Emergent Equivariance in Deep Ensembles

Jan E. Gerken

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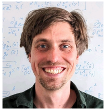
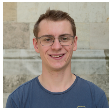
in collaboration with



Pan Kessel



Philipp Misof

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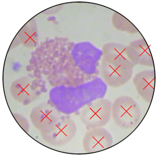

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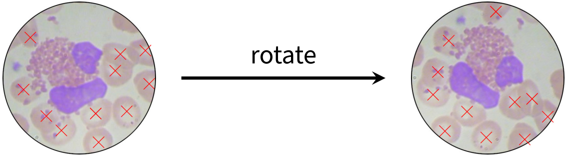

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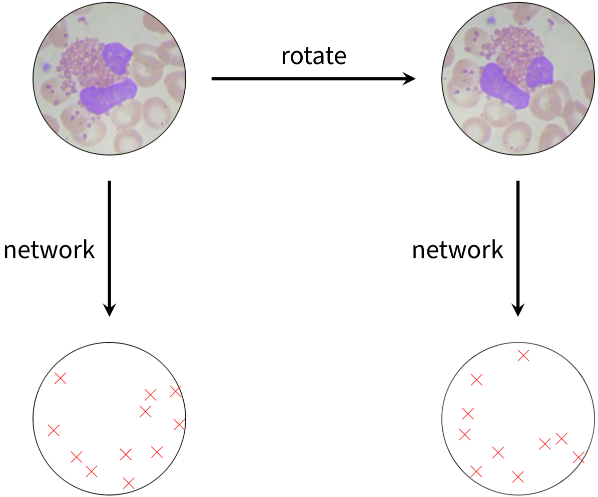

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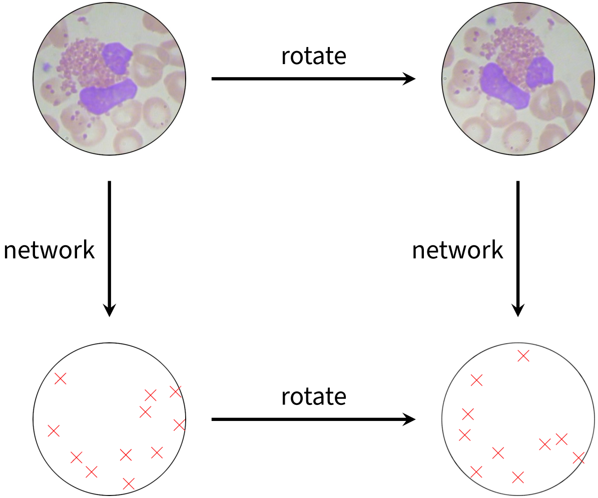

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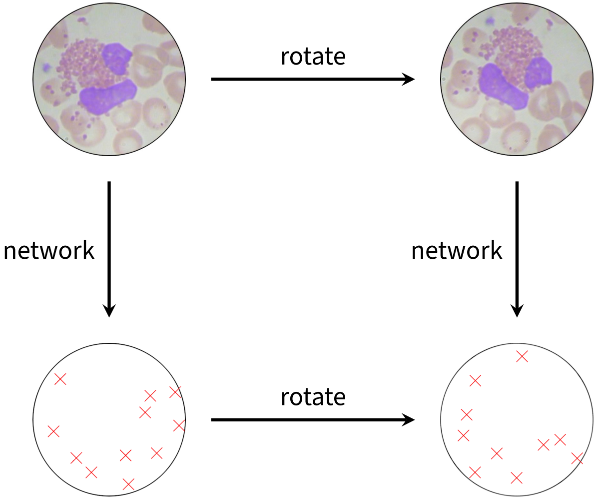

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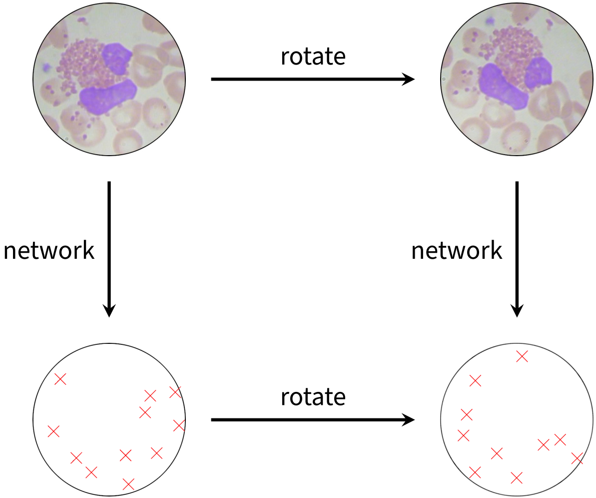

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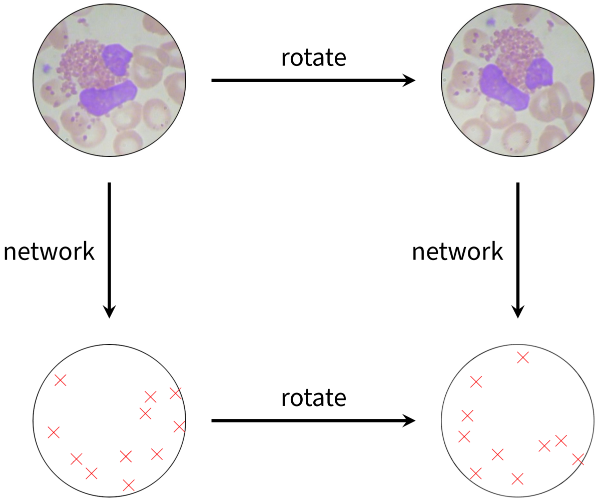
rotation image

Equivariance



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Equivariant neural networks

Equivariant neural networks

Group Equivariant Convolutional Networks

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E(3)-Equivariant Graph Neural Networks for Data-Efficient and Accurate Interatomic Potentials

Simon Batzner*,[1] Albert Musaelian,[1] Lixin Sun,[1] Mario Geiger,[2] Jonathan P. Mailoa,[3] Mordechai Kornbluth,[3] Nicola Molinari,[1] Tess E. Smidt,[4,5] and Boris Kozinsky*[1,3]

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HIERARCHICAL, ROTATION-EQUIVARIANT NEURAL NETWORKS TO SELECT STRUCTURAL MODELS OF PROTEIN COMPLEXES

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Department of Applied Physics	Department of Computer Science	Department of Physics
Stanford University	Stanford University	Stanford University
seismann@stanford.edu	raphael@cs.stanford.edu	nthomas103@gmail.com
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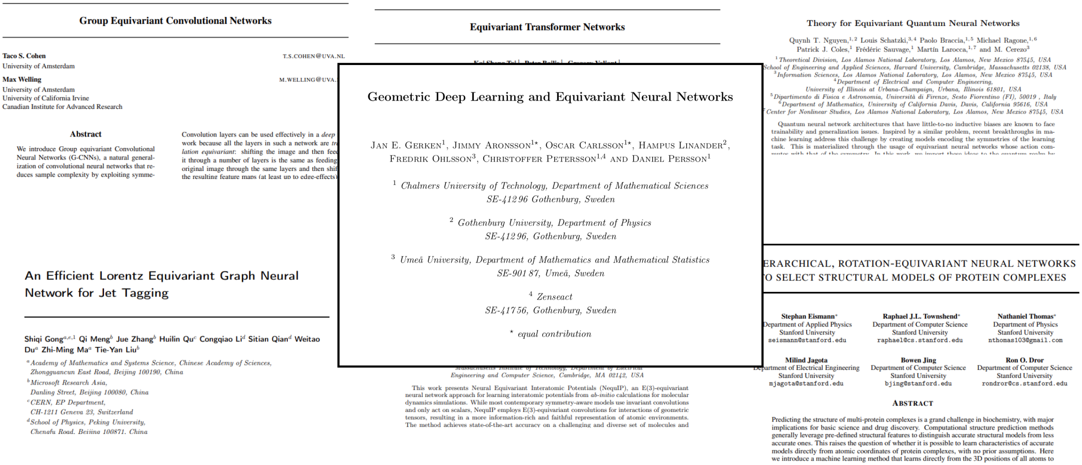

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* *equal contribution*

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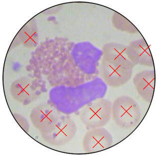

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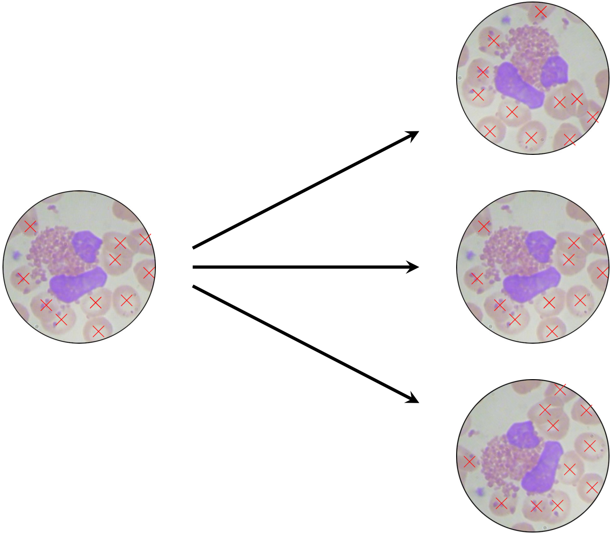

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Article

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The Importance of Being Scalable: Improving the Speed and Accuracy of Neural Network Interatomic Potentials Across Chemical Domains

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Probing the effects of broken symmetries in machine learning

Marcel F Langer, Sergey N Pozdnyakov and Michele Ceriotti*
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Keywords: machine learning, symmetry-constrained models, atomistic modeling, molecular simulations
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Abstract

Symmetry is one of the most central concepts in physics, and it is no surprise that it has also been widely adopted as an inductive bias for machine-learning models applied to the physical sciences. This is especially true for models targeting the properties of matter at the atomic scale. Both established and state-of-the-art approaches, with almost no exceptions, are built to be exactly equivariant to translations, permutations, and rotations of the atoms. Incorporating symmetries—rotations in particular—constrains the model design space and implies more complicated architectures that are often also computationally demanding. There are indications that unconstrained models can easily learn symmetries from data, and that doing so can even be

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Two for One: Diffusion Models and Force Fields for Coarse-Grained Molecular Dynamics

Marloes Arts,*,†,‡,@ Victor Garcia Satorras,*,¶,@ Chin-Wei Huang,¶ Daniel Zügner,§ Marco Federici,†,‖ Cecilia Clementi,§,⊥ Frank Noé,§ Robert Pinsler,# and Rianne van den Berg¶

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@*Equal contribution.*

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Coarse-grained (CG) molecular dynamics enables the study of biological processes at temporal and spatial scales that would be intractable at an atomistic resolution. However, accurately learning a CG force field remains a challenge. In this work, we leverage connections between score-based generative models, force fields and molecular

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Does equivariance matter at scale?

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Abstract

Given large data sets and sufficient compute, is it beneficial to design neural architectures for the structure and symmetries of each problem? Or is it more efficient to learn them from data? We study empirically how equivariant and non-equivariant networks scale with compute and training samples. Focusing on a benchmark problem of rigid-body interactions and on general-purpose transformer architectures, we perform a series of experiments, varying the model size, training steps, and dataset size. We find evidence for three conclusions. First, equivariance improves data efficiency, but training non-equivariant models with data augmentation can close this gap given sufficient epochs. Second, scaling with compute follows a power law, with equivariant models outperforming non-equivariant ones at each tested compute budget. Finally, the optimal allocation of a compute budget onto model size and training duration differs between equivariant and non-equivariant models.

Data augmentation

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- 👍 No specialized architecture necessary

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Can we understand data augmentation theoretically?

