Neural Tangent Kernels:

Data augmentation and Feynman diagrams

Jan E. Gerken

CHALMERS
UNIVERSITY OF TECHNOLOGY

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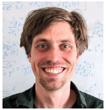
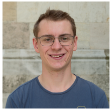
WASP WALLENBERG AI, AUTONOMOUS SYSTEMS AND SOFTWARE PROGRAM

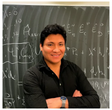
in collaboration with



Pan Kessel



Philipp Misof



Max Guillen

Symmetries in deep learning

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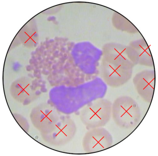

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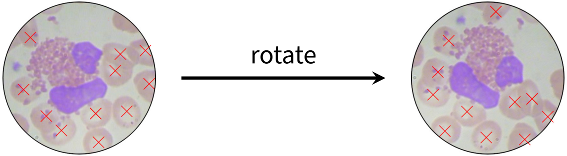

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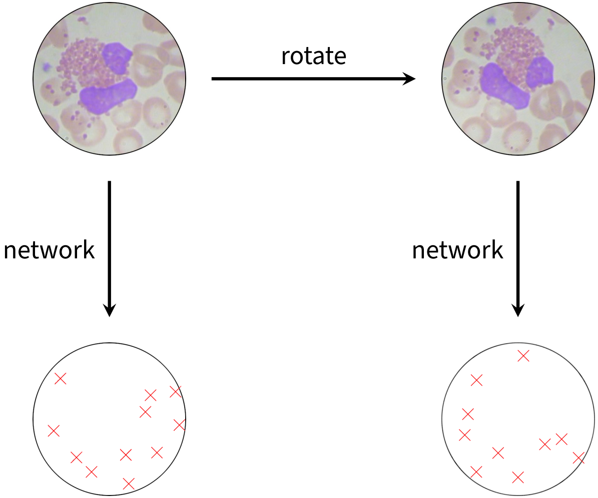

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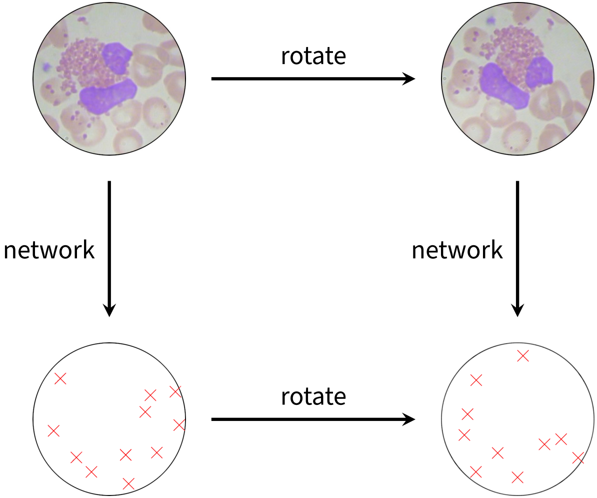

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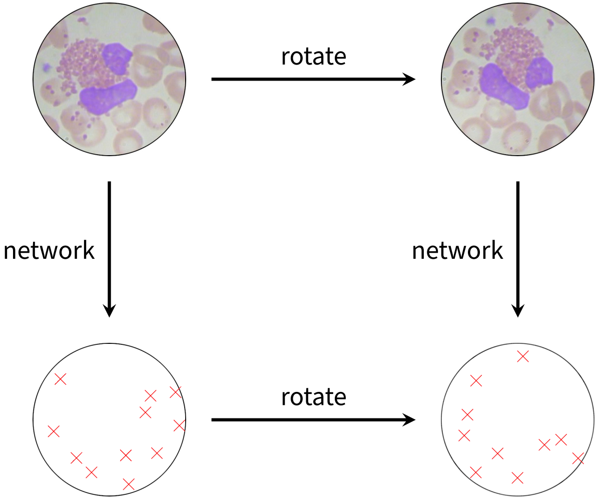

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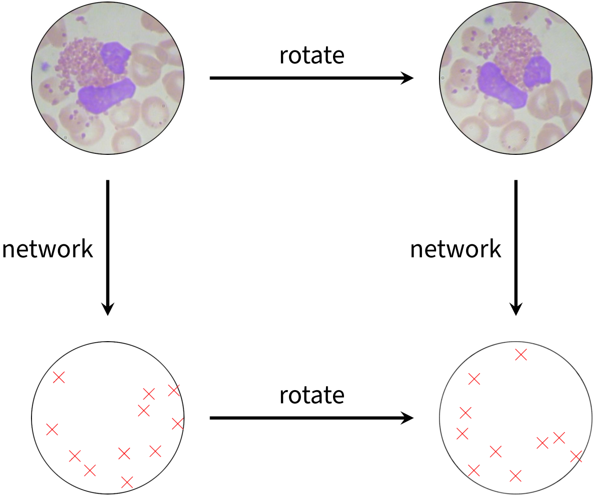

network

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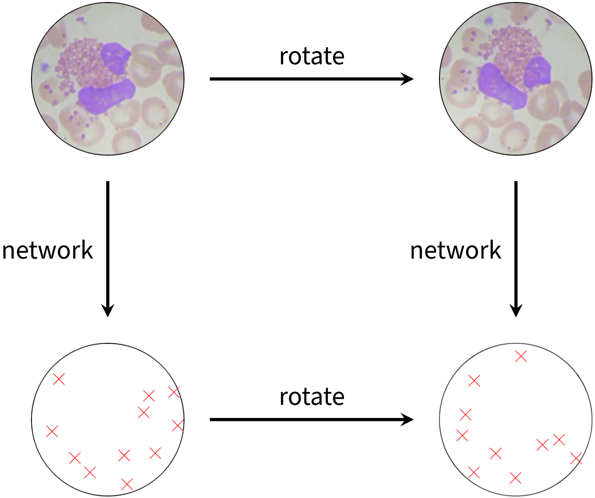
rotation

image

Equivariance



network

$$\Longleftrightarrow \quad \mathcal{N}(\rho_{\text{in}}(g)x) = \rho_{\text{out}}(g)\mathcal{N}(x)$$

rotation

image

Equivariant neural networks

Equivariant neural networks

Group Equivariant Convolutional Networks

Taco S. Cohen T.S.COHEN@UVA.NL
University of Amsterdam

Max Welling M.WELLING@UVA.NL
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Abstract

We introduce Group equivariant Convolutional Neural Networks (G-CNNs), a natural generalization of convolutional neural networks that reduces sample complexity by exploiting symme-

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

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[4] *Computational Research Division and Center for Advanced Mathematics for Energy Research Applications, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA*
[5] *Massachusetts Institute of Technology, Department of Electrical Engineering and Computer Science, Cambridge, MA 02142, USA*

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

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ABSTRACT

Predicting the structure of multi-protein complexes is a grand challenge in biochemistry, with major implications for basic science and drug discovery. Computational structure prediction methods generally leverage pre-defined structural features to distinguish accurate structural models from less accurate ones. This raises the question of whether it is possible to learn characteristics of accurate models directly from atomic coordinates of protein complexes, with no prior assumptions. Here we introduce a machine learning method that learns directly from the 3D positions of all atoms to

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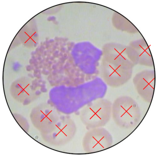

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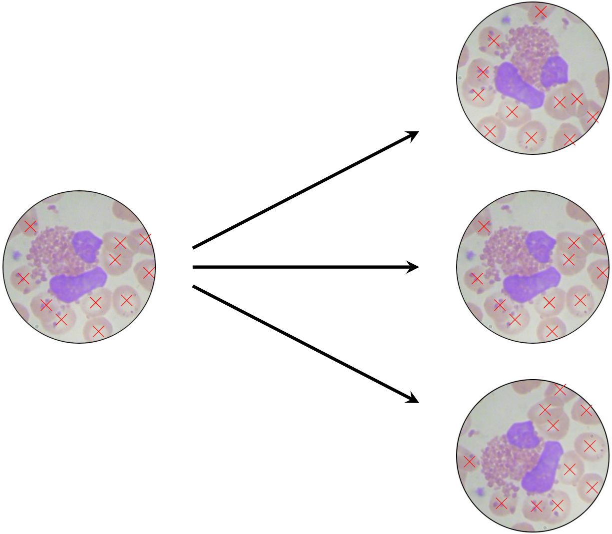

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Article

Accurate structure prediction of biomolecular interactions with AlphaFold 3

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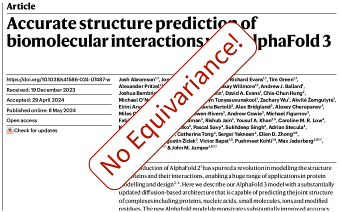

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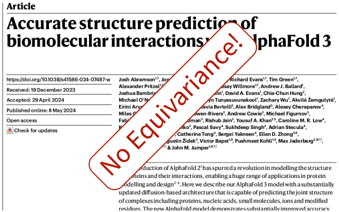

Article

Accurate structure predictio[n] of biomolecular interactions w[ith Al]phaFold 3

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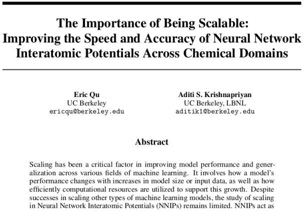

The Importance of Being Scalable: Improving the Speed and Accuracy of Neural Network Interatomic Potentials Across Chemical Domains

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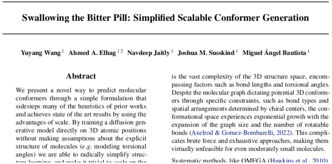

Swallowing the Bitter Pill: Simplified Scalable Conformer Generation

Yuyang Wang[1] Ahmed A. Elhag[1 2] Navdeep Jaitly[1] Joshua M. Susskind[1] Miguel Ángel Bautista[1]

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Systematic methods, like OMEGA (Hawkins et al., 2010),

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Systematic methods, like OMEGA (Hawkins et al., 2010),

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
Supplementary material for this article is available online

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

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@*Equal contribution.*

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Does Equivariance Matter at Scale?

