Emergent Equivariance in Deep Ensembles

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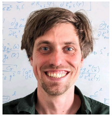
WASP WALLENBERG AI, AUTONOMOUS SYSTEMS AND SOFTWARE PROGRAM

in collaboration with



Pan Kessel*

from Prescient Design

A Genentech Accelerator

Data augmentation

- 👍 Easy to implement
- 👍 No specialized architecture necessary

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Can we understand data augmentation theoretically?

Empirical NTK

Training dynamics under continuous gradient descent:

learning rate

loss

$$\frac{\mathrm{d}\mathcal{N}_\theta(x)}{\mathrm{d}t} = -\frac{\eta}{N}\sum_{i=1}^{N} \Theta_\theta(x, x_i) \frac{\partial L}{\partial \mathcal{N}(x_i)}$$

training sample

Empirical NTK

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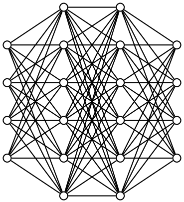
training sample

with the empirical neural tangent kernel (NTK)

$$\Theta_\theta(x, x') = \sum_\mu \frac{\partial \mathcal{N}(x)}{\partial \theta_\mu}\frac{\partial \mathcal{N}(x')}{\partial \theta_\mu}$$

Infinite width limit

[Jacot et al. 2018]



Infinite width limit

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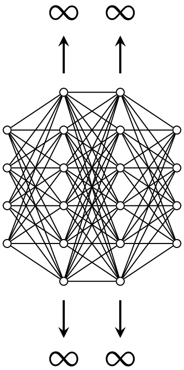

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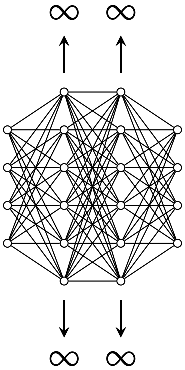

NTK becomes independent of initialization

Infinite width limit

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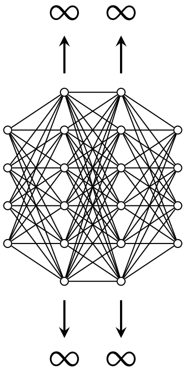

- 👍 NTK becomes independent of initialization
- 👍 NTK becomes constant in training

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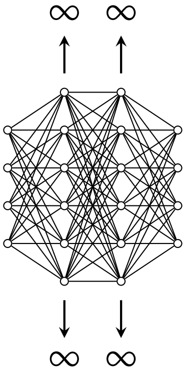

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- NTK can be computed for most networks

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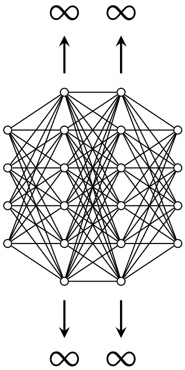

- NTK becomes independent of initialization
- NTK becomes constant in training
- NTK can be computed for most networks
- ✓ Training dynamics can be solved

Mean prediction from NTK

[Jacot et al. 2018]

At infinite width, the mean prediction is given by

$$\mu_t(x) = \Theta(x, X)\Theta(X, X)^{-1}(\mathbb{I} - e^{-\eta\Theta(X,X)t})Y$$

Mean prediction from NTK

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At infinite width, the mean prediction is given by

neural tangent kernel

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train data

Mean prediction from NTK

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learning rate

train data

Mean prediction from NTK

[Jacot et al. 2018]

ⓘ At infinite width, the mean prediction is given by

neural tangent kernel train labels

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Data augmentation

Data augmentation at infinite width

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augmented data

augmented labels

Data augmentation at infinite width

group transformation

$$\mu_t(\rho(g)x) = \Theta(\rho(g)x, X)\,\Theta(X, X)^{-1}\left(\mathbb{I} - e^{-\eta\Theta(X,X)t}\right)Y$$

augmented data

augmented labels

Data augmentation at infinite width

group transformation

for augmented data

$$\mu_t(\rho(g)x) = \Theta(\rho(g)x, X)\,\Theta(X, X)^{-1}\left(\mathbb{I} - e^{-\eta\Theta(X,X)t}\right)Y$$

augmented data

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Data augmentation at infinite width

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$$\mu_t(\rho(g)x) = \Theta(x, X)\Theta(X, X)^{-1}(\mathbb{I} - e^{-\eta\Theta(X,X)t})\rho(g)Y$$

augmented data

augmented labels

Data augmentation at infinite width

group transformation

augmented labels

$$\mu_t(\rho(g)x) = \Theta(x, X)\Theta(X, X)^{-1}(\mathbb{I} - e^{-\eta\Theta(X,X)t})\underbrace{\rho(g)Y}_{=Y}$$

for invariance

Data augmentation at infinite width

group transformation

$$\mu_t(\rho(g)x) = \Theta(x,X)\Theta(X,X)^{-1}(\mathbb{I} - e^{-\eta\Theta(X,X)t})\underbrace{\rho(g)Y}_{=Y}$$
$$= \mu_t(x)$$

for invariance

Mean prediction

$$\mu_t(x)$$

Mean prediction

$$\mu_t(x) = \mathbb{E}_{\theta_0 \sim \text{initializations}}[\mathcal{N}_{\theta_t}(x)]$$

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$$\mu_t(x) = \mathbb{E}_{\theta_0 \sim \text{initializations}}[\mathcal{N}_{\theta_t}(x)] = \lim_{n\to\infty} \frac{1}{n} \sum_{\theta_0=\text{init}_1}^{\text{init}_n} \mathcal{N}_{\theta_t}(x)$$

Mean prediction

$$\mu_t(x) = \mathbb{E}_{\theta_0 \sim \text{initializations}}\left[\mathcal{N}_{\theta_t}(x)\right] = \lim_{n\to\infty} \underbrace{\frac{1}{n} \sum_{\theta_0=\text{init}_1}^{\text{init}_n} \mathcal{N}_{\theta_t}(x)}_{\text{mean prediction of deep ensemble}}$$

Main conclusion

Deep ensembles trained with data augmentation are equivariant.