Empirical NTK

- Consider continuous gradient descent

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

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- Then, the network evolves according to

$$\frac{\mathrm{d}\mathcal{N}_\theta(x)}{\mathrm{d}t} = \sum_\mu \frac{\partial \mathcal{N}_\theta(x)}{\partial \theta_\mu} \frac{\mathrm{d}\theta_\mu}{\mathrm{d}t}$$

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

With the empirical neural tangent kernel (NTK)

$$\Theta^\theta_{ij}(x, x') = \sum_\mu \frac{\partial \mathcal{N}_i(x)}{\partial \theta_\mu}\frac{\partial \mathcal{N}_j(x')}{\partial \theta_\mu}$$

Empirical NTK

Training dynamics under continuous gradient descent:

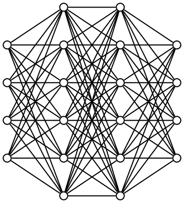
learning rate loss

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

training sample

Infinite width limit

[Jacot et al. 2018]



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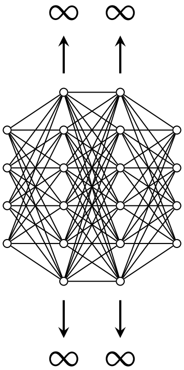

Infinite width limit

Consider an MLP in NTK parametrization

$$z^{(\ell)} = \frac{1}{\sqrt{n_{\ell-1}}} W^{(\ell)} \sigma\left(z^{(\ell-1)}(x)\right), \quad W^{(\ell)} \in \mathbb{R}^{n_\ell \times n_{\ell-1}}, \quad W_{ij}^{(\ell)} \sim \mathcal{N}(0,1)$$

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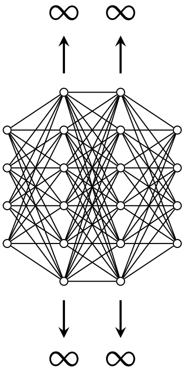

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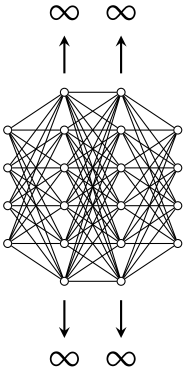
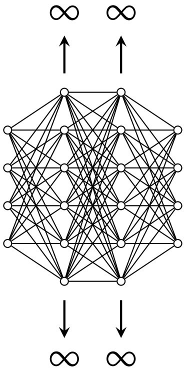


👍 NTK becomes independent of initialization

Infinite width limit

[Jacot et al. 2018]



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

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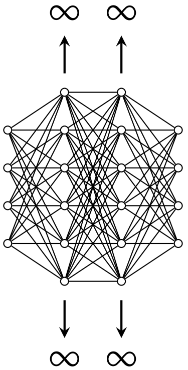

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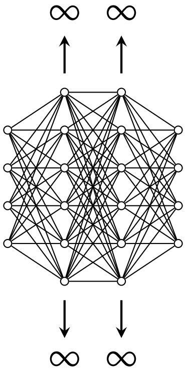
Infinite width limit

[Jacot et al. 2018]



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- NTK can be computed for most networks
- Training dynamics can be solved

NTK at initialization

[Jacot et al. 2020]

When taking the layer widths to infinity sequentially, the empirical NTK $\Theta^{\theta}_{ij}(x,x')$ at initialization converges in probability to a deterministic kernel $\Theta(x,x')\delta_{ij}$

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- The deterministic kernel is given in terms of a recursion over layers
- For most common architectures, this recursion can be performed explicitly,
  e.g. using `neural-tangents` Python package [Novak et al. 2020]

Frozen NTK

[Jacot et al. 2020]

For a nonlinearity which is Lipschitz, twice differentiable and has bounded second derivative,

$$\Theta_{ij}^{\theta_t}(x,x') \to \Theta(x,x')\delta_{ij}$$

uniformly in t as the layer widths go to infinity sequentially.

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- However, the network still learns

Mean prediction from NTK

[Jacot et al. 2018]

- At infinite width, the mean prediction is given by

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

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train labels

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Data augmentation

Data augmentation at infinite width

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Data augmentation at infinite width

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

augmented data

augmented labels

Data augmentation at infinite width

group transformation

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

augmented data

augmented labels

Kernel transformation

The neural tangent kernel Θ as well as the NNGP kernel K transform according to

$$\Theta(\rho(g)x, \rho(g)x') = \rho_K(g)\Theta(x, x')\rho_K^\top(g)\,,$$
$$K(\rho(g)x, \rho(g)x') = \rho_K(g)K(x, x')\rho_K^\top(g)\,,$$

for all $g \in G$ and $x, x' \in X$.

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for all $g \in G$ and $x, x' \in X$.

Hence, for MLPs,

$$\Theta(\rho(g)x, \rho(g)x') = \Theta(x, x') \quad \Rightarrow \quad \Theta(\rho(g)x, x') = \Theta(x, \rho^{-1}(g)x')$$

Permutation shift

- On the training data, group transformations permute the samples

$$\rho(g)x_i = x_{\pi_g(i)}\,, \qquad \pi_g \in S_N$$

Permutation shift

- On the training data, group transformations permute the samples

$$\rho(g)x_i = x_{\pi_g(i)}\,, \qquad \pi_g \in S_N$$

- Therefore, for a permutation of training samples associate to g

$$\begin{aligned}
\Pi(g)\Theta(X,X) &= \Theta(\rho(g)X,X) \\
&= \Theta(X,\rho^{-1}(g)X) \\
&= \Theta(X,X)(\Pi^{-1}(g))^\top \\
&= \Theta(X,X)\Pi(g)
\end{aligned}$$

Data augmentation at infinite width

group transformation

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

augmented data

augmented labels

Data augmentation at infinite width

group transformation

for augmented data

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

augmented data

augmented labels

Data augmentation at infinite width

group transformation

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

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

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

Mean prediction

$$\mu_t(x)$$

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

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Mean prediction

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

Main conclusion

Deep ensembles trained with data augmentation are equivariant.

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

[Nordenfors, Flinth 2024]

Intuitive explanation

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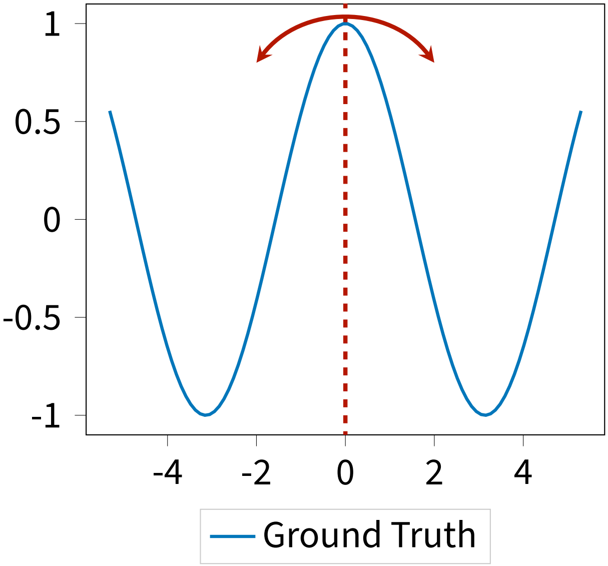
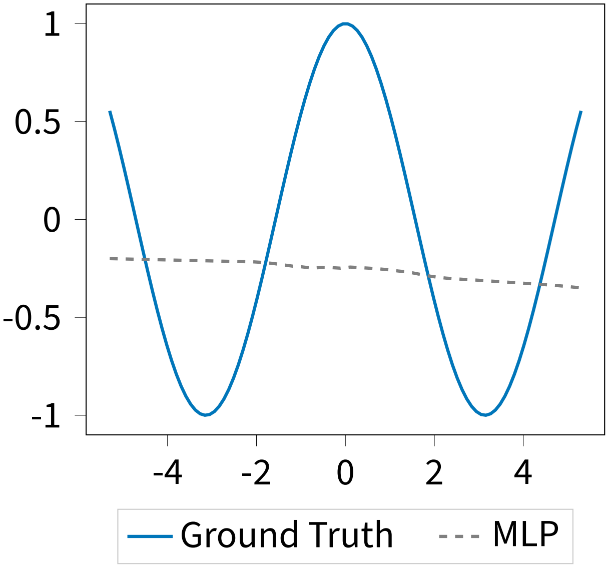
! At infinite width, the mean output at initialization is zero everywhere.