Johann Brehmer* Sönke Behrends Pim de Haan* Taco Cohen*
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mail@johannbrehmer.de

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

- 👍 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:

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

learning rate → η

loss → L

training sample → x_i

Empirical NTK

Training dynamics under continuous gradient descent:

learning rate

loss

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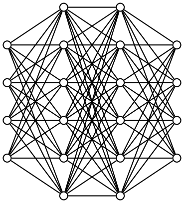
training sample

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]



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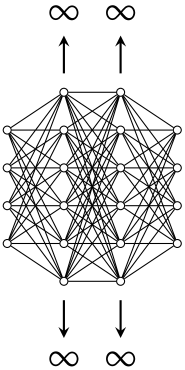

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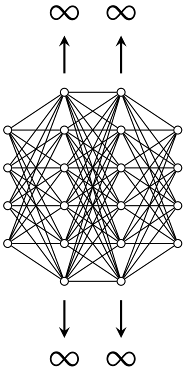

👍 NTK becomes independent of initialization

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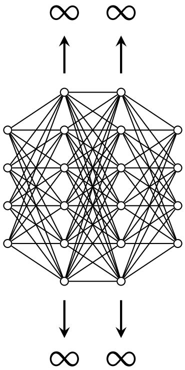

- NTK becomes independent of initialization
- NTK becomes constant in training

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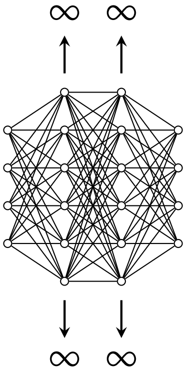

- 👍 NTK becomes independent of initialization
- 👍 NTK becomes constant in training
- 👍 NTK can be computed for most networks

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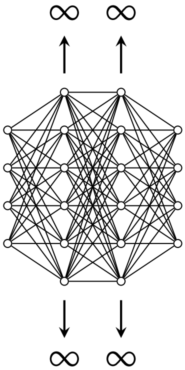

- 👍 NTK becomes independent of initialization
- 👍 NTK becomes constant in training
- 👍 NTK can be computed for most networks
- ✓ Training dynamics can be solved

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

[Jacot et al. 2018]

ⓘ 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]

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train labels

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

learning rate

train data

Data augmentation

Data augmentation at infinite width

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

Data augmentation at infinite width

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

augmented data

augmented labels

Data augmentation at infinite width

group transformation

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

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

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- 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

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Data augmentation at infinite width

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

augmented data

augmented labels

Data augmentation at infinite width

group transformation

augmented labels

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

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

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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

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

Main conclusion

Deep ensembles trained with data augmentation are equivariant.

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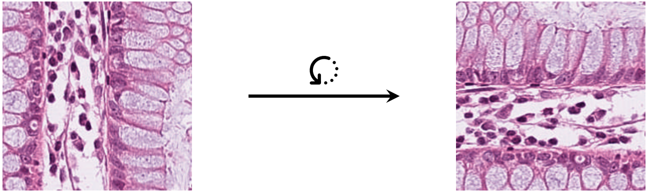
⇨ Training with full data augmentation leads to an equivariant function.

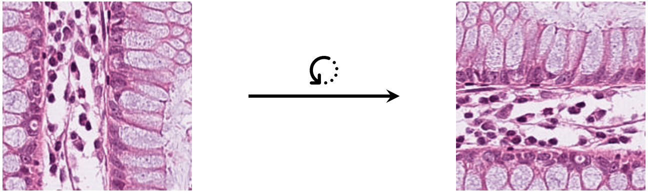
What Does An Augmented Ensemble Converge To?

Rotating images

Rotating images



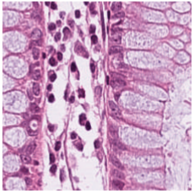
Rotating images

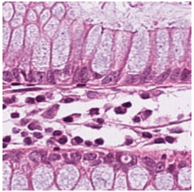


$f(x)$

f : pixels $\rightarrow$ colors

Rotating images





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

f : pixels $\to$ 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

Data augmentation and NTKs

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trained without data augmentation

trained with data augmentation

If

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

Data augmentation and NTKs

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trained without data augmentation — trained with data augmentation

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Then

$$\mu_t^{\text{non-aug}}(x) = \mu_t^{\text{aug}}(x)$$

at infinite width.

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Consider two ensembles:

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$$\mu_t^{\text{non-aug}}(x) = \mu_t^{\text{aug}}(x) \quad \forall t$$

at infinite width.

Data augmentation and NTKs

Consider two ensembles:

trained without data augmentation ↓ trained with data augmentation ↓

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Then

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(!) Given an architecture with NTK Θ^{aug},
find an architecture with NTK $\Theta^{\text{non-aug}}$

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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- Ordinary convolutions

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

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

lifting

Group convolutions

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

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

Group convolutions

[Cohen, Welling 2016]

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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

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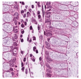

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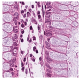
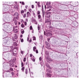


→ lifting

GCNNs

Stack GConv-layers to obtain an invariant network

 ⟶ lifting ⟶ σ

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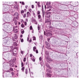 ⟶ lifting ⟶ σ ⟶ GConv

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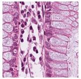 ⟶ lifting ⟶ σ ⟶ GConv ⟶ σ

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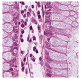 $\longrightarrow$ lifting $\longrightarrow$ σ $\longrightarrow$ GConv $\longrightarrow$ σ $\longrightarrow$ GConv

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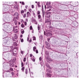
Stack GConv-layers to obtain an invariant network

 ⟶ lifting ⟶ σ ⟶ GConv ⟶ σ ⟶ GConv ⟶ GPool

NTKs for GCNNs

For GCNN-layers, define the NNGP and NTK via

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

NTKs for GCNNs

For GCNN-layers, define the NNGP and NTK via

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

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

NTKs for GCNNs

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

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

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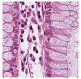
$$\Theta^{(\ell+1)}_{g,g'}(f,f') = K^{(\ell+1)}_{g,g'}(f,f') + \frac{1}{|S_\kappa|} \int_{S_\kappa} \mathrm{d}h\, \Theta^{(\ell)}_{gh,g'h}(f,f')$$

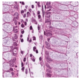
GCNNs

Stack GConv-layers to obtain an invariant network

 ⟶ lifting ⟶ σ ⟶ GConv ⟶ σ ⟶ GConv ⟶ GPool

NTKs for GCNNs

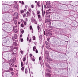
Stack GConv-layers to obtain an invariant network

 ⟶ lifting ⟶ σ ⟶ GConv ⟶ σ ⟶ GConv ⟶ GPool

Compute NTK with layer-wise recursion

NTKs for GCNNs

Stack GConv-layers to obtain an invariant network

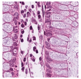
 $\longrightarrow$ lifting $\longrightarrow \sigma \longrightarrow$ GConv $\longrightarrow \sigma \longrightarrow$ GConv $\longrightarrow$ GPool

Compute NTK with layer-wise recursion

0

NTKs for GCNNs

Stack GConv-layers to obtain an invariant network



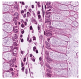
lifting → σ → GConv → σ → GConv → GPool

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

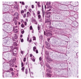
 $\longrightarrow$ lifting $\longrightarrow$ σ $\longrightarrow$ GConv $\longrightarrow$ σ $\longrightarrow$ GConv $\longrightarrow$ GPool

Compute NTK with layer-wise recursion

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

NTKs for GCNNs

Stack GConv-layers to obtain an invariant network

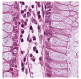
 $\longrightarrow$ lifting $\longrightarrow$ σ $\longrightarrow$ GConv $\longrightarrow$ σ $\longrightarrow$ GConv $\longrightarrow$ GPool

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



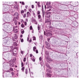
$\longrightarrow$ lifting $\longrightarrow$ σ $\longrightarrow$ GConv $\longrightarrow$ σ $\longrightarrow$ GConv $\longrightarrow$ GPool