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- ✓ Proof of exact equivariance for
    - full data augmentation
    - infinite ensembles
    - at infinite width
- ✓ Equivariance holds for all training times
- ✓ Equivariance holds away from the training data

Intuitive explanation

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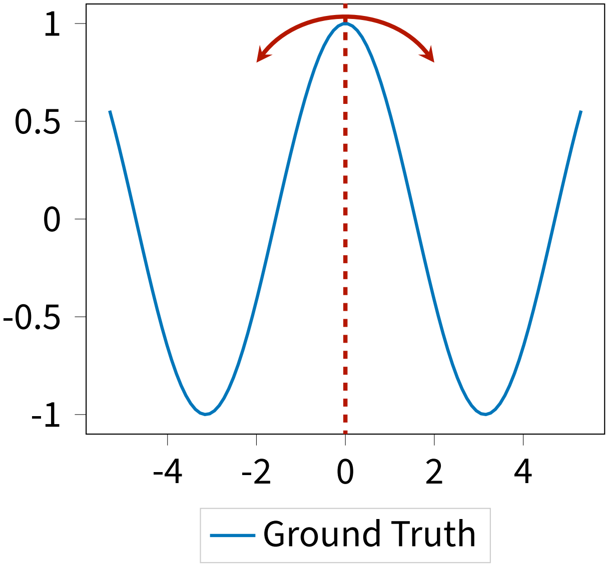
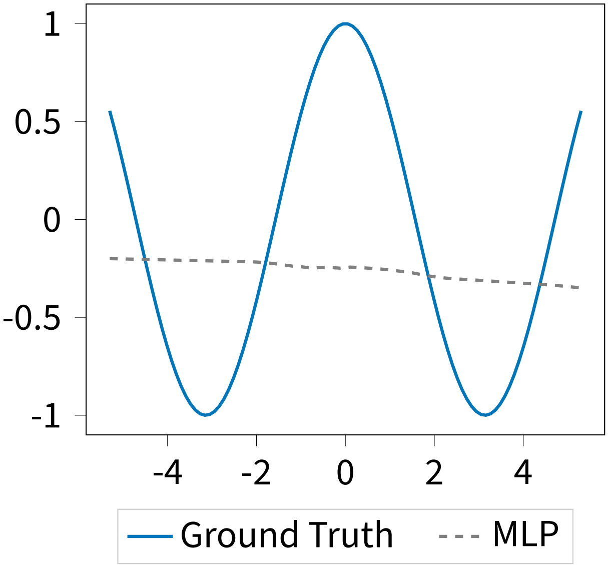
ⓘ At infinite width, the mean output at initialization is zero everywhere.

⇨ Training with full data augmentation leads to an equivariant function.