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

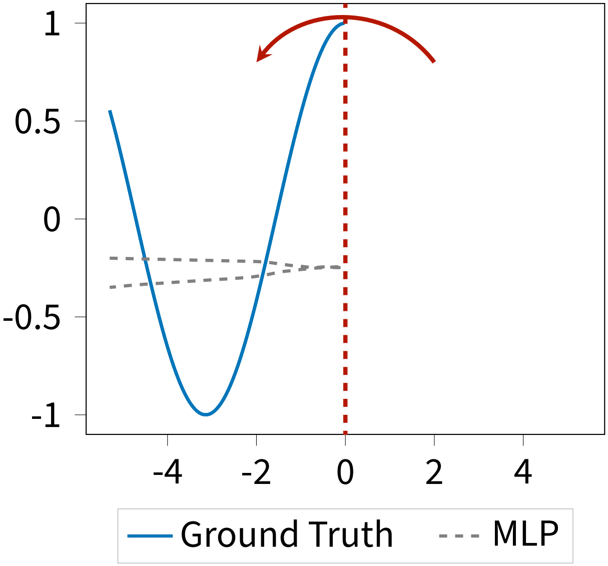
Toy example


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

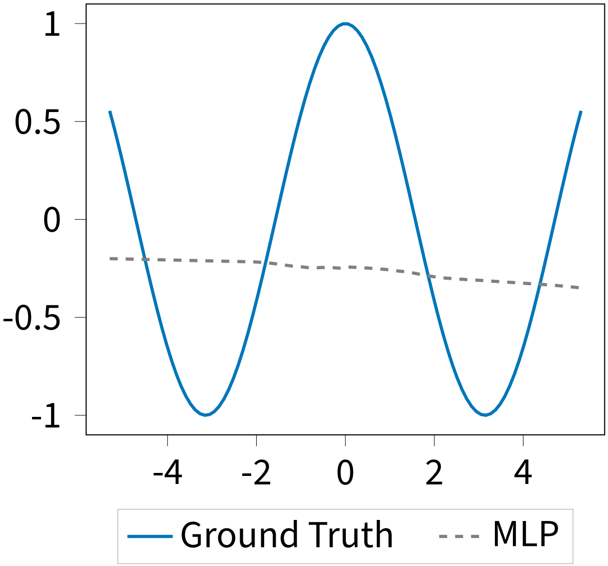
Initialization



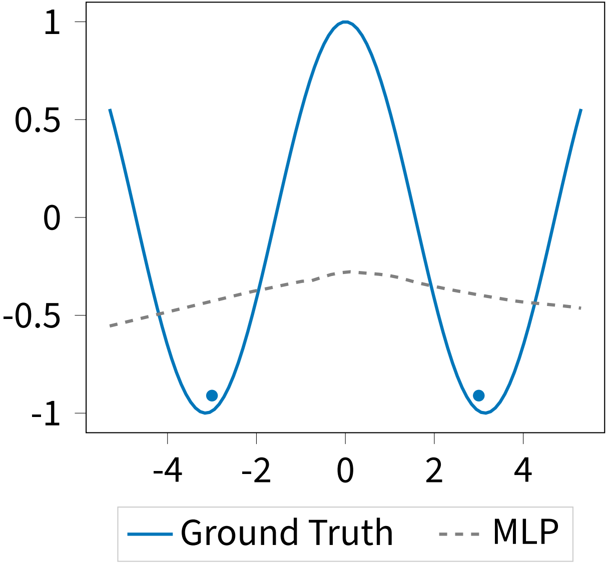
Initialization



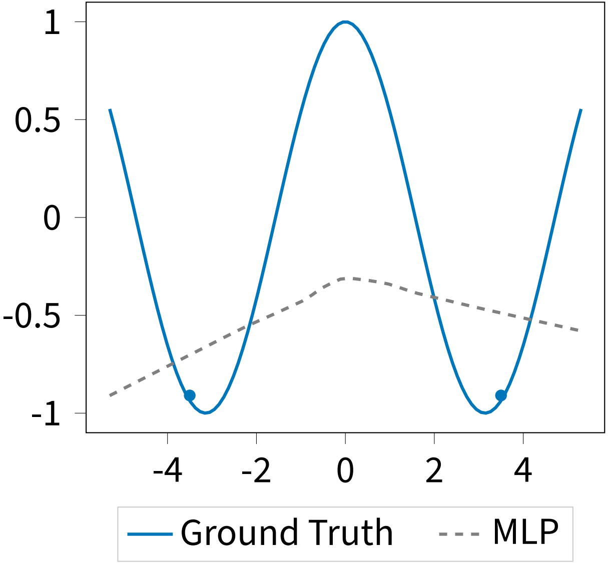
Initialization



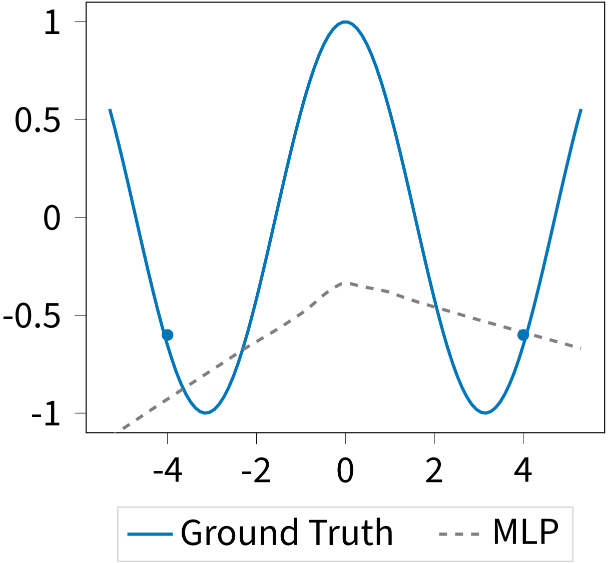
After 1 Training Step



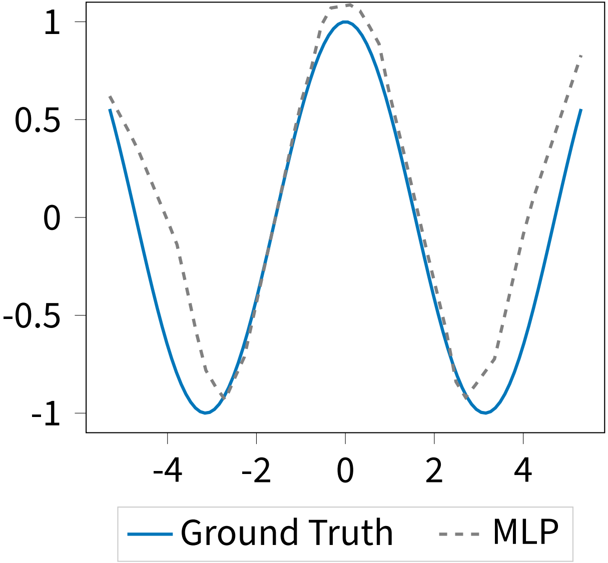
After 2 Training Steps



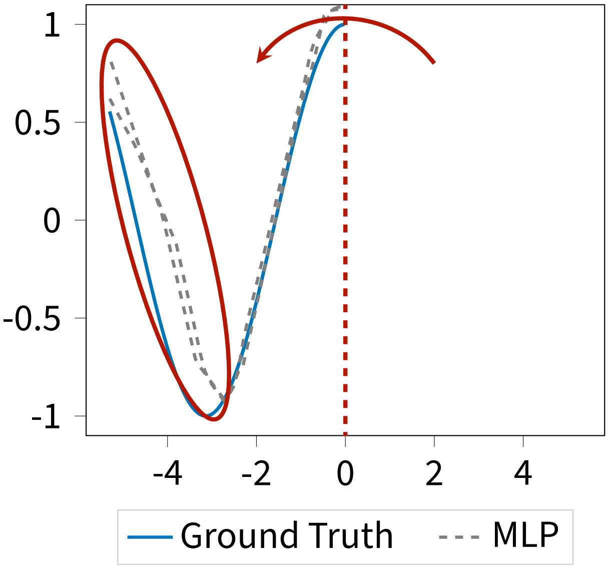
After 3 Training Steps



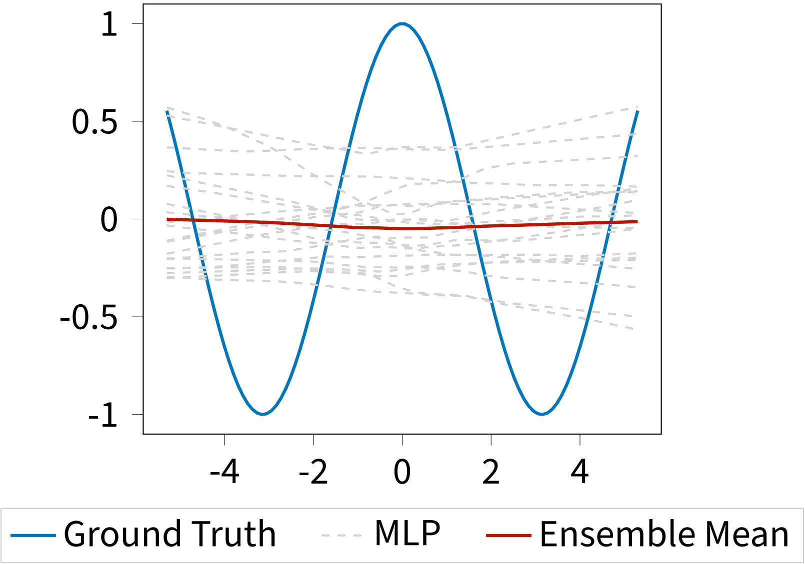
After 2000 Training Steps



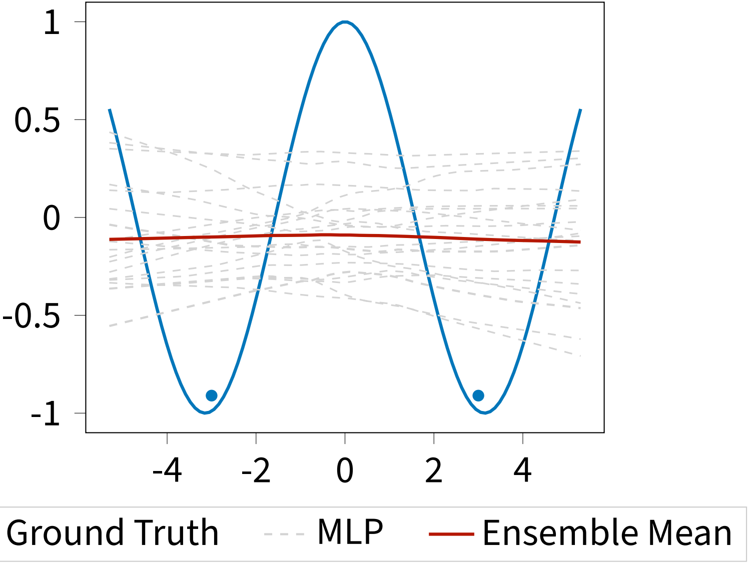
After 2000 Training Steps



Initialization



After 1 Training Step



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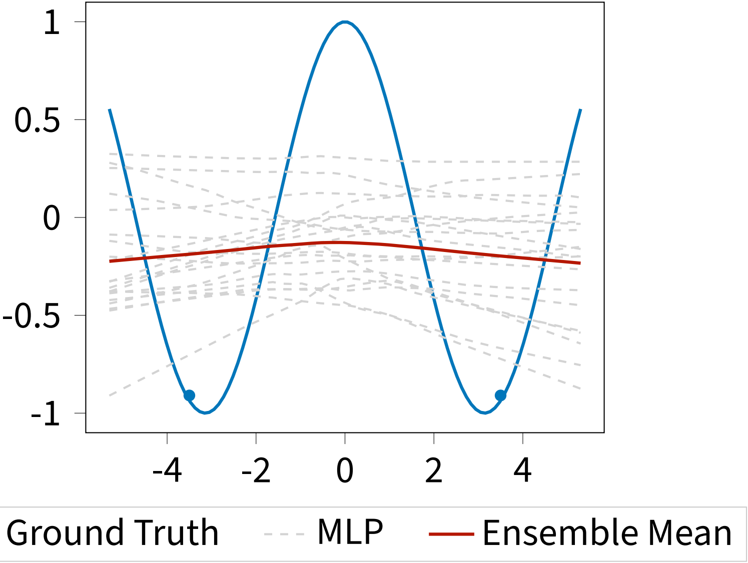

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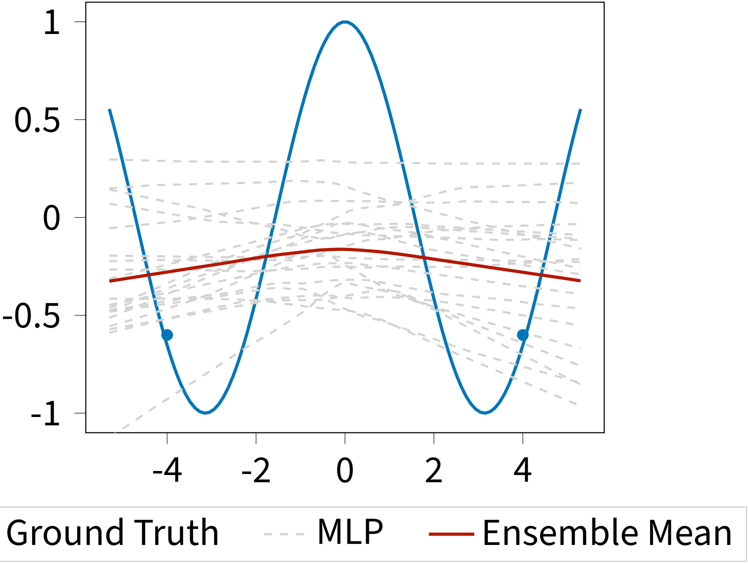

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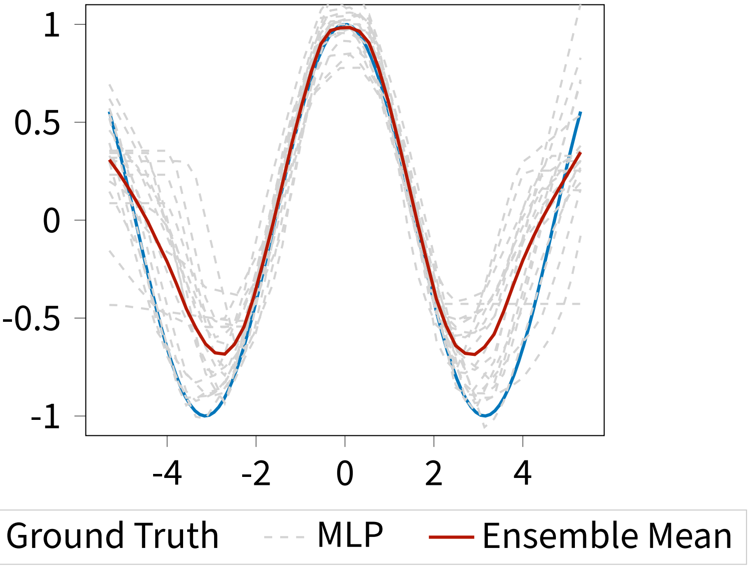