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

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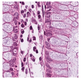 $\longrightarrow$ lifting $\longrightarrow \sigma \longrightarrow$ GConv $\longrightarrow \sigma \longrightarrow$ GConv $\longrightarrow$ GPool

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

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- Consider two neural networks

NTKs of MLPs and GCNNs

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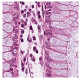
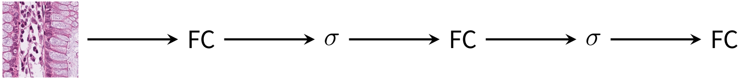
An MLP

 ⟶ FC ⟶ σ ⟶ FC ⟶ σ ⟶ FC

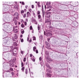
NTKs of MLPs and GCNNs

- Consider two neural networks

An MLP



A GCNN



NTKs of MLPs and GCNNs

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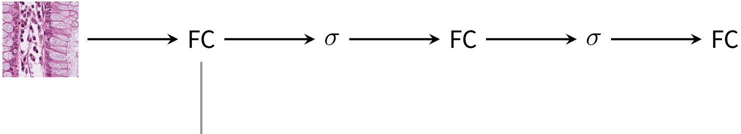
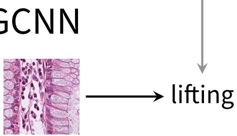
An MLP



A GCNN

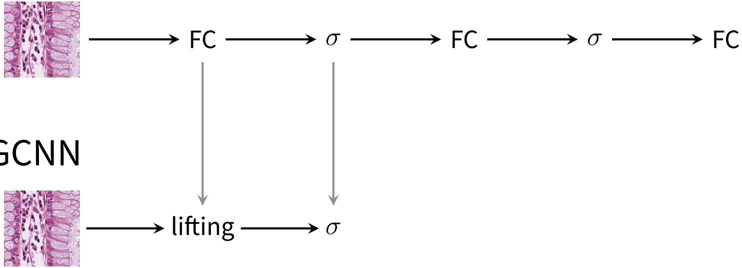


NTKs of MLPs and GCNNs

- Consider two neural networks

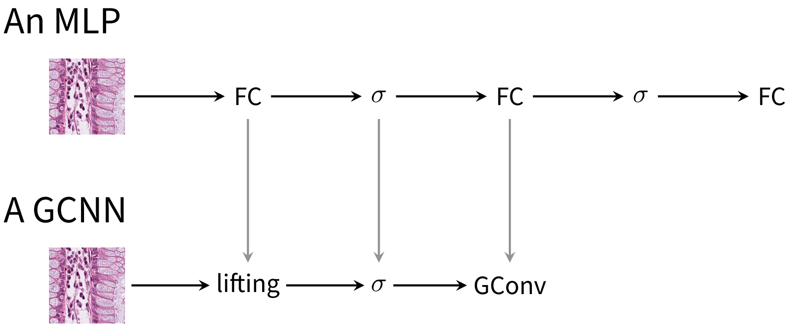
An MLP

A GCNN



NTKs of MLPs and GCNNs

- Consider two neural networks



NTKs of MLPs and GCNNs

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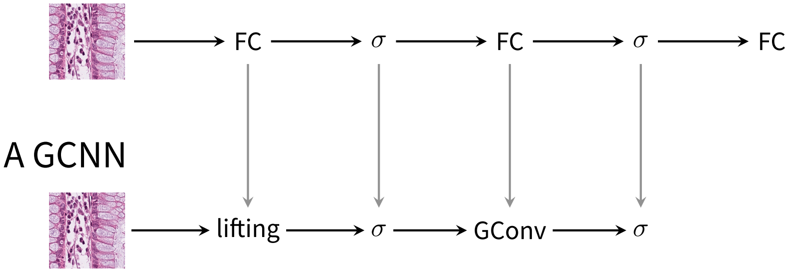
An MLP



NTKs of MLPs and GCNNs

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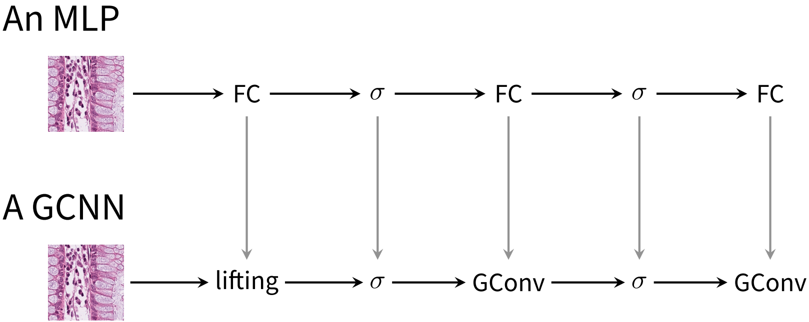

NTKs of MLPs and GCNNs

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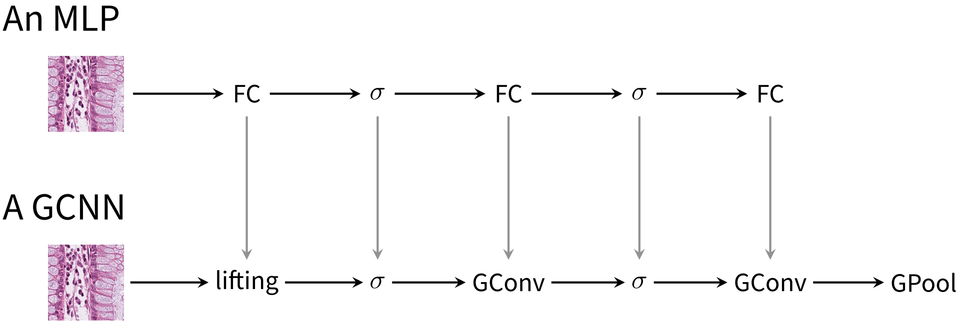

NTKs of MLPs and GCNNs

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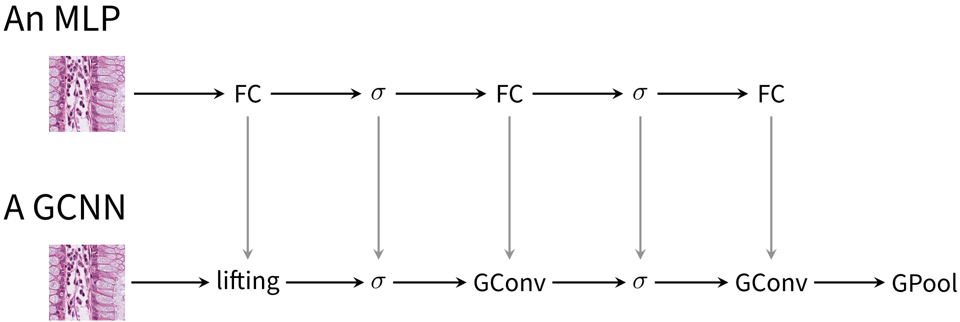


- Then

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

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 → Θ^{GCNN}; before: aug → Θ^{MLP}

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

⇨ training the MLP on G-augmented data

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 → Θ^{GCNN}; before: aug → Θ^{MLP}

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

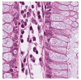
⇨ training the MLP on G-augmented data = training the GCNN on unaugmented data

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

Data augmentation of CNNs

Data augmentation of CNNs

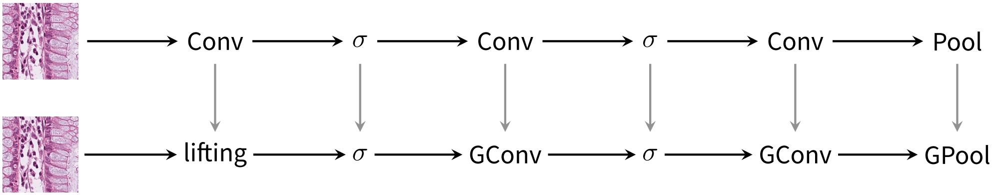
- Consider a CNN



→ Conv → σ → Conv → σ → Conv → Pool

Data augmentation of CNNs

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



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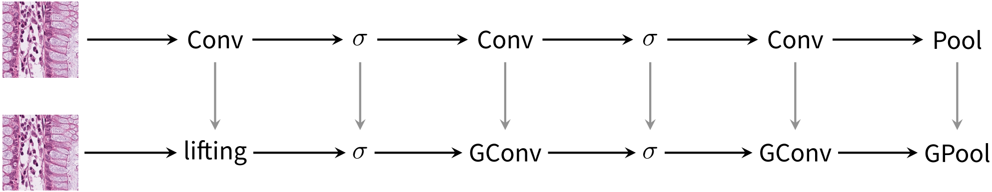

- Then

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

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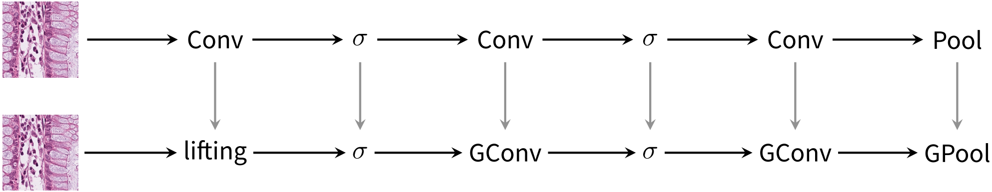