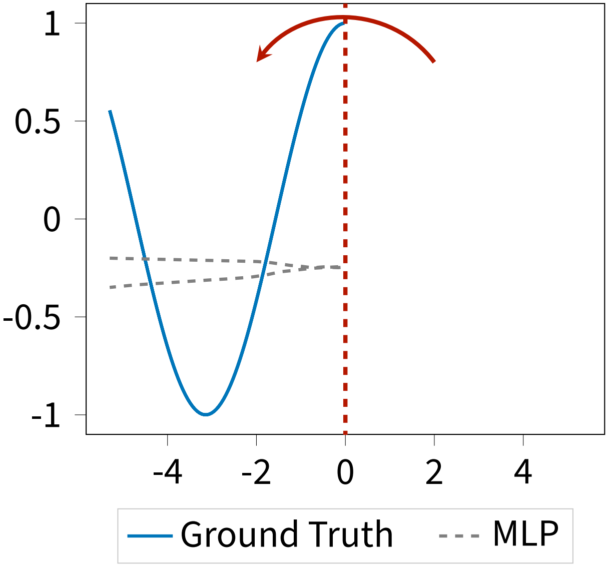
Toy example


1
0.5
0
-0.5
-1
-4
-2
0
2
4
Ground Truth

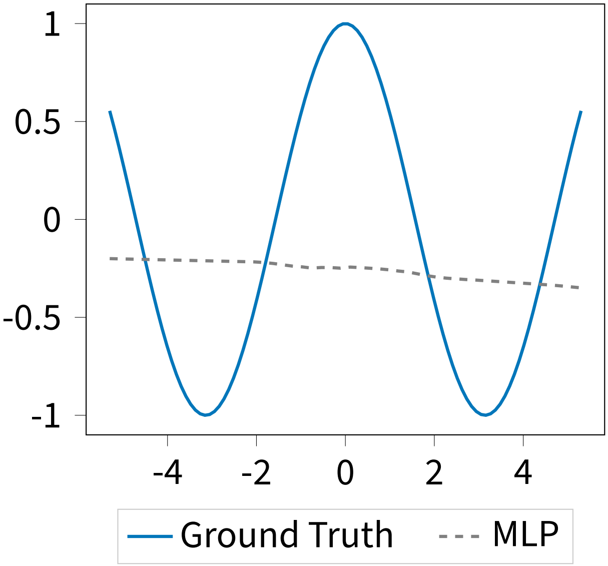
Initialization



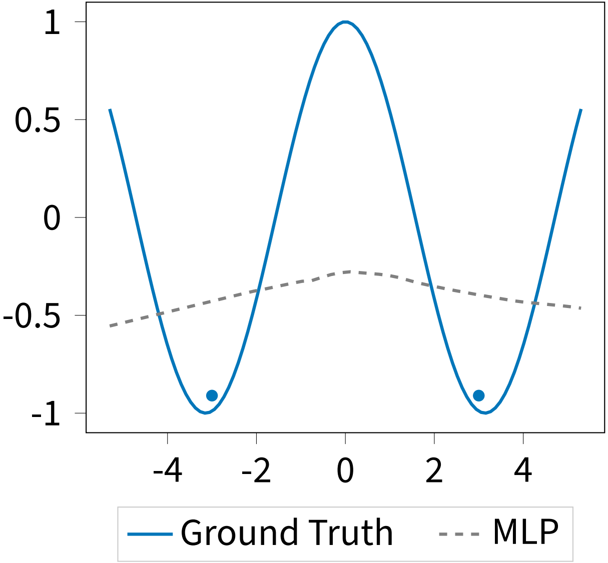
Initialization



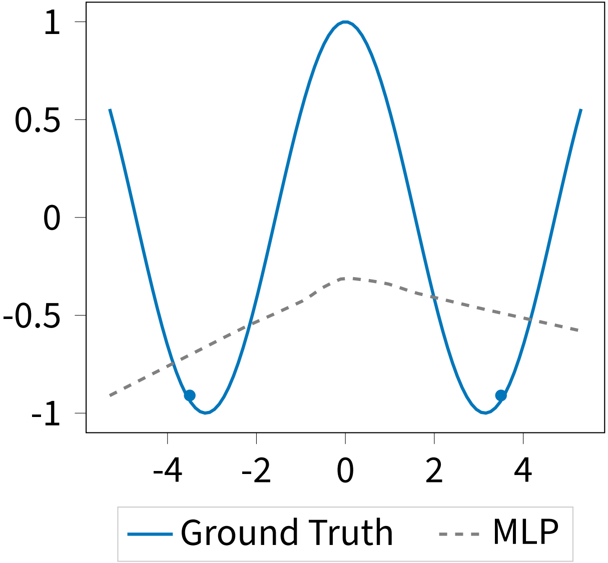
Initialization



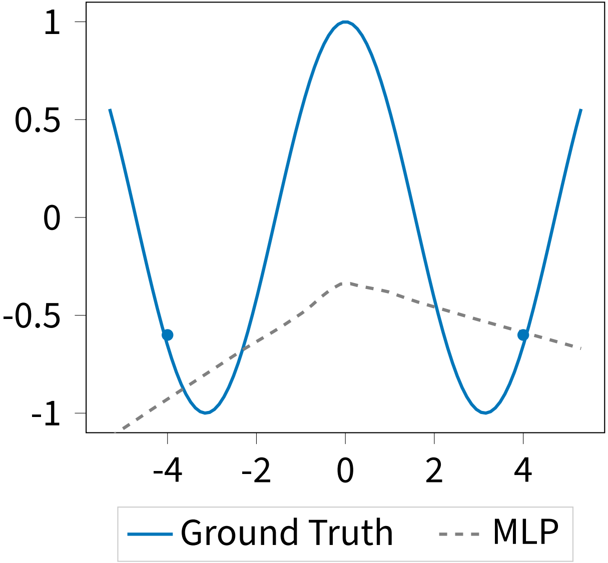
After 1 Training Step



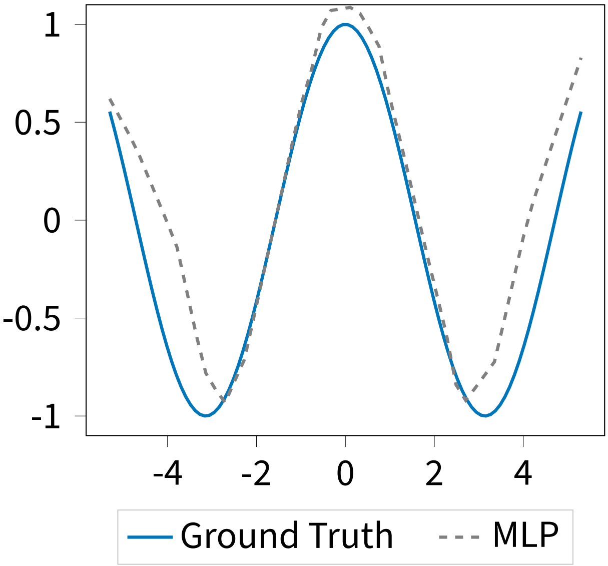
After 2 Training Steps



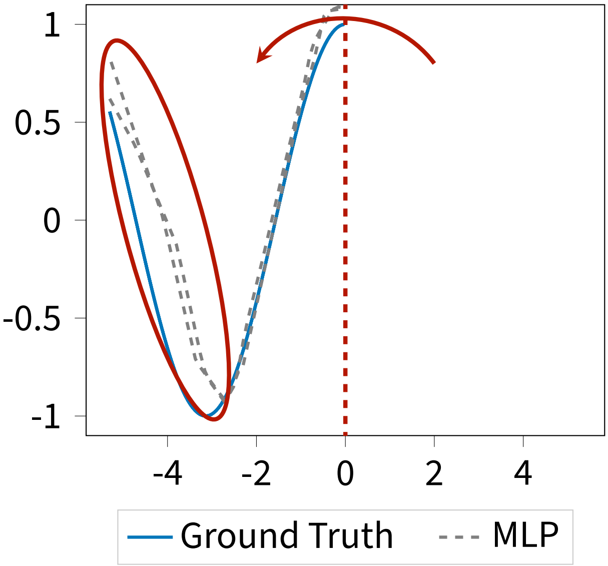