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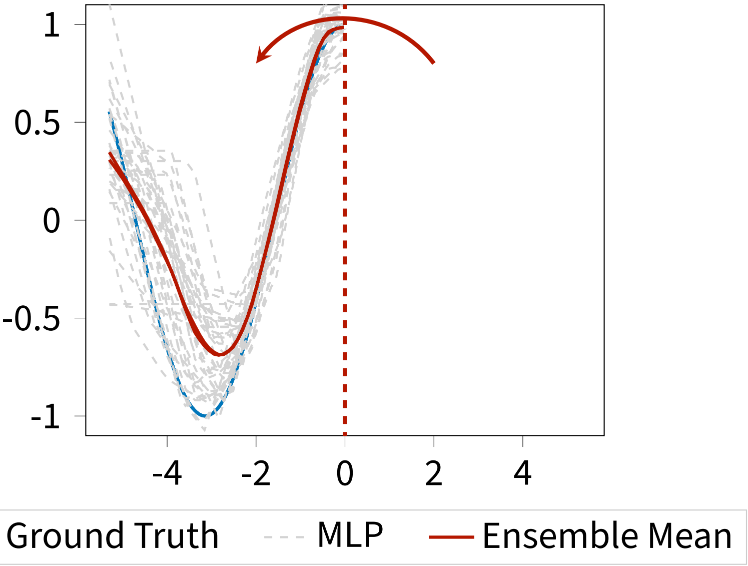
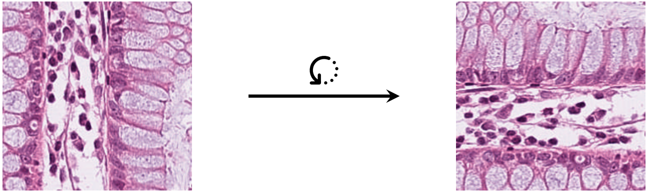


What Does An Augmented Ensemble Converge To?

Rotating images

Rotating images



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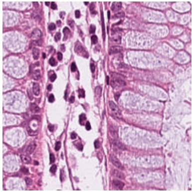
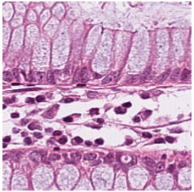
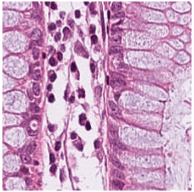


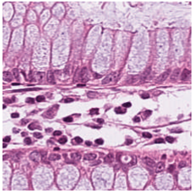


$f(x)$

f : pixels $\rightarrow$ colors

Rotating images





$$f(x) \longrightarrow f(\rho(g^{-1})x)$$

f : pixels $\rightarrow$ colors

$$= [\rho_{\text{reg}}(g)f](x)$$

Data augmentation and NTKs

Data augmentation and NTKs

Consider two ensembles:

trained without data augmentation | trained with data augmentation

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If

$$\Theta^{\mathrm{non-aug}}(f, f') = \frac{1}{|G|} \sum_{g \in G} \Theta^{\mathrm{aug}}(f, \rho_{\mathrm{reg}}(g) f')$$

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at infinite width.

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Given an architecture with NTK Θ^{aug},
find an architecture with NTK $\Theta^{\mathrm{non-aug}}$

Group convolutions

[Cohen, Welling 2016]

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Group conv's are the (unique) linear layers equivariant wrt ρ_{reg}

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$$f'(y) = \int_X \mathrm{d}x\, \kappa(x - y)\, f(x)$$

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- Group convolutions

$$f'(g) = \int_X \mathrm{d}x\, \kappa(\rho(g^{-1})x)\, f(x) \qquad \text{lifting}$$

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$$f'(g) = \int_G \mathrm{d}g\, \kappa(g^{-1}h)\, f(h) \qquad \text{group convolution}$$

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$$f'(g) = \int_G \mathrm{d}g\, \kappa(g^{-1}h)\, f(h) \qquad \text{group convolution}$$

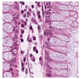
$$f' = \frac{1}{\mathrm{vol}(G)} \int_G \mathrm{d}g\, f(g) \qquad \text{group pooling}$$

GCNNs

Stack GConv-layers to obtain an invariant network

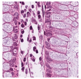
GCNNs

Stack GConv-layers to obtain an invariant network



GCNNs

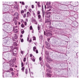
Stack GConv-layers to obtain an invariant network



lifting

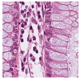
GCNNs

Stack GConv-layers to obtain an invariant network

 $\longrightarrow$ lifting $\longrightarrow$ σ

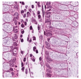
GCNNs

Stack GConv-layers to obtain an invariant network

 $\longrightarrow$ lifting $\longrightarrow$ σ $\longrightarrow$ GConv

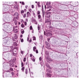
GCNNs

Stack GConv-layers to obtain an invariant network

 $\longrightarrow$ lifting $\longrightarrow \sigma \longrightarrow$ GConv $\longrightarrow \sigma$

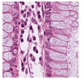
GCNNs

Stack GConv-layers to obtain an invariant network

 $\longrightarrow$ lifting $\longrightarrow$ σ $\longrightarrow$ GConv $\longrightarrow$ σ $\longrightarrow$ GConv

GCNNs

Stack GConv-layers to obtain an invariant network

 $\longrightarrow$ lifting $\longrightarrow \sigma \longrightarrow$ GConv $\longrightarrow \sigma \longrightarrow$ GConv $\longrightarrow$ GPool

NTKs for GCNNs

For GCNN-layers, define the NNGP and NTK via

$$K^{(\ell)}_{g,g'}(f,f') = \mathbb{E}\left[[\mathcal{N}^{(\ell)}(f)](g)\left([\mathcal{N}^{(\ell)}(f')](g')\right)^{\top}\right]$$

NTKs for GCNNs

For GCNN-layers, define the NNGP and NTK via

$$K^{(\ell)}_{g,g'}(f,f') = \mathbb{E}\left[[\mathcal{N}^{(\ell)}(f)](g)\left([\mathcal{N}^{(\ell)}(f')](g')\right)^\top\right]$$

$$\Theta^{(\ell)}_{g,g'}(f,f') = \mathbb{E}\left[\sum_{\ell'=1}^{\ell}\frac{\partial[\mathcal{N}^{(\ell)}(f)](g)}{\partial\theta^{(\ell')}}\left(\frac{\partial[\mathcal{N}^{(\ell)}(f')](g')}{\partial\theta^{(\ell')}}\right)^\top\right]$$

NTKs for GCNNs

$$\boxed{[\mathcal{N}^{(\ell)}(f)](g) = \int_G \mathrm{d}g\, \kappa(g^{-1}h)\, [\mathcal{N}^{(\ell-1)}(f)](h)}$$

The layer-recursion for a GCNN-layer is given by

$$K^{(\ell+1)}_{g,g'}(f,f') = \frac{1}{|S_\kappa|} \int_{S_\kappa} \mathrm{d}h\, K^{(\ell)}_{gh,g'h}(f,f')$$

NTKs for GCNNs

$$[\mathcal{N}^{(\ell)}(f)](g) = \int_G \mathrm{d}g\, \kappa(g^{-1}h)\, [\mathcal{N}^{(\ell-1)}(f)](h)$$

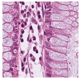
The layer-recursion for a GCNN-layer is given by

$$K^{(\ell+1)}_{g,g'}(f,f') = \frac{1}{|S_\kappa|} \int_{S_\kappa} \mathrm{d}h\, K^{(\ell)}_{gh,g'h}(f,f')$$

$$\Theta^{(\ell+1)}_{g,g'}(f,f') = K^{(\ell+1)}_{g,g'}(f,f') + \frac{1}{|S_\kappa|} \int_{S_\kappa} \mathrm{d}h\, \Theta^{(\ell)}_{gh,g'h}(f,f')$$

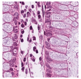
GCNNs

Stack GConv-layers to obtain an invariant network

 $\longrightarrow$ lifting $\longrightarrow \sigma \longrightarrow$ GConv $\longrightarrow \sigma \longrightarrow$ GConv $\longrightarrow$ GPool

NTKs for GCNNs

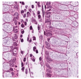
Stack GConv-layers to obtain an invariant network

 $\longrightarrow$ lifting $\longrightarrow$ σ $\longrightarrow$ GConv $\longrightarrow$ σ $\longrightarrow$ GConv $\longrightarrow$ GPool

Compute NTK with layer-wise recursion

NTKs for GCNNs

Stack GConv-layers to obtain an invariant network

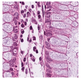
 $\longrightarrow$ lifting $\longrightarrow$ σ $\longrightarrow$ GConv $\longrightarrow$ σ $\longrightarrow$ GConv $\longrightarrow$ GPool

Compute NTK with layer-wise recursion

0

NTKs for GCNNs

Stack GConv-layers to obtain an invariant network



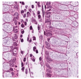
$\longrightarrow$ lifting $\longrightarrow \sigma \longrightarrow$ GConv $\longrightarrow \sigma \longrightarrow$ GConv $\longrightarrow$ GPool

Compute NTK with layer-wise recursion

$$0 \longrightarrow \Theta^{(1)}_{g,g'}(f,f')$$

NTKs for GCNNs

Stack GConv-layers to obtain an invariant network



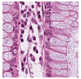
$$\longrightarrow \text{lifting} \longrightarrow \sigma \longrightarrow \text{GConv} \longrightarrow \sigma \longrightarrow \text{GConv} \longrightarrow \text{GPool}$$

Compute NTK with layer-wise recursion

$$0 \longrightarrow \Theta^{(1)}_{g,g'}(f,f') \longrightarrow \Theta^{(2)}_{g,g'}(f,f')$$

NTKs for GCNNs

Stack GConv-layers to obtain an invariant network

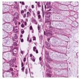
 $\longrightarrow$ lifting $\longrightarrow$ σ $\longrightarrow$ GConv $\longrightarrow$ σ $\longrightarrow$ GConv $\longrightarrow$ GPool

Compute NTK with layer-wise recursion

$$0 \longrightarrow \Theta^{(1)}_{g,g'}(f,f') \longrightarrow \Theta^{(2)}_{g,g'}(f,f') \longrightarrow \Theta^{(3)}_{g,g'}(f,f')$$

NTKs for GCNNs

Stack GConv-layers to obtain an invariant network

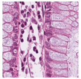
 $\longrightarrow$ lifting $\longrightarrow$ σ $\longrightarrow$ GConv $\longrightarrow$ σ $\longrightarrow$ GConv $\longrightarrow$ GPool

Compute NTK with layer-wise recursion

$$0 \longrightarrow \Theta^{(1)}_{g,g'}(f,f') \longrightarrow \Theta^{(2)}_{g,g'}(f,f') \longrightarrow \Theta^{(3)}_{g,g'}(f,f') \longrightarrow \Theta^{(4)}_{g,g'}(f,f')$$

NTKs for GCNNs

Stack GConv-layers to obtain an invariant network

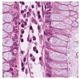
 $\longrightarrow$ lifting $\longrightarrow$ σ $\longrightarrow$ GConv $\longrightarrow$ σ $\longrightarrow$ GConv $\longrightarrow$ GPool

Compute NTK with layer-wise recursion

$$0 \longrightarrow \Theta^{(1)}_{g,g'}(f,f') \longrightarrow \Theta^{(2)}_{g,g'}(f,f') \longrightarrow \Theta^{(3)}_{g,g'}(f,f') \longrightarrow \Theta^{(4)}_{g,g'}(f,f') \longrightarrow \Theta^{(5)}_{g,g'}(f,f')$$