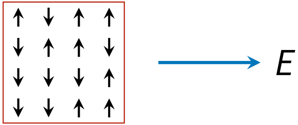
- Then

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

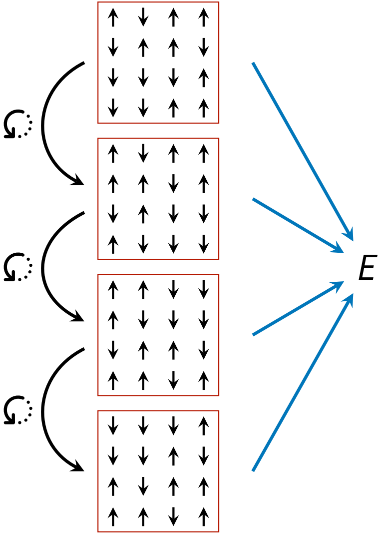
⇨ By training the CNN on rotated images, one obtains a roto-translation invariant GCNN

Experiments

Ising model



Ising model



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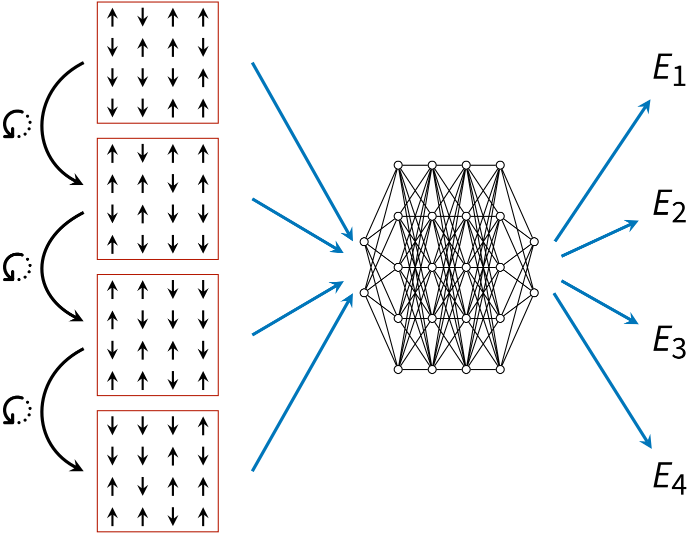

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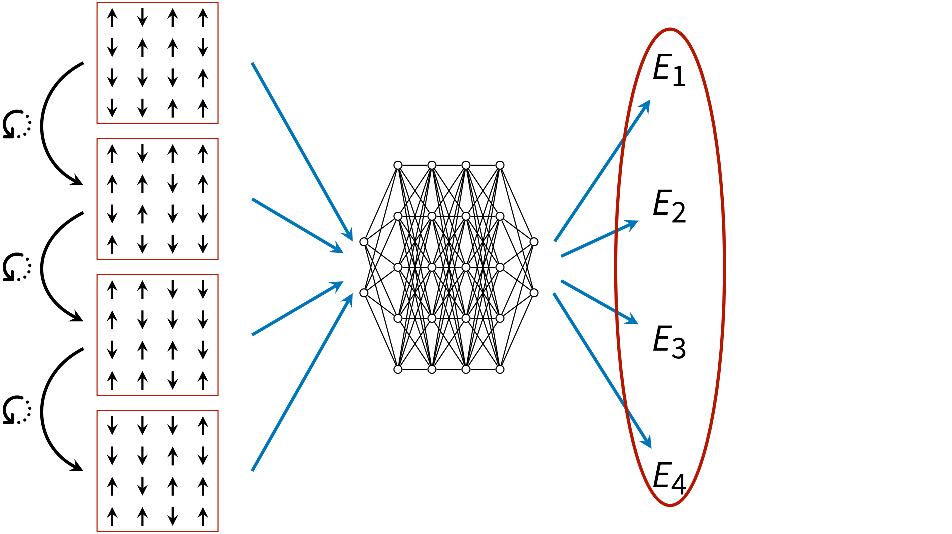
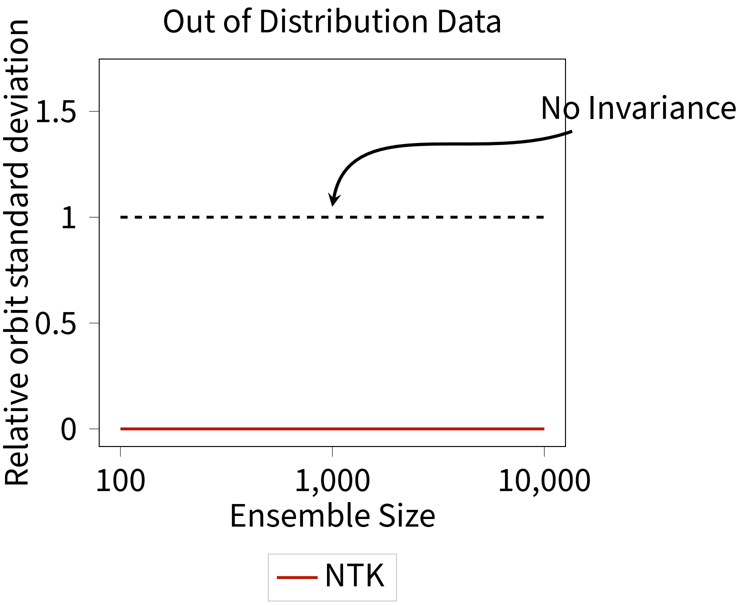
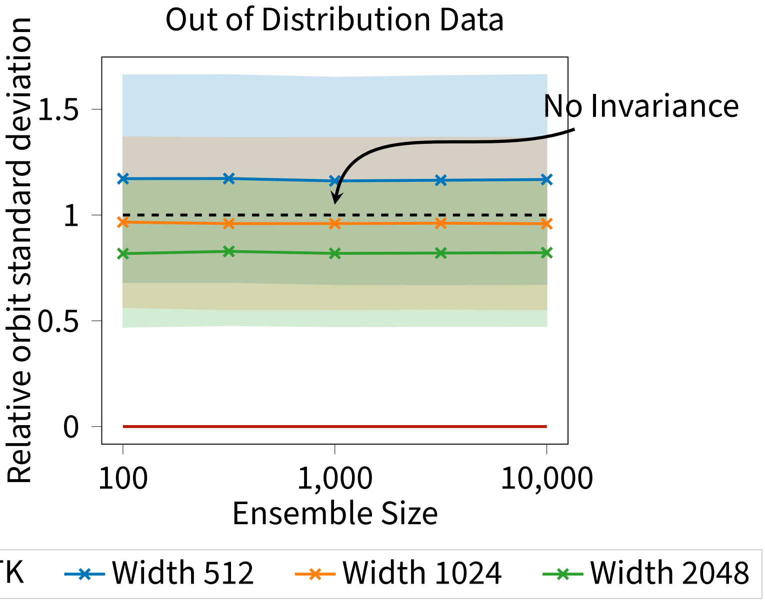
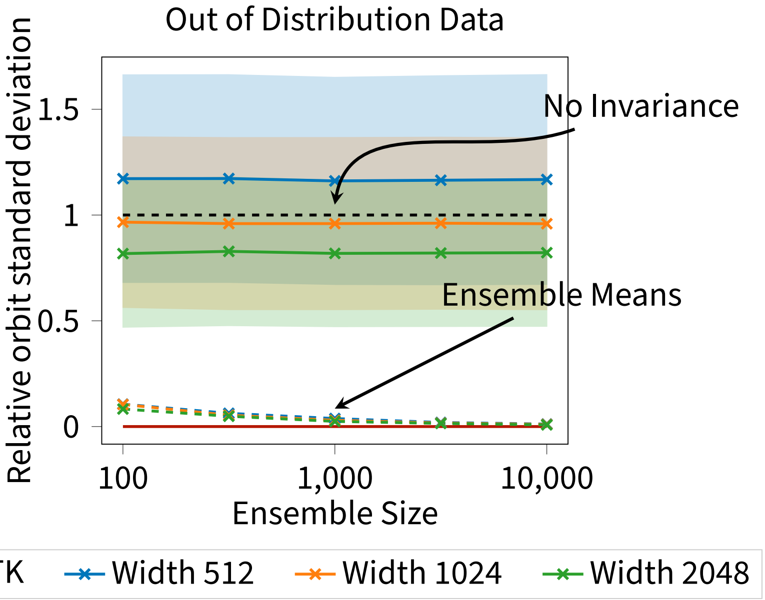



Out of Distribution Data
No Invariance
Relative orbit standard deviation
1.5
1
0.5
0
100
1,000
10,000
Ensemble Size
NTK


