function, All Distributions)

Let  $\mathcal{P} = \{\text{all distributions}\} \diamond \{h^*\}$ . Then:

1.  $\mathcal{N}(\mathcal{A}, \mathcal{P}, \epsilon, \delta) = \Omega((d^2 + \ln \delta)/\epsilon)$ , for all  $\mathcal{A} \in \mathbb{A}_{\mathcal{G}_{\mathcal{X}}}$ .
2. There is a 2-layer CNN architecture s.t.  
 $\mathcal{N}(\text{ERM}_{\text{CNN}}, \mathcal{P}, \epsilon, \delta) = O(\frac{1}{\epsilon} (\log \frac{1}{\epsilon} + \log \frac{1}{\delta}))$

This lower bound does not show a separation *for a single task*. While some  $\mathcal{P}_{\mathcal{X}}^1 \diamond h^*$  might be hard for some network  $\text{FCNN}_1$ , it might be easy for another. Next result shows that there is a **single task that is hard for all FCNNs**.

### Theorem (Single function, Single Distribution)

Let  $\mathcal{P} = \{N(0, I_{2d})\} \diamond h^*$ . There is a constant  $\epsilon_0 > 0$  (indep. of  $d$ ) s.t.:

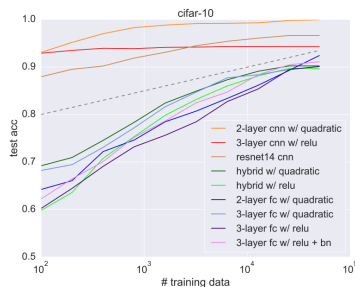
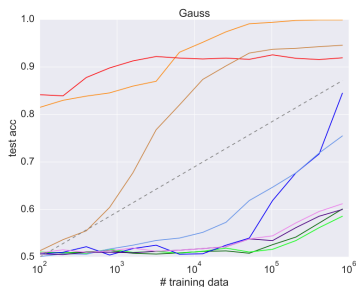
1.  $\mathcal{N}^*(\mathcal{A}, \mathcal{P}, \epsilon_0) = \Omega(d^2)$ , for all  $\mathcal{A} \in \mathbb{A}_{\mathcal{G}_{\mathcal{X}}}$ .
2. There is a 2-layer CNN architecture s.t.  
 $\mathcal{N}(\text{ERM}_{\text{CNN}}, \mathcal{P}, \epsilon, \delta) = O(\frac{1}{\epsilon} (\log \frac{1}{\epsilon} + \log \frac{1}{\delta}))$ .
3. Moreover,  $\text{ERM}_{\text{CNN}}$  could be realized by gradient descent (on the second layer only).

### Theorem (Multiple functions, Single Distribution)

Let  $\mathcal{P} = \{N(0, I_d)\} \diamond \{\text{sign} \left[ \sum_{i=1}^d a_i x_i^2 \right] \mid a_i \in \mathbb{R}\}$ .

1.  $\mathcal{N}^*(\mathcal{A}, \mathcal{P}, \epsilon) = \Omega(d^2/\epsilon)$ , for all  $\mathcal{A} \in \mathbb{A}_{\mathcal{G}_{\mathcal{X}}}$ .
2. There is a 2-layer CNN architecture s.t.  
 $\mathcal{N}(\text{ERM}_{\text{CNN}}, \mathcal{P}, \epsilon, \delta) = O(\frac{1}{\epsilon} (d \log \frac{1}{\epsilon} + \log \frac{1}{\delta}))$ .
3. Moreover,  $\text{ERM}_{\text{CNN}}$  could be realized by gradient descent (on the second layer only).

- ▶ The task is to find whether the Red or the Green channel in CIFAR10 images has larger  $l_2$ -norm.
- ▶ CIFAR10 has 50k images of size  $32 \times 32 \times 3$ . The theory predicts that any FCNN would need around  $32^4 \approx 1M$  images to learn this function. (if the distribution is complex enough to be close to i.i.d. gaussian; which isn't)



## Theorem (Single function, Single Distribution)

Let  $\mathcal{P} = \{N(0, I_{2d})\} \diamond h^*$ , s.t.  $h^*(x) = \text{sign}[\sum_{i=1}^d x_i^2 - \sum_{i=d+1}^{2d} x_i^2]$ .  
 There is a constant  $\epsilon_0 > 0$  (indep. of  $d$ ) s.t.:

$$\mathcal{N}^*(\mathcal{A}, \mathcal{P}, \epsilon_0) = \Omega(d^2), \text{ for all } \mathcal{A} \in \mathbb{A}_{\mathcal{G}_{\mathcal{X}}}.$$

## Sketch of Proof.

1. We have  $\mathcal{H}_o = \{h_U := \text{sign}[x_{1:d}^T U x_{d+1:2d}] | U \in \mathcal{O}(d)\} \subseteq h^* \circ \mathcal{O}(2d)$
2. Use Benedek-Itai on  $\mathcal{P} = N(0, I_{2d}) \diamond \mathcal{H}_o$ . Then,  
 $\mathcal{N}^*(\mathcal{A}, \mathcal{P}, \epsilon_0) \geq \log(1 - \delta) + \log D(\mathcal{H}_o, \rho_{\mathcal{X}}, 2\epsilon)$
3. Show  $\rho_{\mathcal{X}}(h_U, h_V) = \Omega(\frac{\|U - V\|_F}{\sqrt{d}})$ . Larger pairwise distances imply bigger packing.
4. Pack just the elements of  $\mathcal{SO}(d)$ . Again, supersets imply bigger packing.
5. Groups are hard to handle. But (some) Lie groups can be described by their Lie algebra, which is a vector space.
6. Select a 1-1 set (or smaller) on the Lie algebra  $\mathfrak{so}(2d)$  and show that for this set  $\|\exp u - \exp v\|_F = \Omega(\|u - v\|_F)$ .
7. Inverse Santalo's inequality to show  $\geq (\frac{c}{\epsilon})^{\binom{d}{2}}$

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- ▶ We can unify a lot of algorithms, with practical relevance, under the umbrella of **algorithmic equivariance**. The authors proved lower bound on their sample complexity.
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- ▶ From the bounds we get that there are even very small CNNs (or tasks that a CNN can approximate) that no FCNN can find them efficiently from samples.
- ▶ The class of CNNs is kind of unnatural. Especially the strided pooling. Also, the distribution might be overly complex relative e.g. to image datasets.
- ▶ The method does not unify CNNs. There might be other CNNs, with more practical relevance, that perform worse than some FCNNs.

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