NTKs for GCNNs

Stack GConv-layers to obtain an invariant network



$\longrightarrow$ lifting $\longrightarrow \sigma \longrightarrow$ GConv $\longrightarrow \sigma \longrightarrow$ GConv $\longrightarrow$ GPool

Compute NTK with layer-wise recursion

$$0 \longrightarrow \Theta^{(1)}_{g,g'}(f,f') \longrightarrow \Theta^{(2)}_{g,g'}(f,f') \longrightarrow \Theta^{(3)}_{g,g'}(f,f') \longrightarrow \Theta^{(4)}_{g,g'}(f,f') \longrightarrow \Theta^{(5)}_{g,g'}(f,f') \longrightarrow \Theta(f,f')$$

NTKs of MLPs and GCNNs

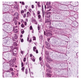
NTKs of MLPs and GCNNs

- Consider two neural networks

NTKs of MLPs and GCNNs

- Consider two neural networks

An MLP

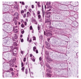


$$\longrightarrow \text{FC} \longrightarrow \sigma \longrightarrow \text{FC} \longrightarrow \sigma \longrightarrow \text{FC}$$

NTKs of MLPs and GCNNs

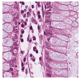
- Consider two neural networks

An MLP



$\longrightarrow$ FC $\longrightarrow \sigma \longrightarrow$ FC $\longrightarrow \sigma \longrightarrow$ FC

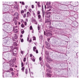
A GCNN



NTKs of MLPs and GCNNs

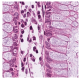
- Consider two neural networks

An MLP



$\longrightarrow \text{FC} \longrightarrow \sigma \longrightarrow \text{FC} \longrightarrow \sigma \longrightarrow \text{FC}$

A GCNN

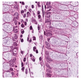


$\longrightarrow \text{lifting}$

NTKs of MLPs and GCNNs

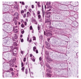
- Consider two neural networks

An MLP



$\longrightarrow \text{FC} \longrightarrow \sigma \longrightarrow \text{FC} \longrightarrow \sigma \longrightarrow \text{FC}$

A GCNN

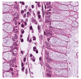


$\longrightarrow \text{lifting} \longrightarrow \sigma$

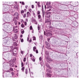
NTKs of MLPs and GCNNs

- Consider two neural networks

An MLP



A GCNN

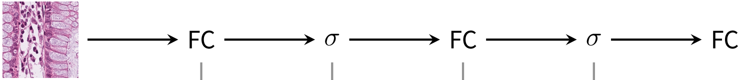


$$
\begin{tikzcd}
{} \arrow[r] & \mathrm{FC} \arrow[r] \arrow[d] & \sigma \arrow[r] \arrow[d] & \mathrm{FC} \arrow[r] \arrow[d] & \sigma \arrow[r] & \mathrm{FC} \\
{} \arrow[r] & \text{lifting} \arrow[r] & \sigma \arrow[r] & \mathrm{GConv} & &
\end{tikzcd}
$$

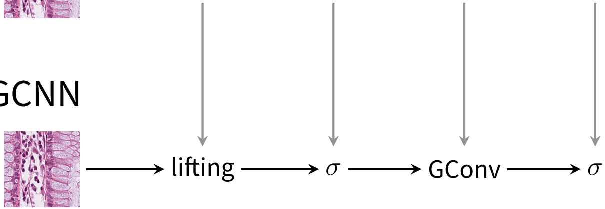
NTKs of MLPs and GCNNs

- Consider two neural networks

An MLP



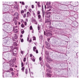
A GCNN



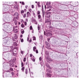
NTKs of MLPs and GCNNs

- Consider two neural networks

An MLP



A GCNN

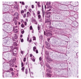


$$\begin{tikzcd}
{} \arrow[r] & \mathrm{FC} \arrow[r] \arrow[d] & \sigma \arrow[r] \arrow[d] & \mathrm{FC} \arrow[r] \arrow[d] & \sigma \arrow[r] \arrow[d] & \mathrm{FC} \arrow[d] \\
{} \arrow[r] & \text{lifting} \arrow[r] & \sigma \arrow[r] & \mathrm{GConv} \arrow[r] & \sigma \arrow[r] & \mathrm{GConv}
\end{tikzcd}$$

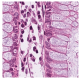
NTKs of MLPs and GCNNs

- Consider two neural networks

An MLP



A GCNN

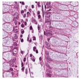


$$\begin{tikzcd}
{} \arrow[r] & \text{FC} \arrow[r] \arrow[d] & \sigma \arrow[r] \arrow[d] & \text{FC} \arrow[r] \arrow[d] & \sigma \arrow[r] \arrow[d] & \text{FC} \arrow[d] & \\
{} \arrow[r] & \text{lifting} \arrow[r] & \sigma \arrow[r] & \text{GConv} \arrow[r] & \sigma \arrow[r] & \text{GConv} \arrow[r] & \text{GPool}
\end{tikzcd}$$

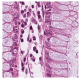
NTKs of MLPs and GCNNs

- Consider two neural networks

An MLP



A GCNN



$$\begin{tikzcd}
\cdot \arrow[r] & \mathrm{FC} \arrow[r] \arrow[d] & \sigma \arrow[r] \arrow[d] & \mathrm{FC} \arrow[r] \arrow[d] & \sigma \arrow[r] \arrow[d] & \mathrm{FC} \arrow[d] & \\
\cdot \arrow[r] & \text{lifting} \arrow[r] & \sigma \arrow[r] & \mathrm{GConv} \arrow[r] & \sigma \arrow[r] & \mathrm{GConv} \arrow[r] & \mathrm{GPool}
\end{tikzcd}$$

- Then

$$\Theta^{\mathrm{GCNN}}(f, f') = \frac{1}{|G|} \sum_{g \in G} \Theta^{\mathrm{MLP}}(f, \rho_{\mathrm{reg}}(g) f')$$

Data augmentation of MLPs

$$\Theta^{\mathrm{GCNN}}(f, f') = \frac{1}{|G|} \sum_{g \in G} \Theta^{\mathrm{MLP}}(f, \rho_{\mathrm{reg}}(g) f')$$

Data augmentation of MLPs

before: non-aug

$$\Theta^{\mathrm{GCNN}}(f, f') = \frac{1}{|G|} \sum_{g \in G} \Theta^{\mathrm{MLP}}(f, \rho_{\mathrm{reg}}(g) f')$$

Data augmentation of MLPs

before: non-aug

before: aug

$$\Theta^{\mathrm{GCNN}}(f, f') = \frac{1}{|G|} \sum_{g \in G} \Theta^{\mathrm{MLP}}(f, \rho_{\mathrm{reg}}(g) f')$$

Data augmentation of MLPs

before: non-aug

before: aug

$$\Theta^{\text{GCNN}}(f, f') = \frac{1}{|G|} \sum_{g \in G} \Theta^{\text{MLP}}(f, \rho_{\text{reg}}(g) f')$$

⇨ training the MLP on G-augmented data

Data augmentation of MLPs

before: non-aug

before: aug

$$\Theta^{\mathrm{GCNN}}(f, f') = \frac{1}{|G|} \sum_{g \in G} \Theta^{\mathrm{MLP}}(f, \rho_{\mathrm{reg}}(g) f')$$

⇨ training the MLP on G-augmented data = training the GCNN on unaugmented data

Data augmentation of MLPs

before: non-aug

before: aug

$$\Theta^{\mathrm{GCNN}}(f, f') = \frac{1}{|G|} \sum_{g \in G} \Theta^{\mathrm{MLP}}(f, \rho_{\mathrm{reg}}(g) f')$$

⇨ training the MLP on G-augmented data = training the GCNN on unaugmented data

in the ensemble mean

Data augmentation of MLPs

before: non-aug

before: aug

$$\Theta^{\mathrm{GCNN}}(f,f') = \frac{1}{|G|}\sum_{g\in G}\Theta^{\mathrm{MLP}}(f,\rho_{\mathrm{reg}}(g)f')$$

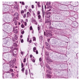
⇨ training the MLP on G-augmented data = training the GCNN on unaugmented data

in the ensemble mean, $\forall t$, $\forall x$

Data augmentation of CNNs

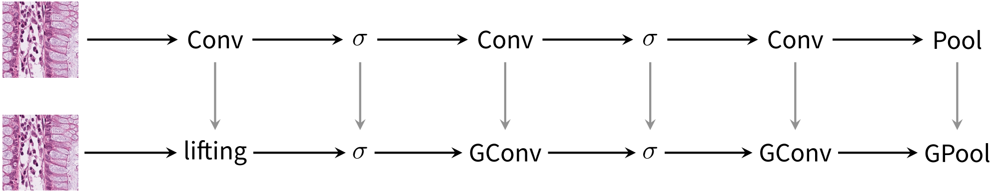
Data augmentation of CNNs

- Consider a CNN

 $\longrightarrow$ Conv $\longrightarrow$ σ $\longrightarrow$ Conv $\longrightarrow$ σ $\longrightarrow$ Conv $\longrightarrow$ Pool

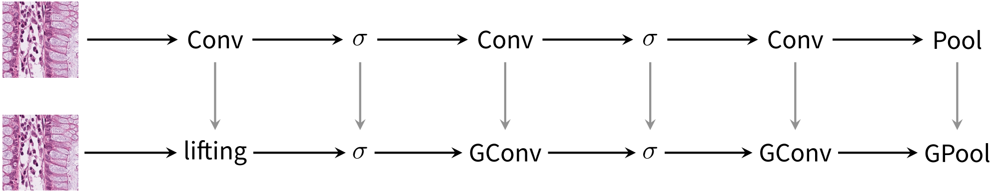
Data augmentation of CNNs

- Consider a CNN and a GCNN invariant wrt. roto-translations



Data augmentation of CNNs

- Consider a CNN and a GCNN invariant wrt. roto-translations

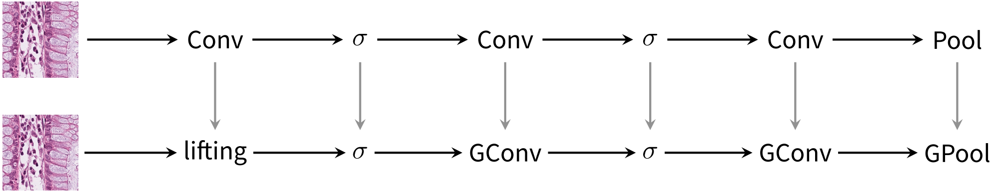


- Then

$$\Theta^{\mathrm{GCNN}}(f, f') = \frac{1}{n} \sum_{r \in C_n} \Theta^{\mathrm{CNN}}(f, \rho_{\mathrm{reg}}(r) f')$$

Data augmentation of CNNs

- Consider a CNN and a GCNN invariant wrt. roto-translations



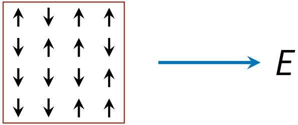
- Then

$$\Theta^{\mathrm{GCNN}}(f, f') = \frac{1}{n} \sum_{r \in C_n} \Theta^{\mathrm{CNN}}(f, \rho_{\mathrm{reg}}(r) f')$$

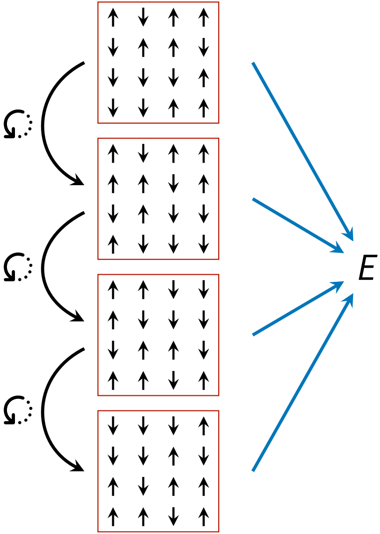
⇨ By training the CNN on rotated images, one obtains a roto-translation invariant GCNN