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


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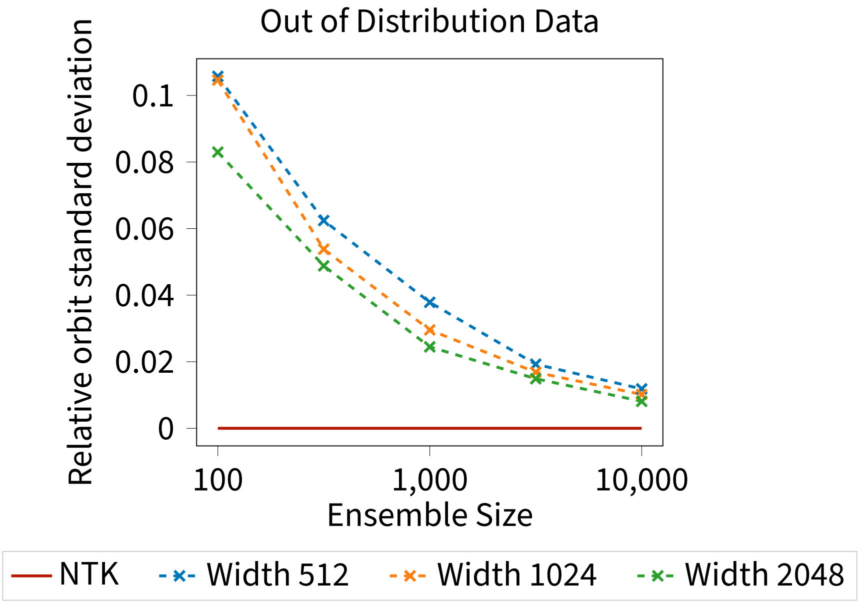
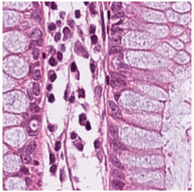

Out of Distribution Data
Relative orbit standard deviation
0.1
0.08
0.06
0.04
0.02
0
100
1,000
10,000
Ensemble Size
NTK
Width 512
Width 1024
Width 2048

Histological slices

[Kather et al. 2018]



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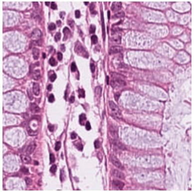
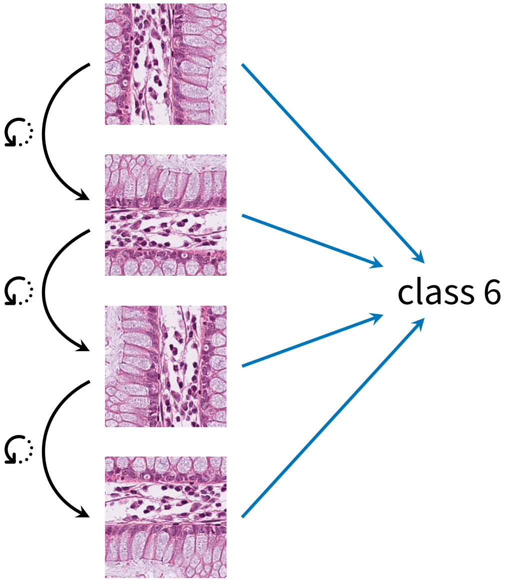


class 6

Histological slices



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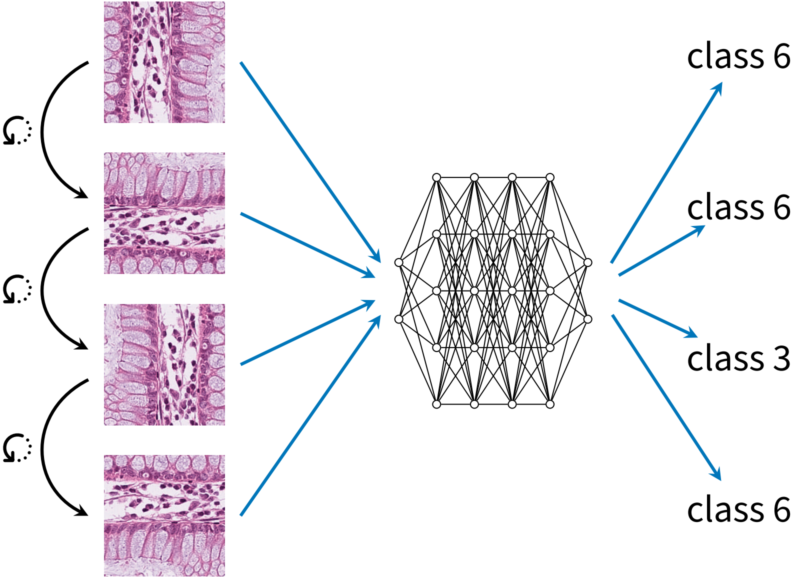

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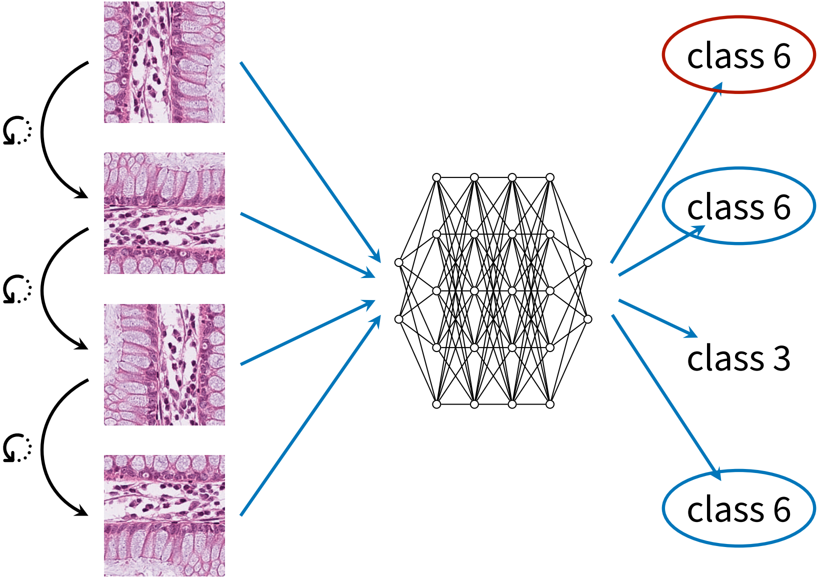
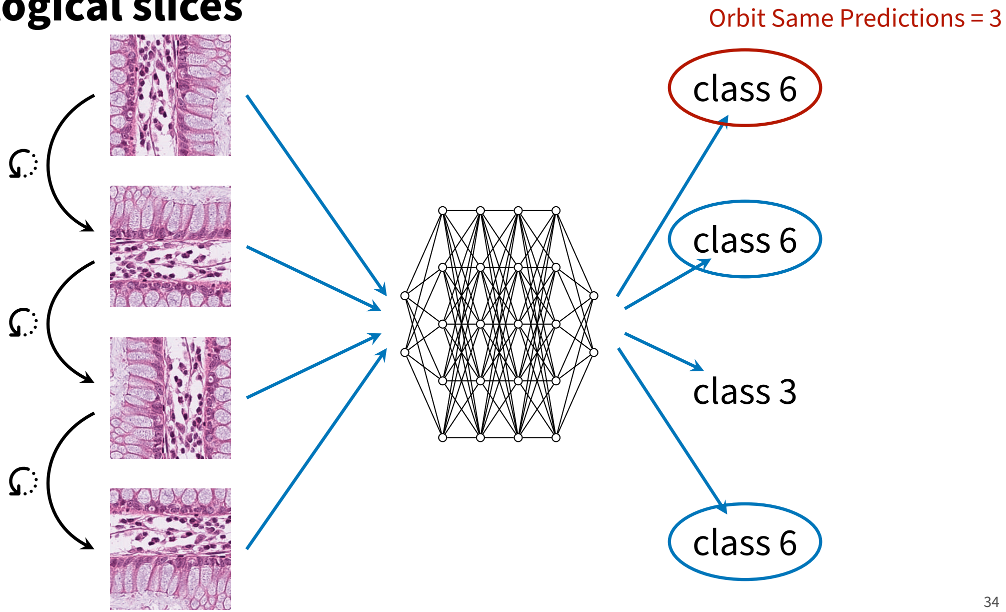
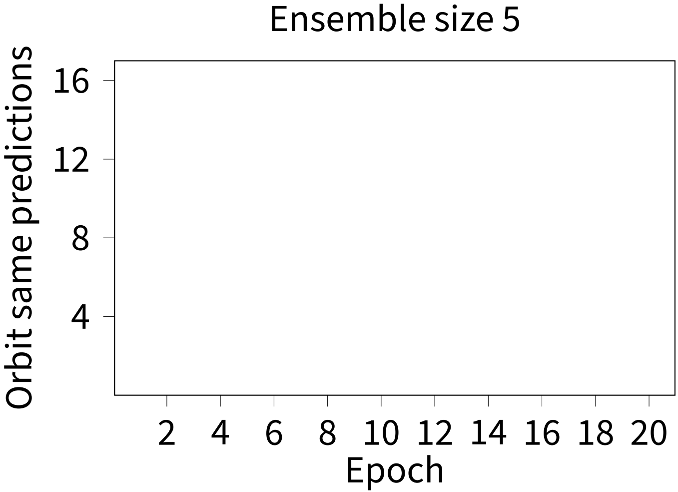