After 3 Training Steps



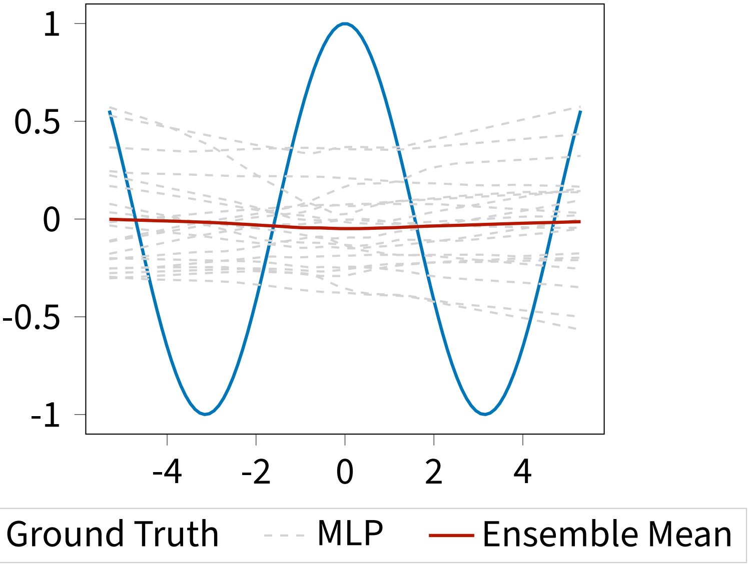
After 2000 Training Steps



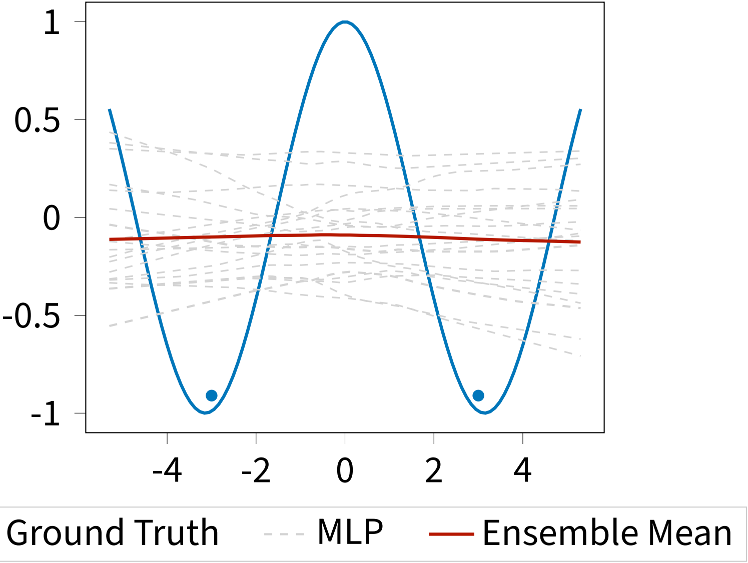
After 2000 Training Steps



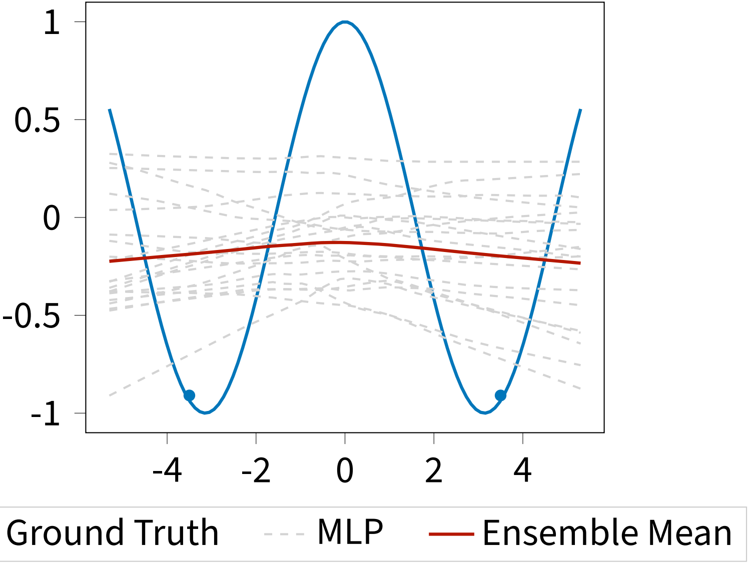
Initialization



After 1 Training Step



After 2 Training Steps



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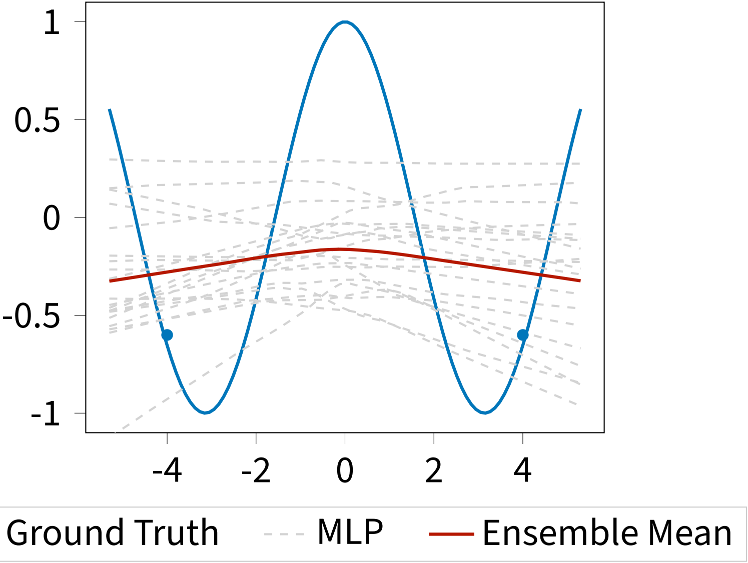
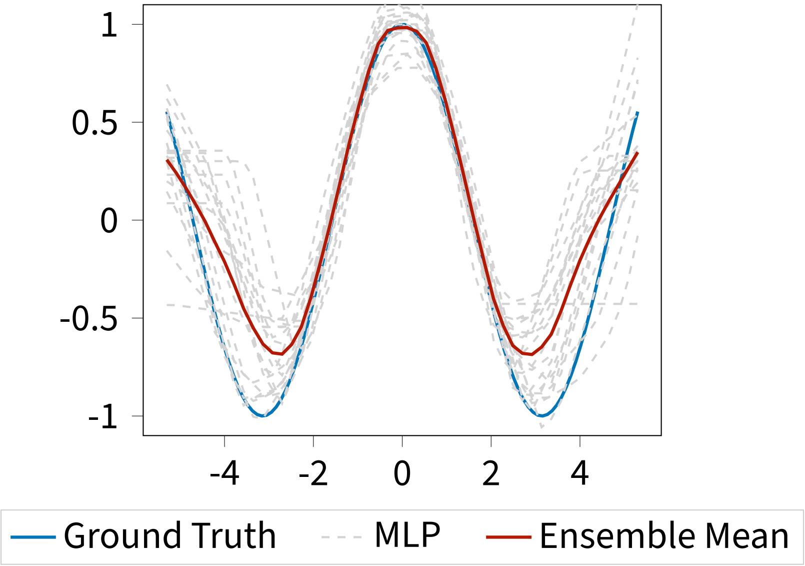
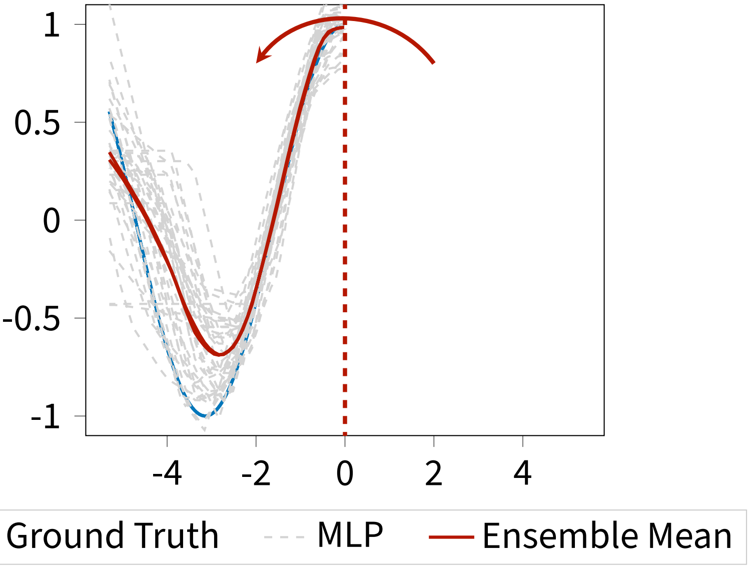