Experiments

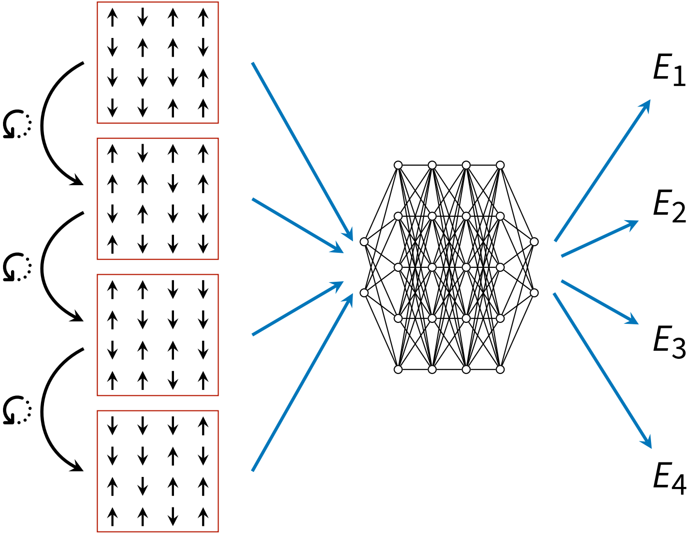
Ising model



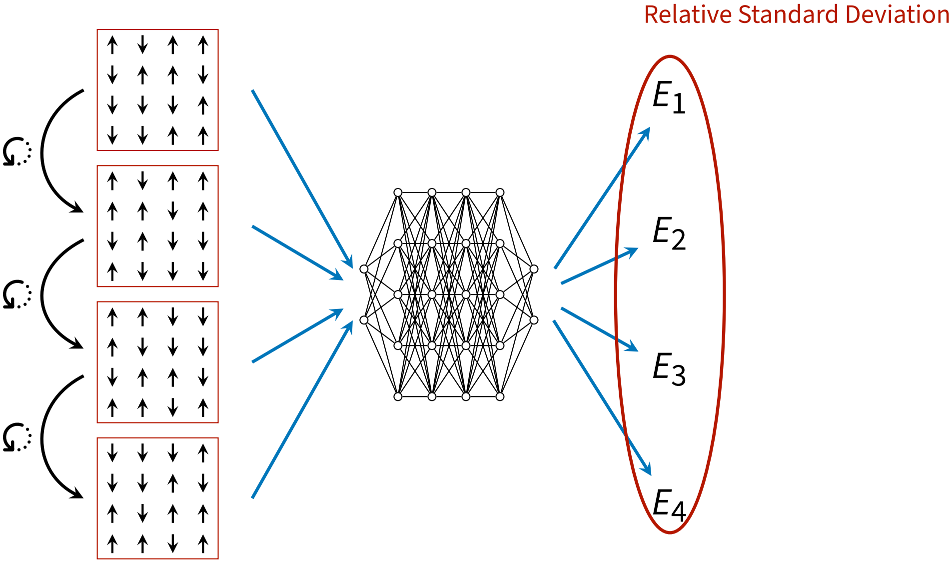
Ising model

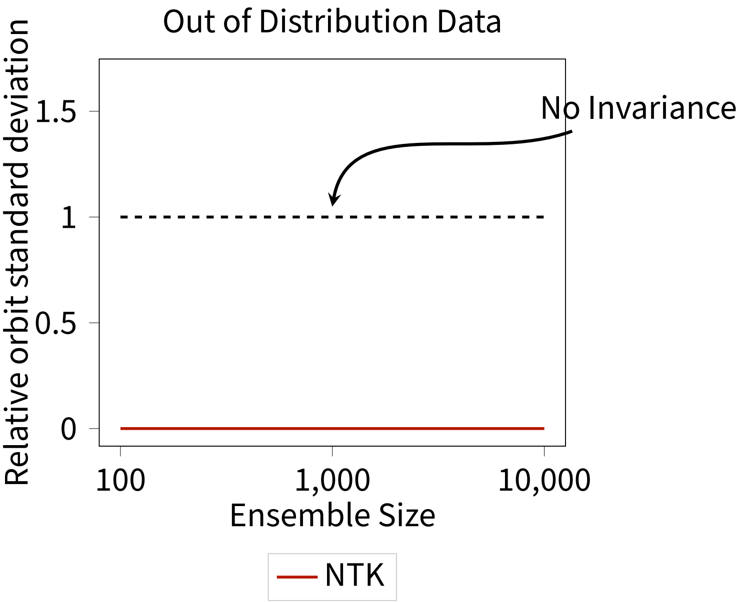


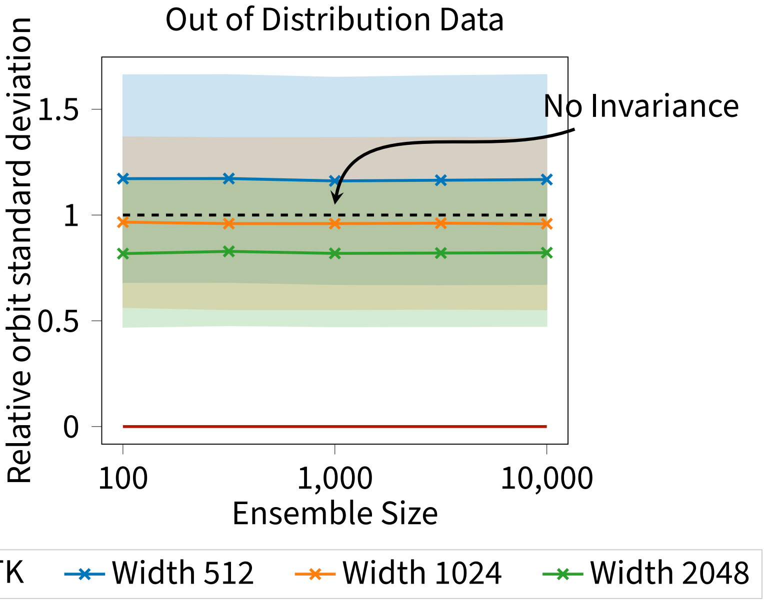
Ising model

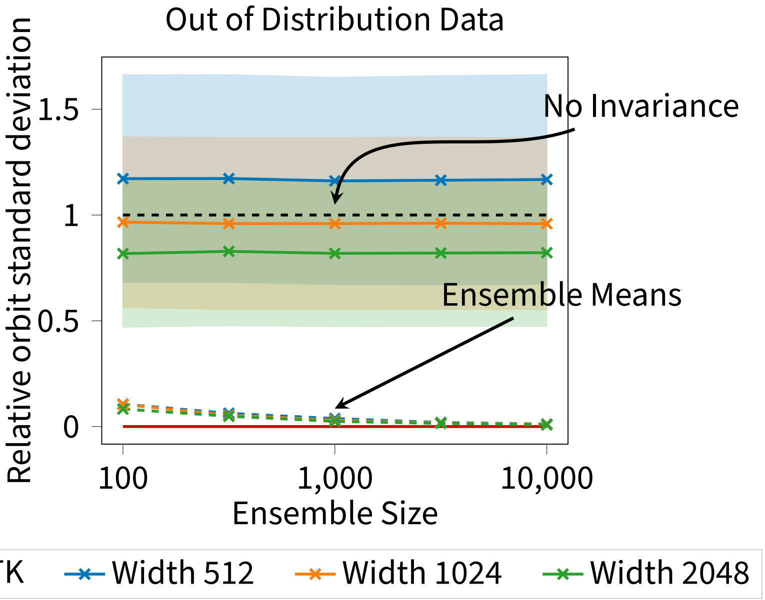


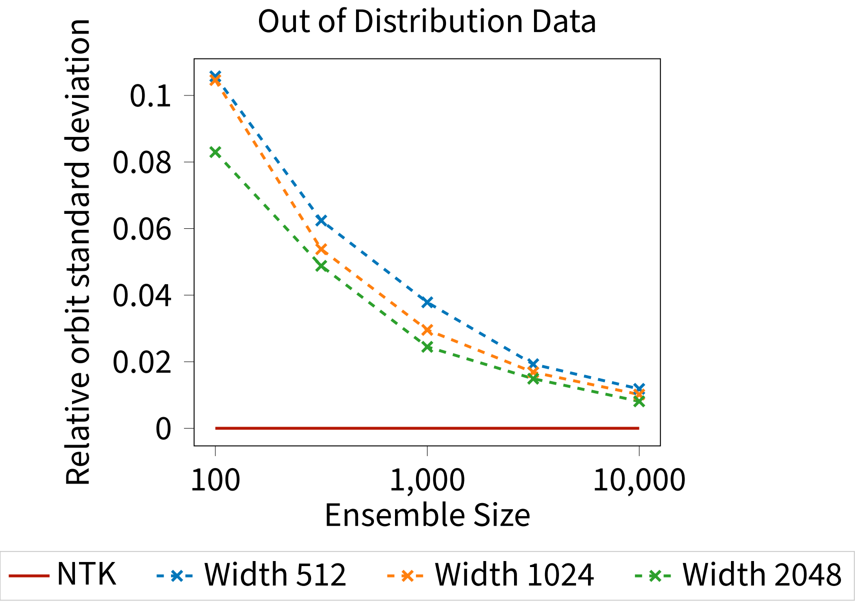
Ising model




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

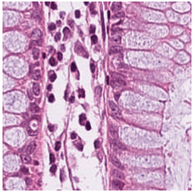

Out of Distribution Data
No Invariance
Relative orbit standard deviation
1.5
1
0.5
0
100
1,000
10,000
Ensemble Size
NTK
Width 512
Width 1024
Width 2048


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


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

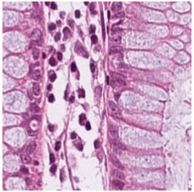
Histological slices

[Kather et al. 2018]



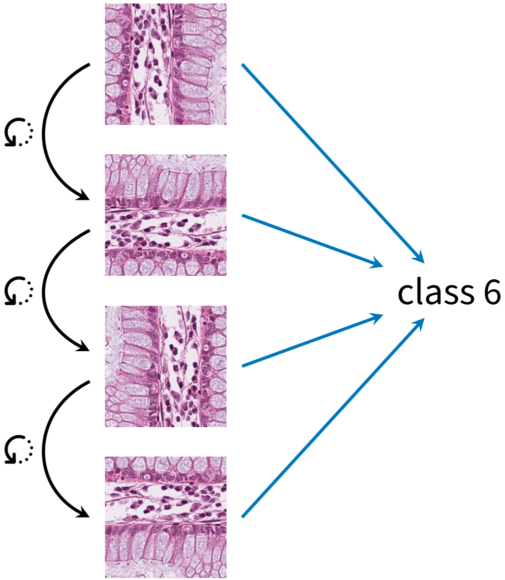
Histological slices

[Kather et al. 2018]