Histological slices



Out of distribution results



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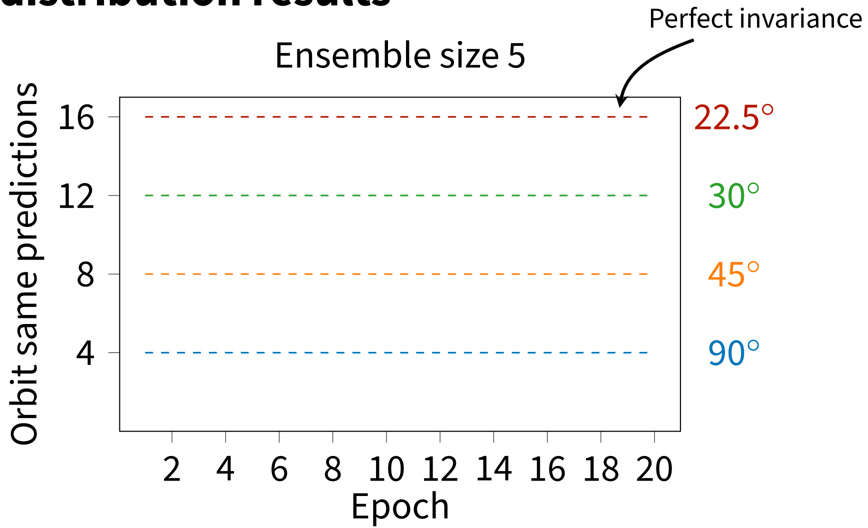

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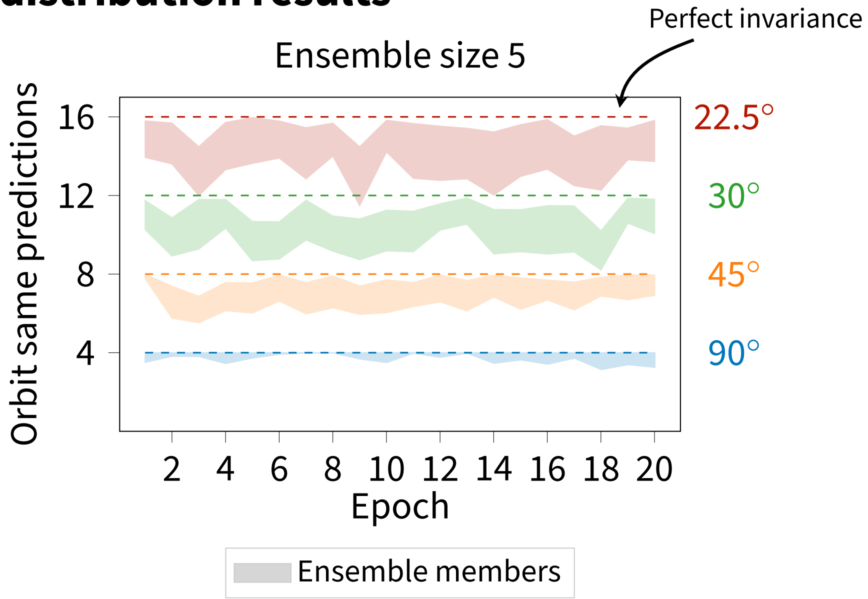

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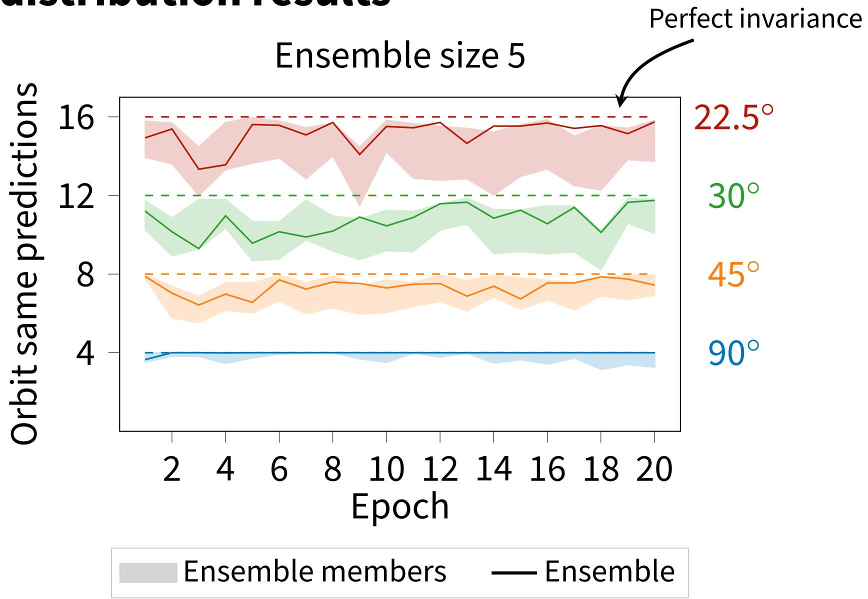

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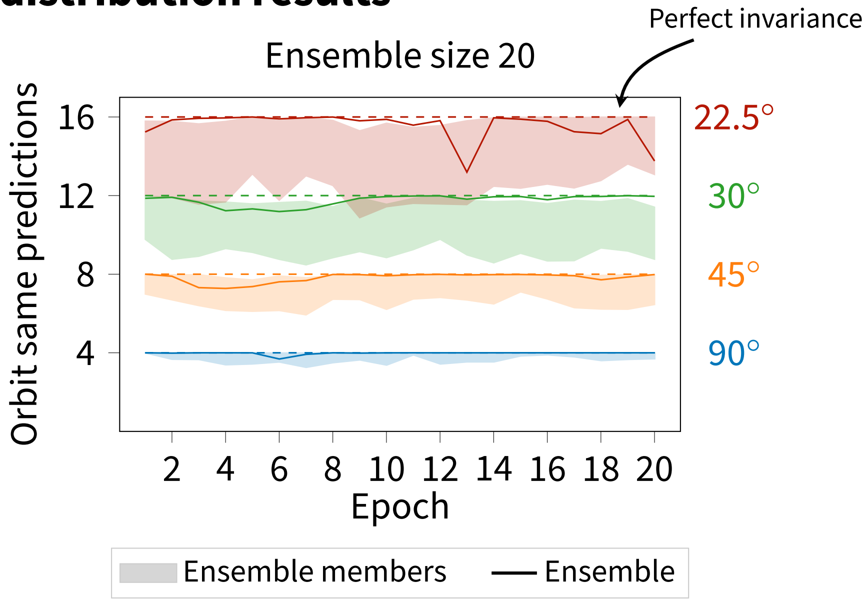

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- ✓ Emergent equivariance (as opposed to invariance)

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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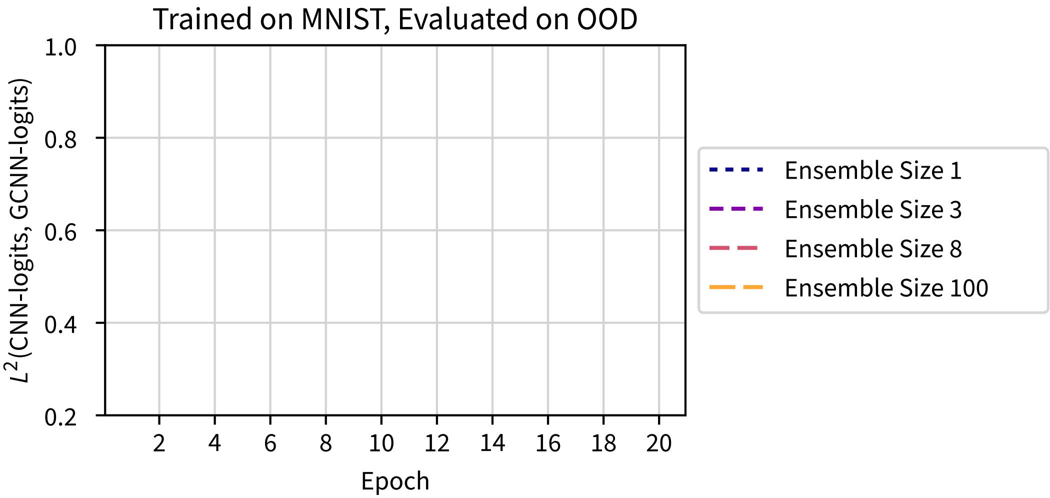