After 2000 Training Steps

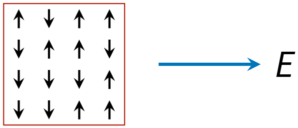


After 2000 Training Steps



Experiments

Ising model



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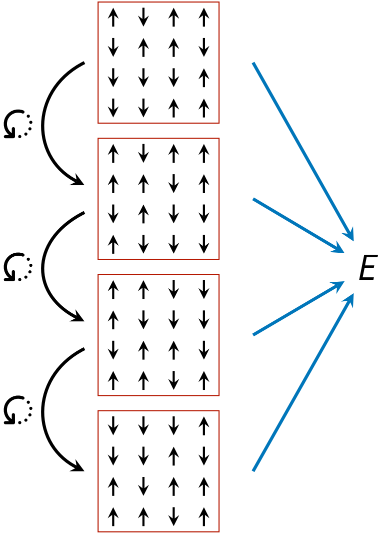
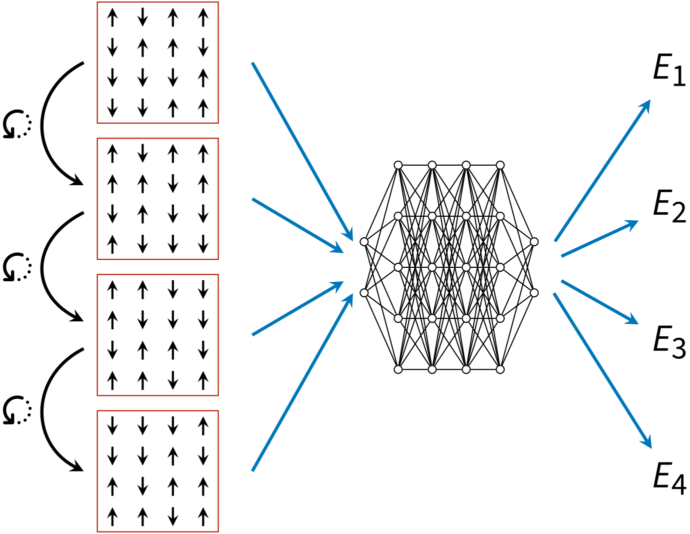
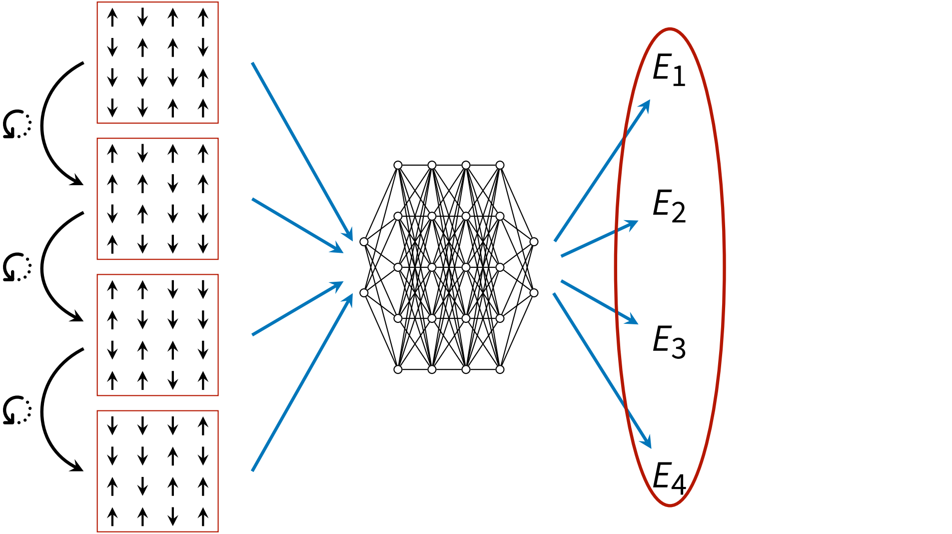
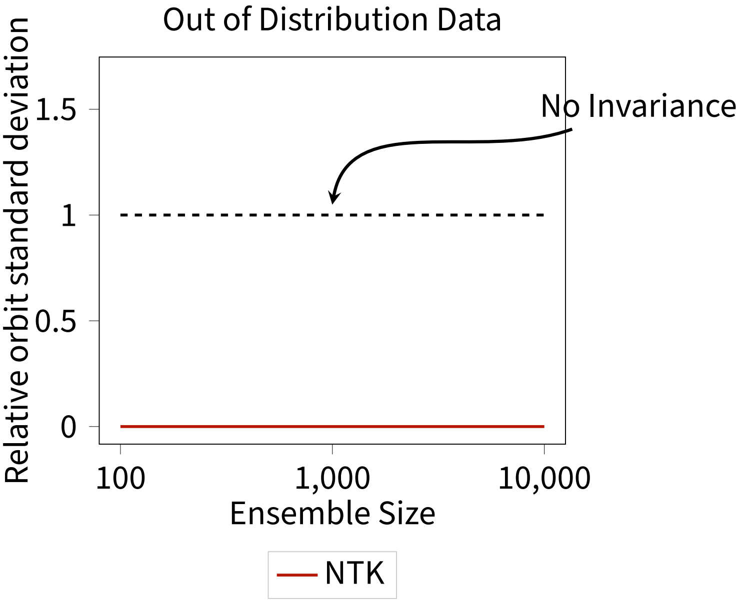