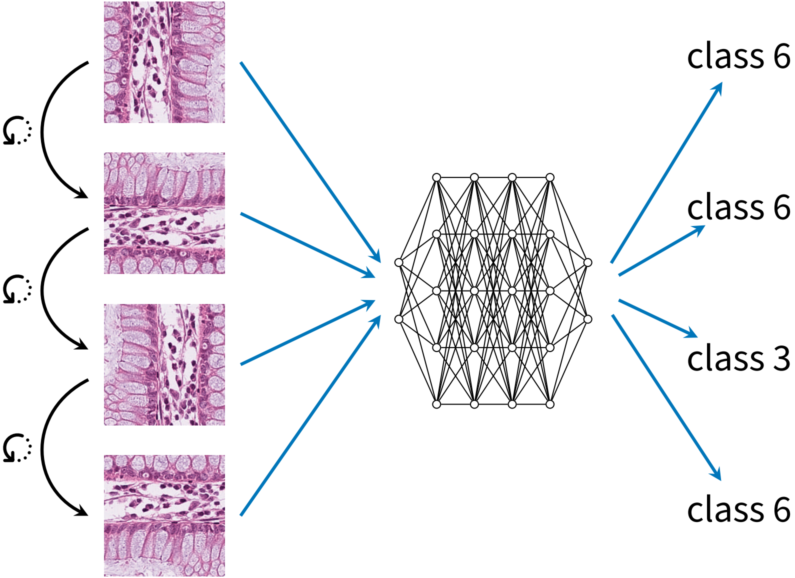


class 6

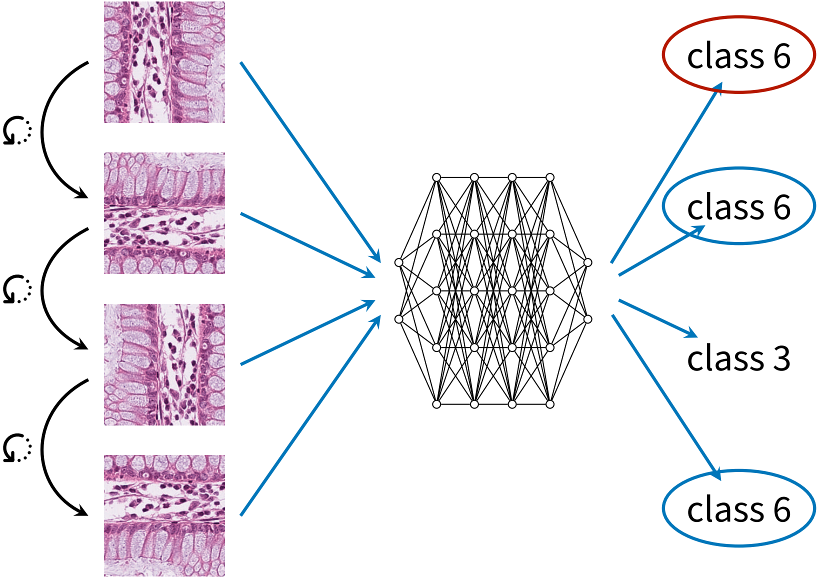
Histological slices



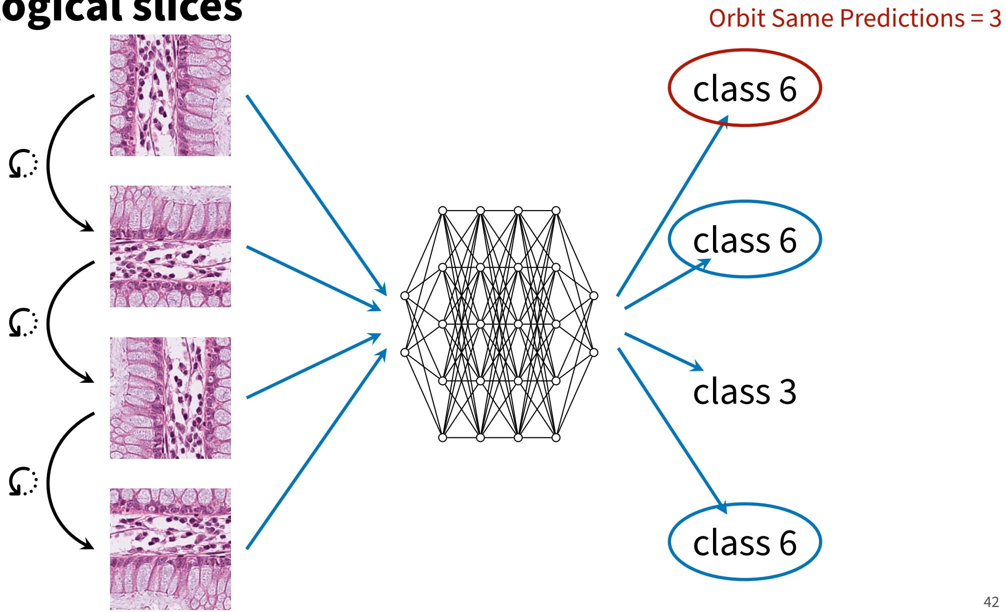
Histological slices



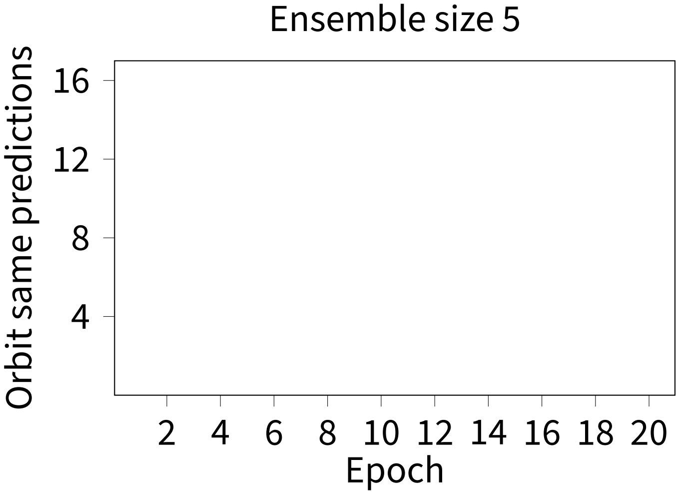
Histological slices



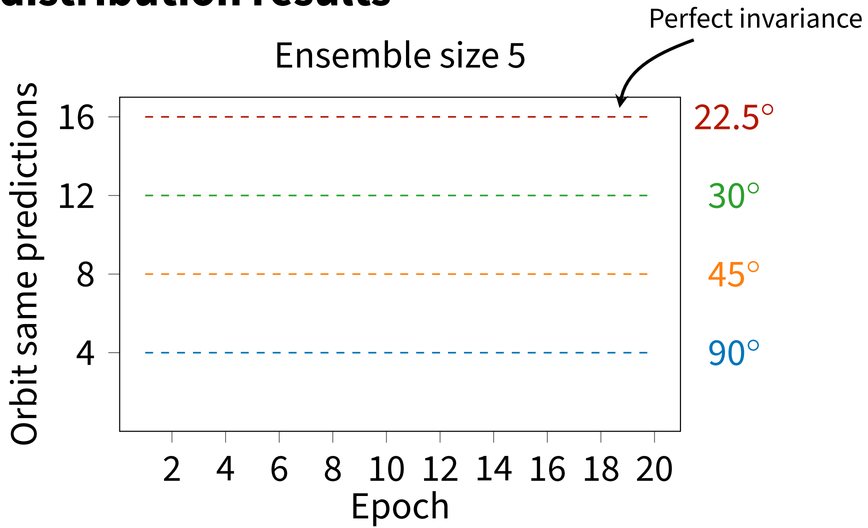
Histological slices



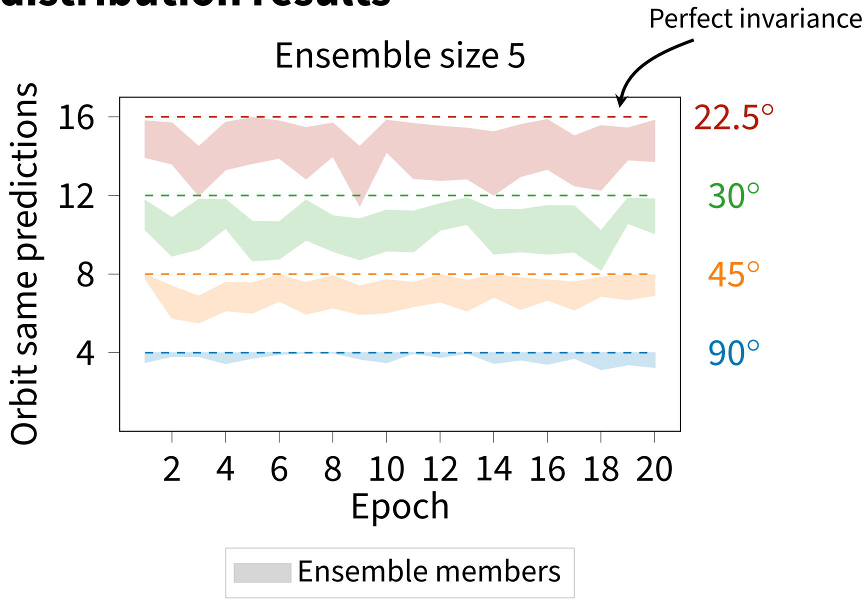
Out of distribution results



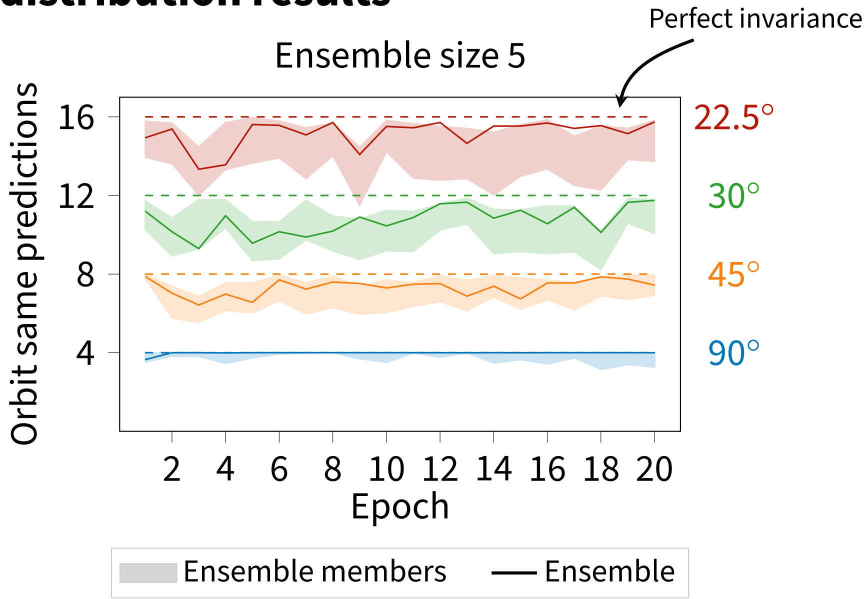
Out of distribution results



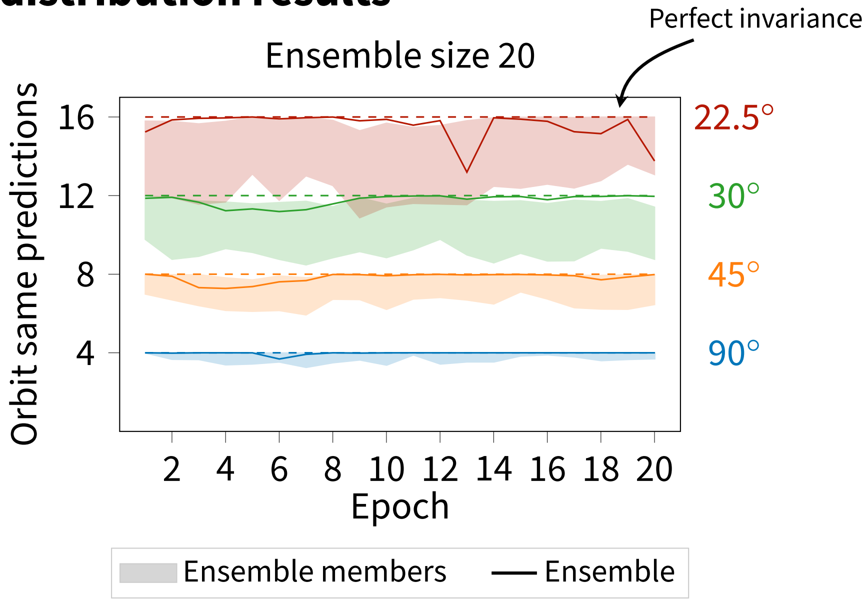
Out of distribution results



Out of distribution results



Out of distribution results



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]