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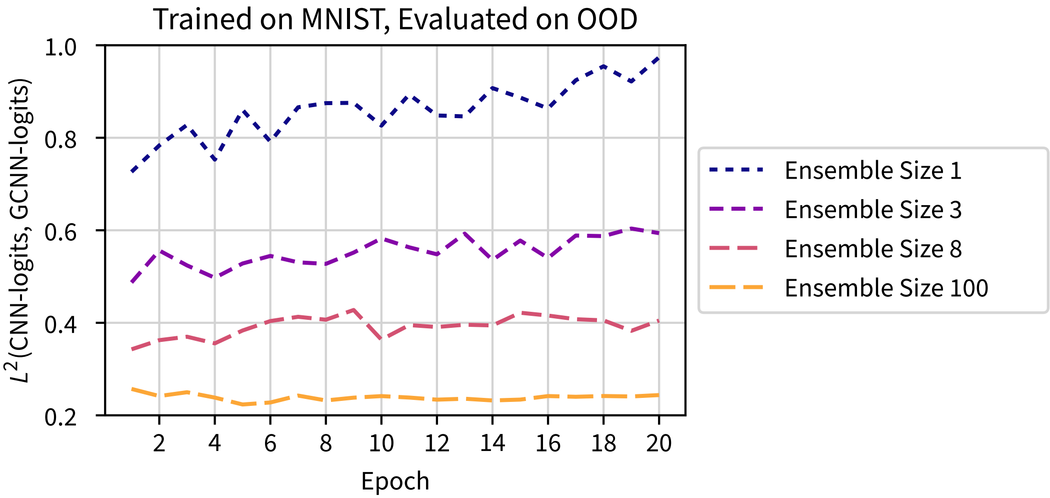

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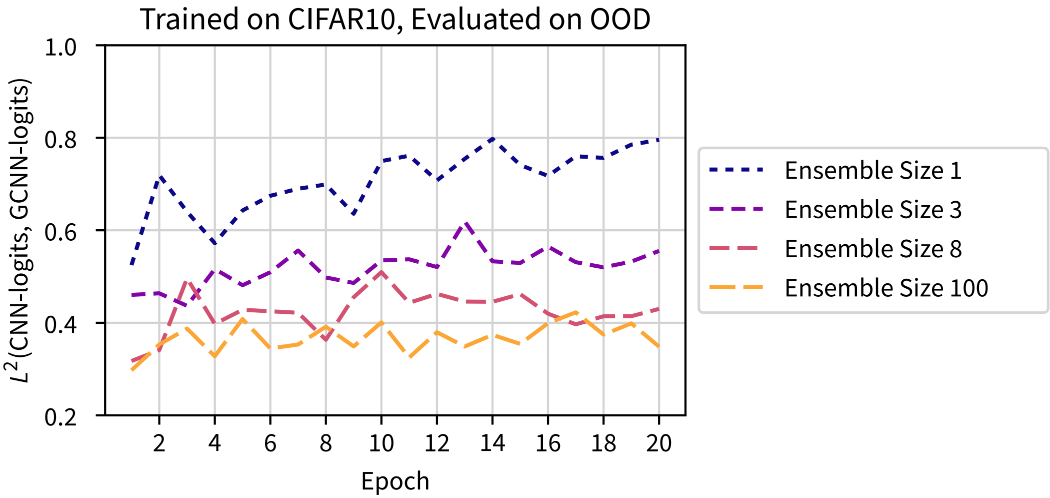

Finite-width from Feynman diagrams

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> ⓘ Use methods from physics to compute finite-width effects

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- In field theory, consider probability distribution over fields (functions)
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- Compute statistics of these fields

Feynman diagrams

Feynman diagrams are used to compute statistics

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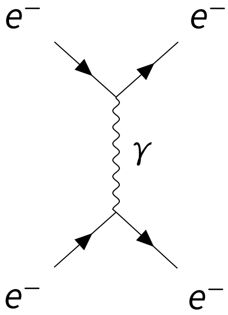
E.g. Electron-electron scattering



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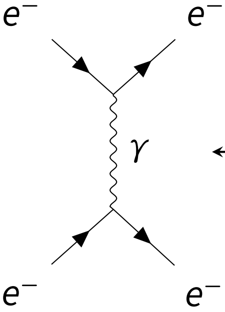

$$\longleftrightarrow \quad -ie^2 \frac{[\bar{u}(p_3)\gamma^\mu u(p_1)][\bar{u}(p_4)\gamma_\mu u(p_2)]}{(p_1 - p_3)^2}$$

Non-Gaussian Corrections from Physics

- Taylor-expand network statistics in 1/width
- Use Feynman diagrams to compute non-Gaussian corrections

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Neural Networks	Field Theory
infinite width	no interactions
Gaussian distribution	free fields
finite-width	interactions

Tensors for neural network statistics

[Roberts, Yaida 2022]

Goal: Compute corrections for all neural network statistics at initialization, e.g.

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cumulant → $\mathbb{E}^c_\theta$; preactivation → z; NTK fluctuation, $\widehat{\Delta\Theta}^{(\ell)} = \widehat{\Theta}^{(\ell)} - \mathbb{E}_\theta[\widehat{\Theta}^{(\ell)}]$

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Decompose these into tensors

$$= \frac{1}{n}\left(D^{(\ell)}_{1234}\delta_{i_1 i_2}\delta_{i_3 i_4} + F^{(\ell)}_{1324}\delta_{i_1 i_3}\delta_{i_2 i_4} + F^{(\ell)}_{1423}\delta_{i_1 i_4}\delta_{i_2 i_3}\right)$$

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Gram tensor, $F^{(\ell)}_{1324} = F^{(\ell)}(x_1, x_3, x_2, x_4)$

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At order $1/n$, we have

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- D and F for mixed statistics
- 6 more for higher derivatives, needed for training

Tensor recursions

For each tensor, there is a layer-wise recursion relation, e.g.

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$$F^{(\ell+1)}_{1324} = \langle \sigma^{(\ell)}_1 \sigma^{(\ell)}_2 \sigma'^{(\ell)}_3 \sigma'^{(\ell)}_4 \rangle_{K^{(\ell)}} \Theta^{(\ell)}_{34}$$

$$+ \sum_{\alpha,\beta,\gamma,\delta=1}^{4} \langle \sigma^{(\ell)}_1 \sigma'^{(\ell)}_3 z^{(\ell)}_\alpha \rangle_{K^{(\ell)}} \langle \sigma^{(\ell)}_2 \sigma'^{(\ell)}_4 z^{(\ell)}_\beta \rangle_{K^{(\ell)}} K^{\alpha\gamma}_{(\ell)} K^{\beta\delta}_{(\ell)} F^{(\ell)}_{\gamma 3 \delta 4}$$

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> ⓘ Computing these recursions analytically is very laborious

Feynman diagrams

Use Feynman diagrams to compute these recursions.

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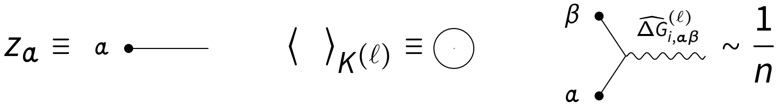
- For preactivations, can read off Feynman rules from NN probability distribution, e.g. [Banta et al. 2024]



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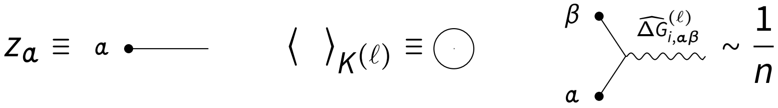
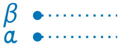
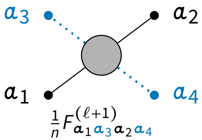


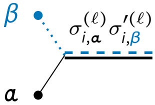
- For derivatives, need to find Feynman rules by inspecting analytic expressions

Feynman rules relevant for the F-tensor

$\widehat{\Delta\Theta}_{\alpha\beta} \equiv$







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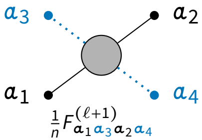

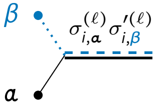

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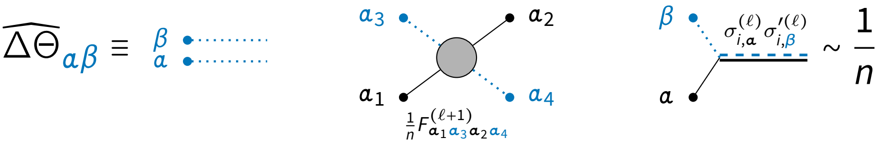

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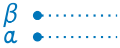
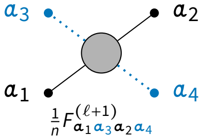
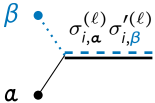
$\widehat{\Delta\Theta}_{\alpha\beta} \equiv$ 





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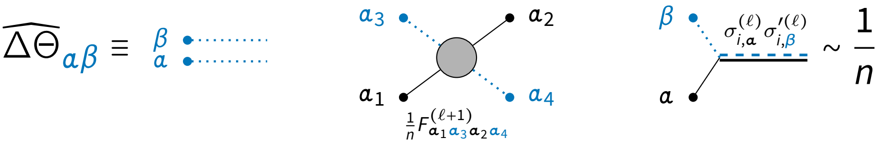
- Dotted lines attached to a propagator do not appear in the Gaussian expectation value

Feynman rules relevant for the F-tensor

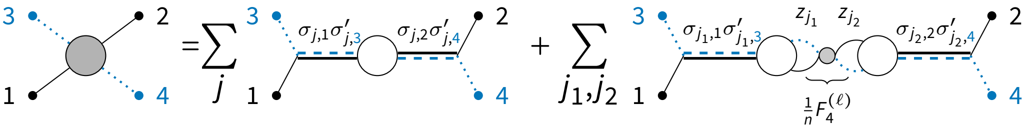


The propagator ◯ satisfies selection rules, e.g.