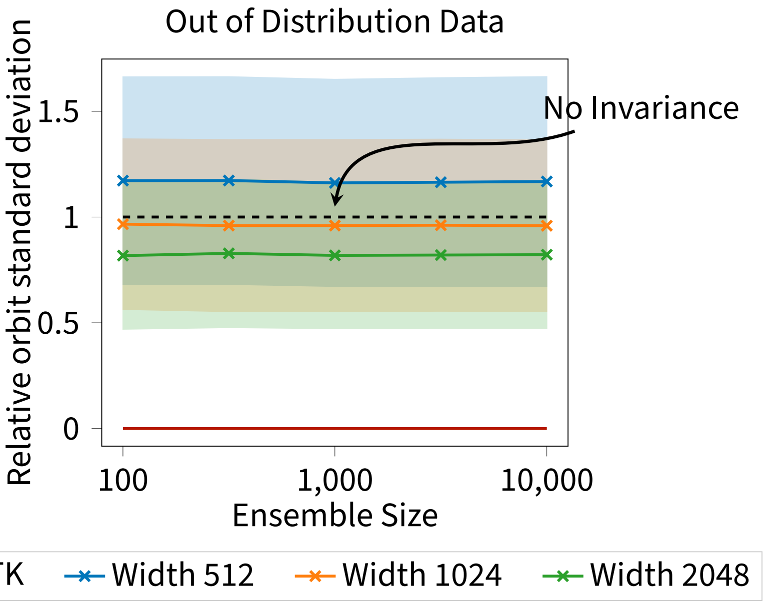
Ising model

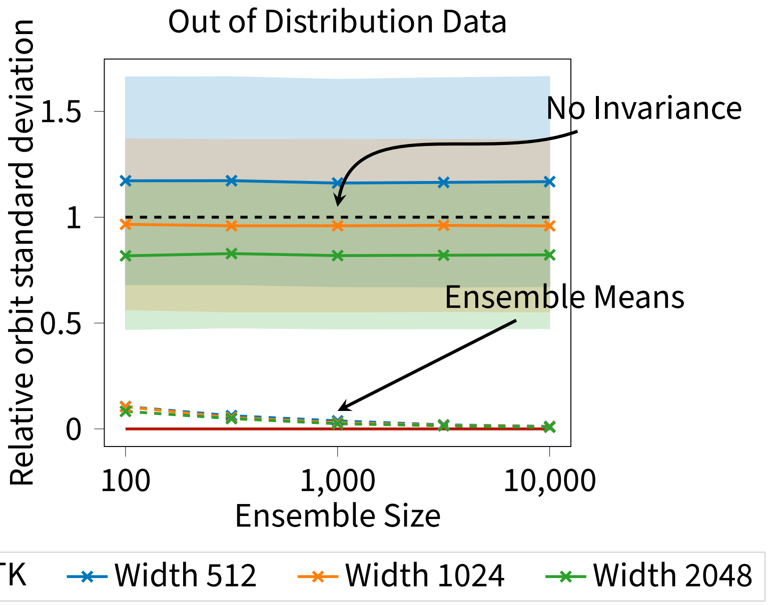


Ising model




Out of Distribution Data
No Invariance
Relative orbit standard deviation
1.5
1
0.5
0
100
1,000
10,000
Ensemble Size
NTK


Out of Distribution Data
Relative orbit standard deviation
1.5
1
0.5
0
No Invariance
100
1,000
10,000
Ensemble Size
NTK
Width 512
Width 1024
Width 2048


Out of Distribution Data
Relative orbit standard deviation
1.5
1
0.5
0
100
1,000
10,000
Ensemble Size
No Invariance
Ensemble Means
NTK
Width 512
Width 1024
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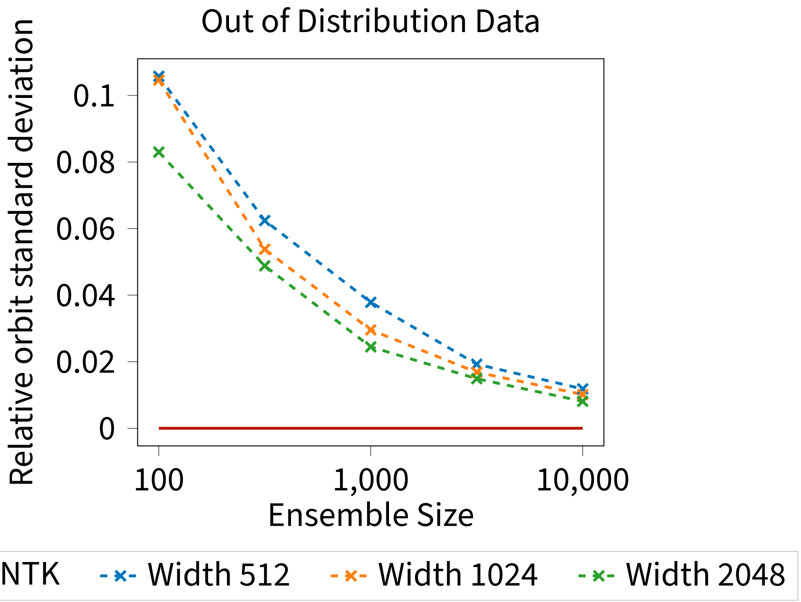
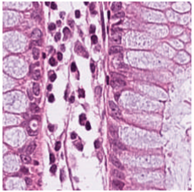


Out of Distribution Data
Relative orbit standard deviation
0.1
0.08
0.06
0.04
0.02
0
100
1,000
10,000
Ensemble Size
NTK
Width 512
Width 1024
Width 2048

Histological slices

[Kather et al. 2018]



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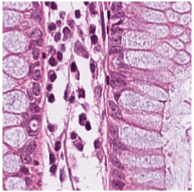
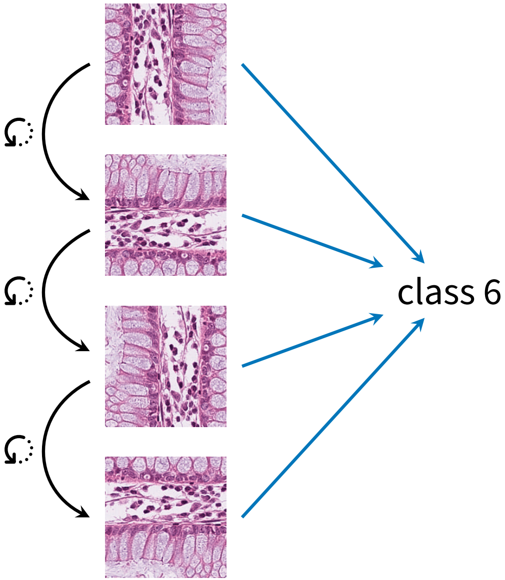
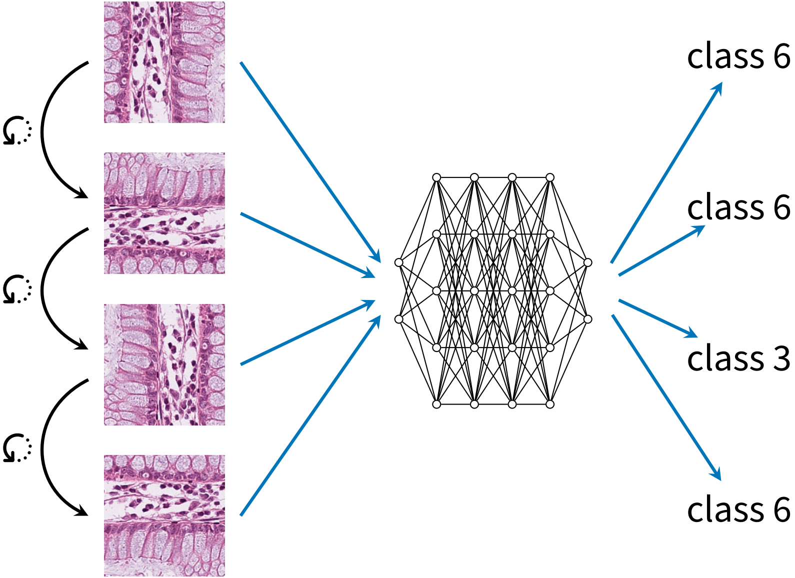