Convergence of augmented CNNs to GCNNs

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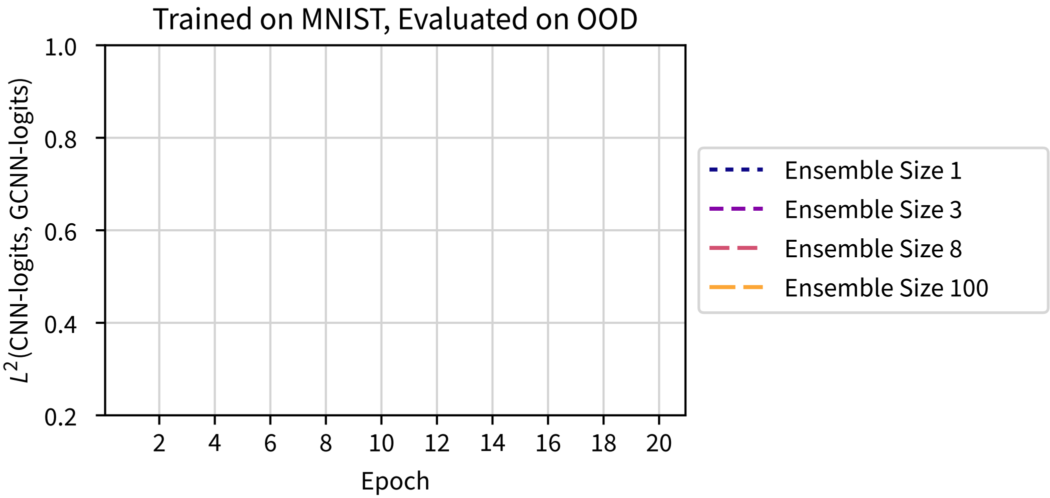
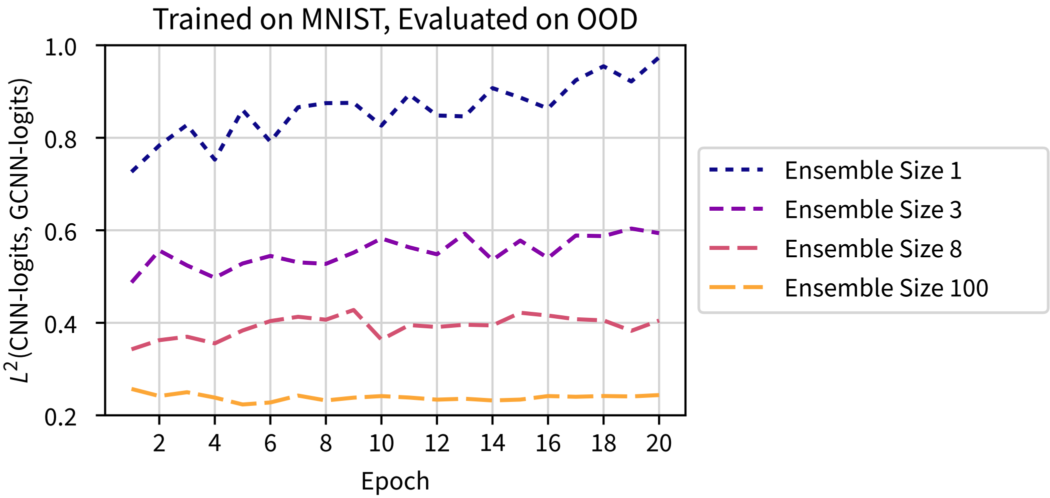
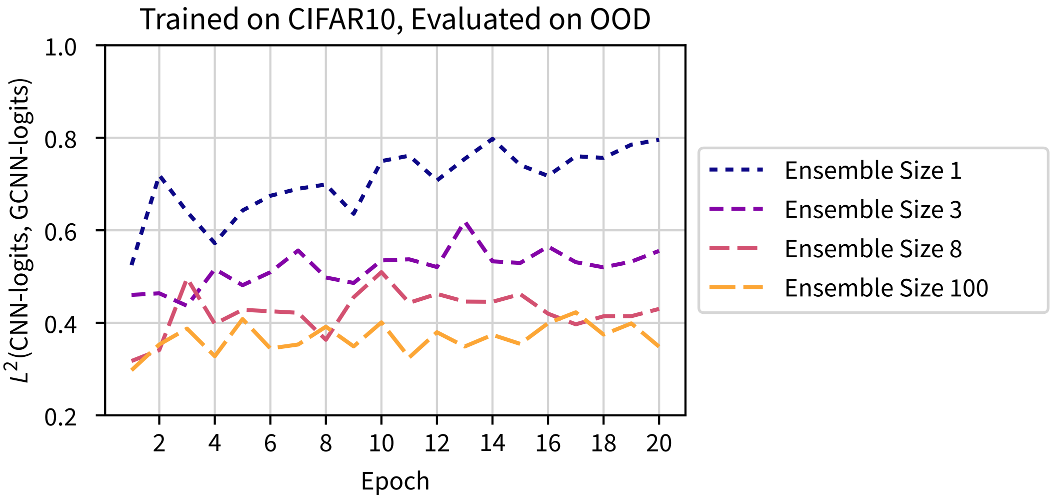


Convergence of augmented CNNs to GCNNs



Convergence of augmented CNNs to GCNNs



Key takeaways

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If you need ensembles

👍 use data augmentation to obtain an equivariant model.

Key takeaways

If you need ensembles

- 👍 use data augmentation to obtain an equivariant model.

If you need data augmentation

- 👍 use an ensemble to boost the equivariance.

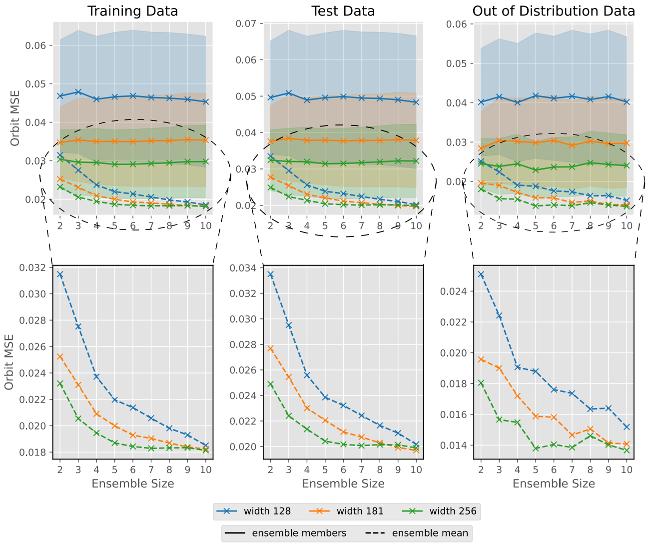
Papers

- Emergent Equivariance in Deep Ensembles
  Jan E. Gerken*, Pan Kessel*
  ICML 2024 (Oral)
  * Equal contribution
- Equivariant Neural Tangent Kernels
  Philipp Misof, Pan Kessel, Jan E. Gerken
  ICML 2025

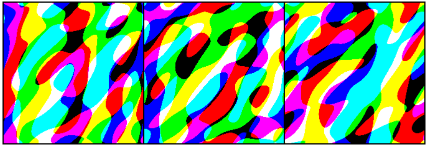
Thank you

Backup

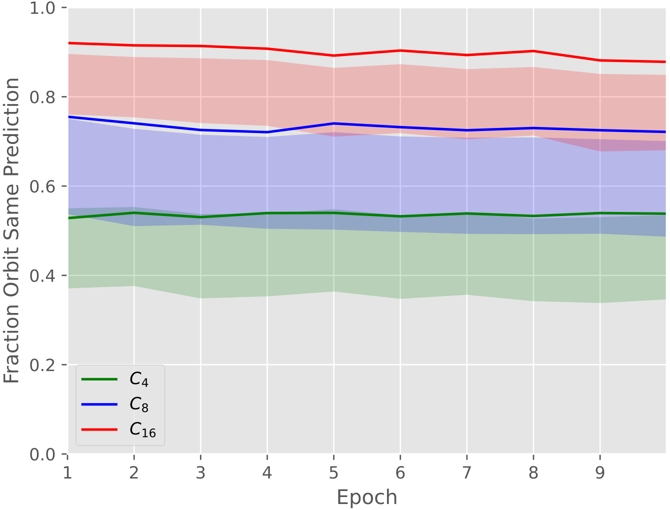
Emergent equivariance of cross products



Histological Data – OOD samples

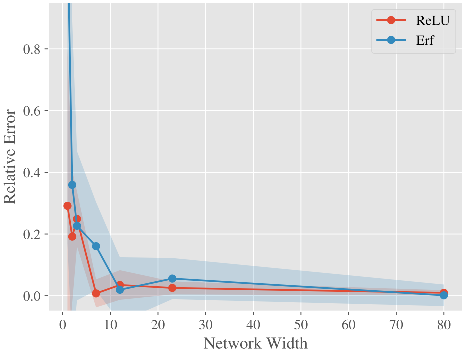


Emergent continuous symmetry on FashionMNIST

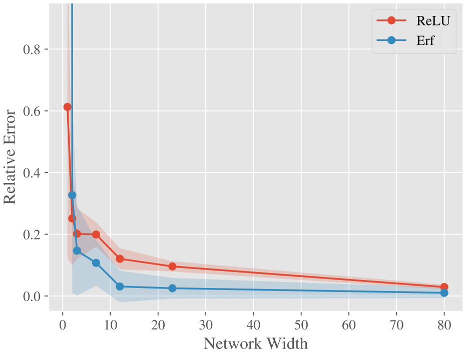


Kernel convergence

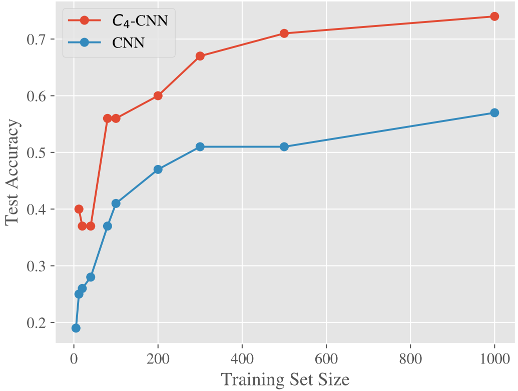
NNGP



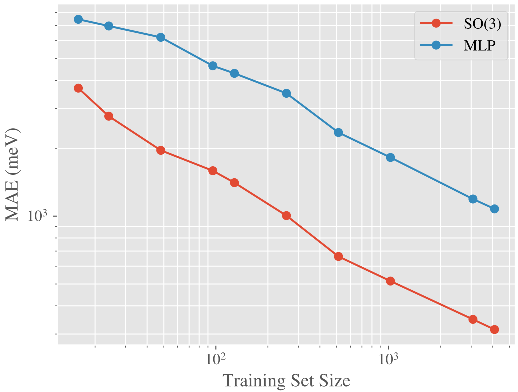
NTK



Equivariant NTKs for medical image classification

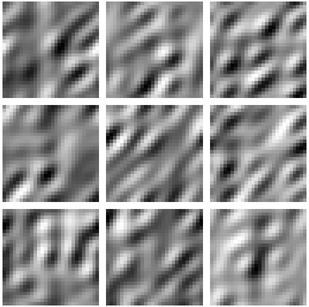


Equivariant NTKs for molecular property regression



OOD samples for CNN to GCNN convergence

MNIST



CIFAR10