- It cannot be directly connected to other propagators
- Dotted lines attached to a propagator do not appear in the Gaussian expectation value
- Pairs of dashed lines of the same color connected to the propagator add a factor of Θ

The F-recursion

Draw all diagrams possible for the F-tensor at order $1/n$



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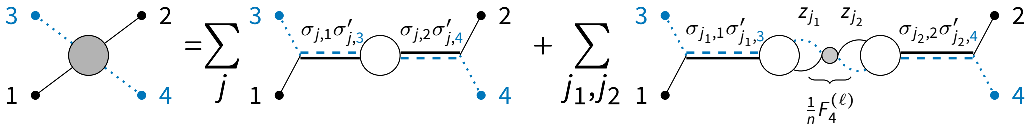
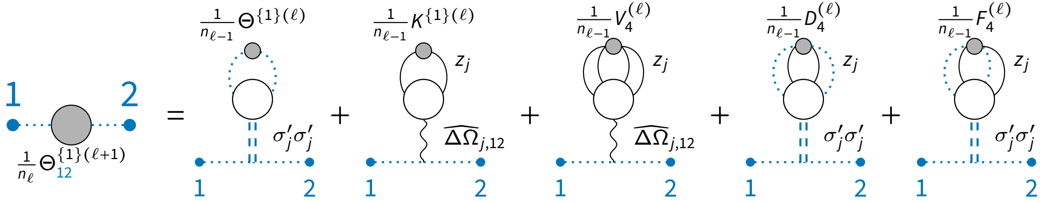


Compare to the analytical expression

$$\frac{1}{n}F^{(\ell+1)}_{1324} = \frac{1}{n}\langle \sigma^{(\ell)}_1 \sigma^{(\ell)}_2 \sigma'^{(\ell)}_3 \sigma'^{(\ell)}_4 \rangle_{K^{(\ell)}} \Theta^{(\ell)}_{34}$$

$$+ \frac{1}{n}\sum_{\alpha,\beta,\gamma,\delta=1}^{4} \langle \sigma^{(\ell)}_1 \sigma'^{(\ell)}_3 z^{(\ell)}_\alpha \rangle_{K^{(\ell)}} \langle \sigma^{(\ell)}_2 \sigma'^{(\ell)}_4 z^{(\ell)}_\beta \rangle_{K^{(\ell)}} K^{\alpha\gamma}_{(\ell)} K^{\beta\delta}_{(\ell)} F^{(\ell)}_{\gamma 3 \delta 4}$$

The NTK recursion at finite width



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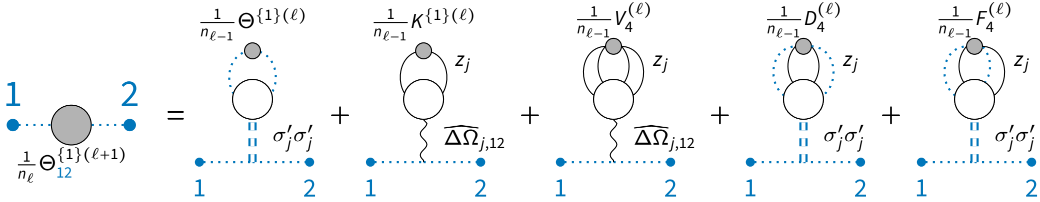
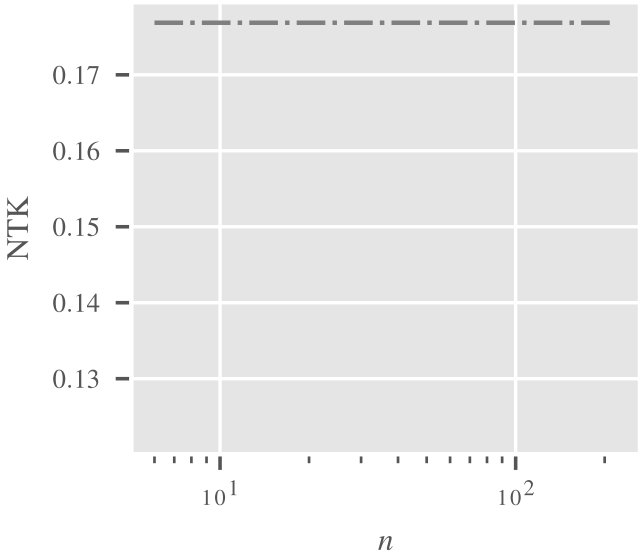


ⓘ Feynman diagrams allow for much simpler derivation of recursion relations

Numerical results



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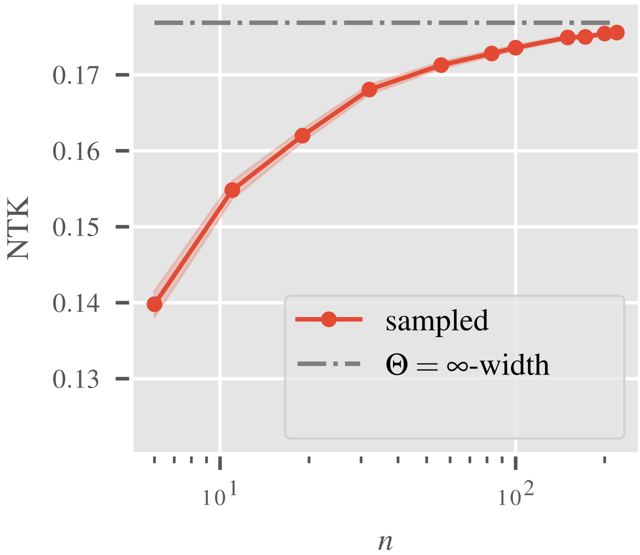

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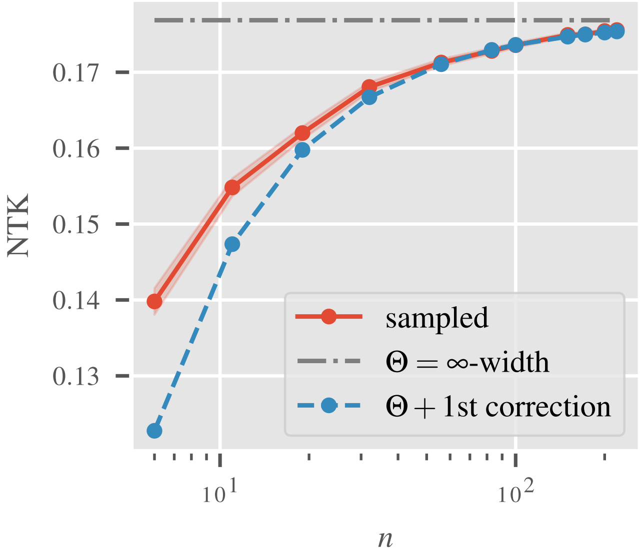

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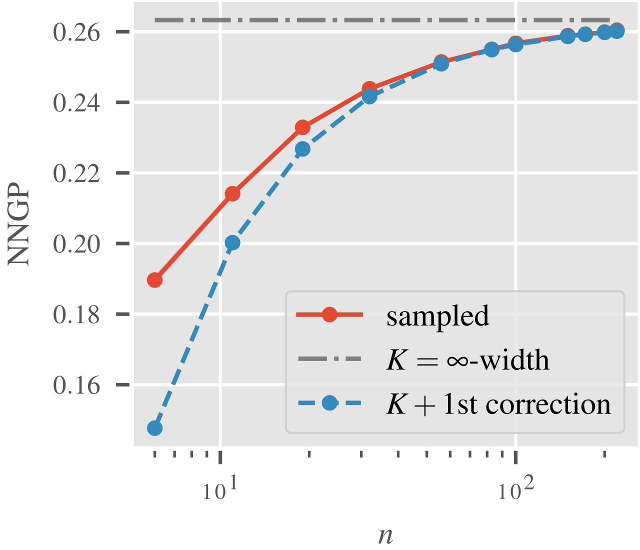

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- Neural tangent kernels at infinite width can be used to understand data augmentation of deep ensembles:
  - Deep ensembles become exactly equivariant
  - Deep ensembles trained with data augmentation are group convolutional networks

- To consider non-Gaussian corrections away from infinite width, consider 1/width expansion

- The corrections can be computed conveniently using Feynman diagrams

Papers

- Emergent Equivariance in Deep Ensembles
  Jan E. Gerken*, Pan Kessel*
  ICML 2024 (Oral)
- Equivariant Neural Tangent Kernels
  Philipp Misof, Pan Kessel, Jan E. Gerken
  ICML 2025
- Finite-Width Neural Tangent Kernels from Feynman Diagrams
  Max Guillen*, Philipp Misof*, Jan E. Gerken
  arXiv: 2508.11522

* Equal contribution

Thank you!