class 6

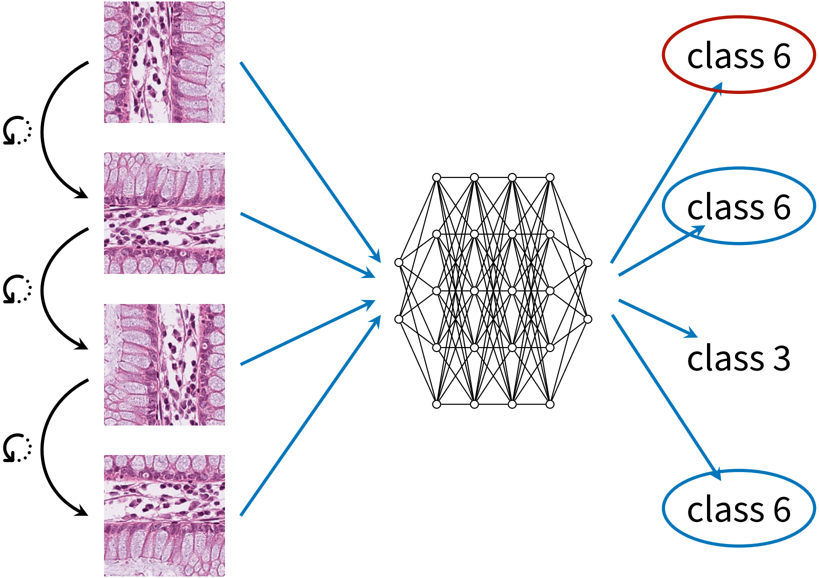
Histological slices



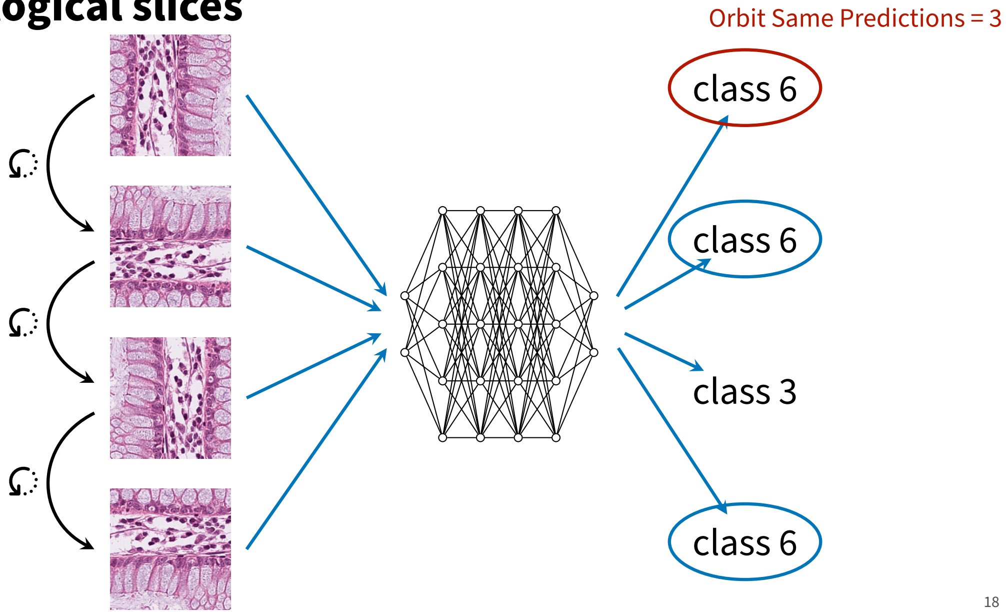
Histological slices



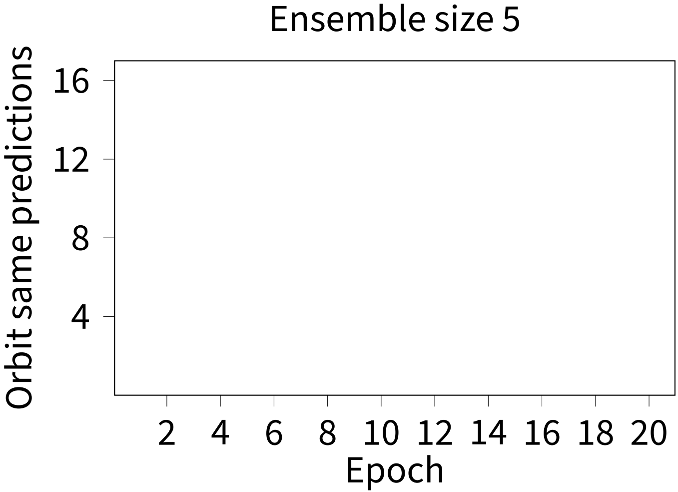
Histological slices



Histological slices



Out of distribution results



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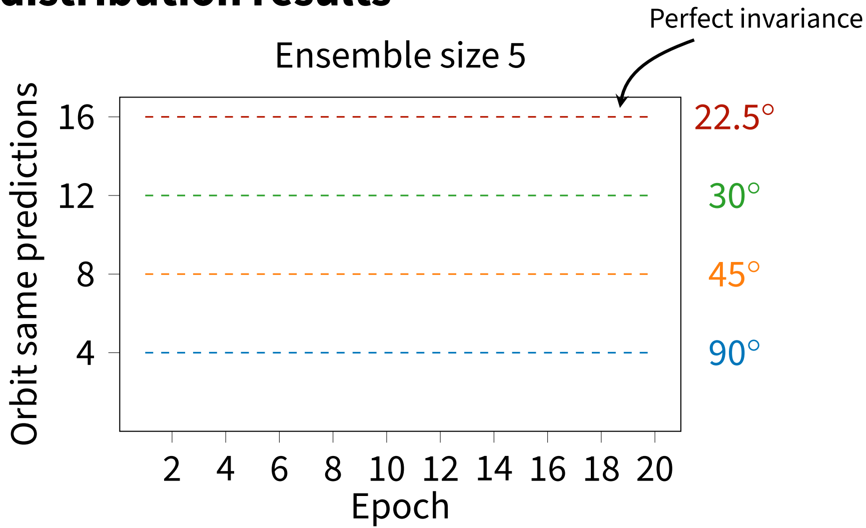
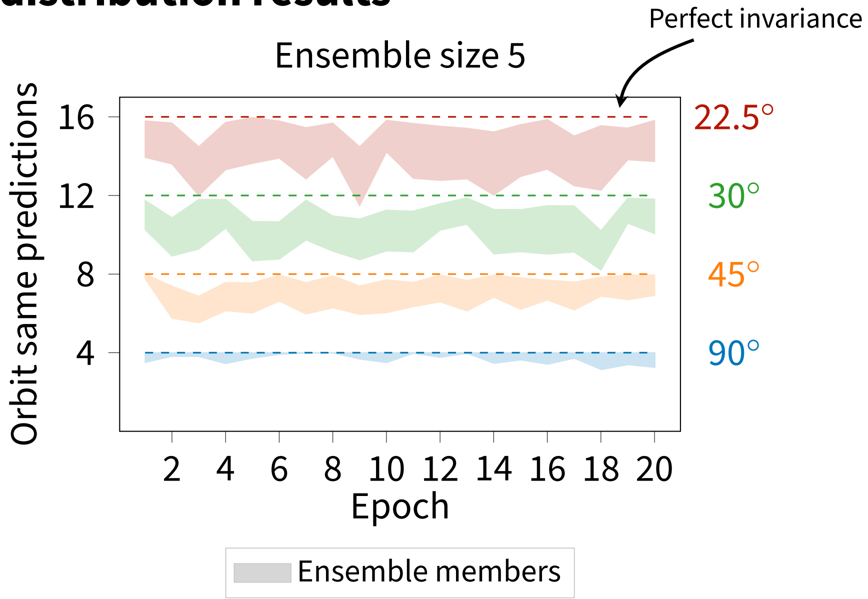


Out of distribution results



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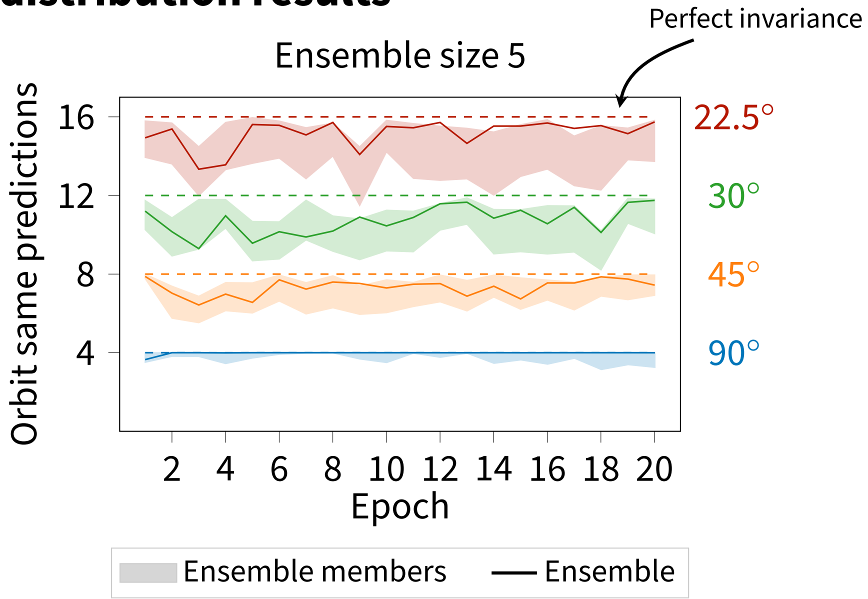

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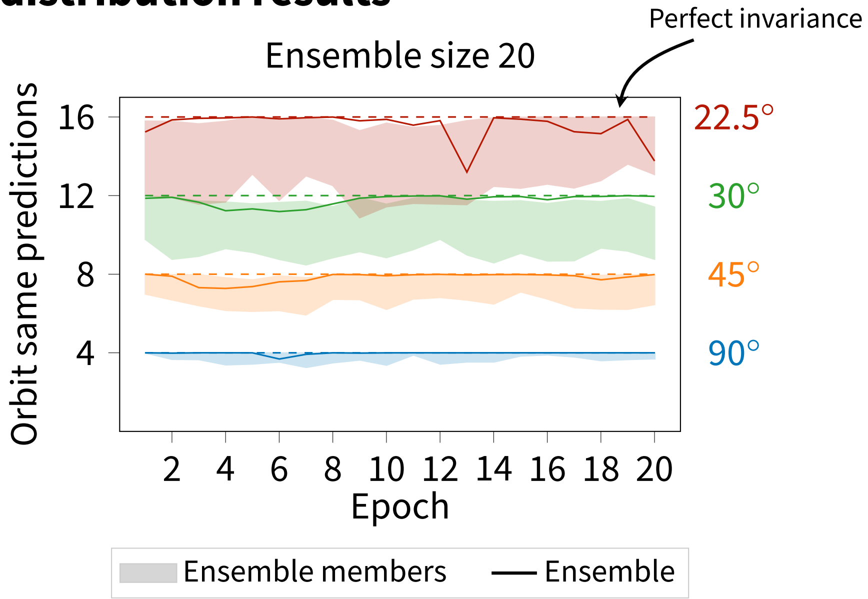

Further experimental results

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- ✓ Emergent invariance for rotated FashionMNIST

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- ✓ Partial augmentation for continuous symmetries

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- ✓ Emergent invariance for rotated FashionMNIST
- ✓ Partial augmentation for continuous symmetries
- ✓ Emergent equivariance (as opposed to invariance)

Comparison to other methods

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➪ Models trained on rotated FashionMNIST

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Orbit same predictions out of distribution:

	C_4	C_8	C_{16}
DeepEns+DA	3.85±0.12	**7.72±0.34**	**15.24±0.69**
only DA	3.41±0.18	6.73±0.24	12.77±0.71
E2CNN[1]	**4±0.0**	**7.71±0.21**	**15.08±0.34**
Canon[2]	**4±0.0**	**7.45±0.14**	12.41±0.85

[1] [Weiler et al. 2019], [2] [Kaba et al. 2022]

Key takeaways

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👍 use data augmentation to obtain an equivariant model.

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If you need data augmentation

👍 use an ensemble to boost the equivariance.

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If you need data augmentation
- 👍 use an ensemble to boost the equivariance.

Analysis of neural tangent kernel can lead to powerful practical insights!

Paper

Emergent Equivariance in Deep Ensembles

Jan E. Gerken*, Pan Kessel*

ICML 2024 (Oral)

* Equal contribution

Thank you