Equivariant Neural Tangent Kernels

Connecting data augmentation and equivariant architectures

by Philipp Misof

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CHALMERS
UNIVERSITY OF TECHNOLOGY

WASP WALLENBERG AI, AUTONOMOUS SYSTEMS AND SOFTWARE PROGRAM

Joint work with

Jan Gerken
(Chalmers)

Pan Kessel
(Prescient Design, Switzerland)

1. The Neural Tangent Kernel
2. NTK of Equivariant NNs
3. Concrete Examples
4. Data Augmentation vs GCNNs

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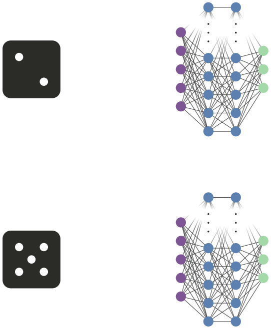

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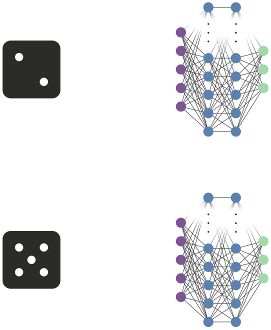
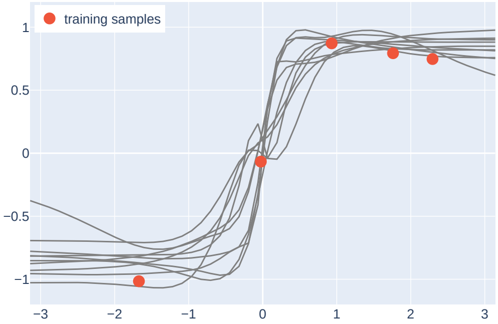


Let's learn $\sin(x)$

3-layer MLPs with width 8



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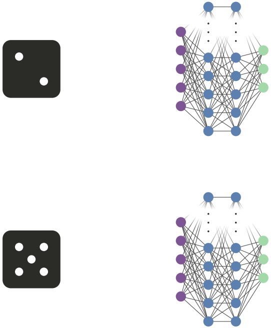

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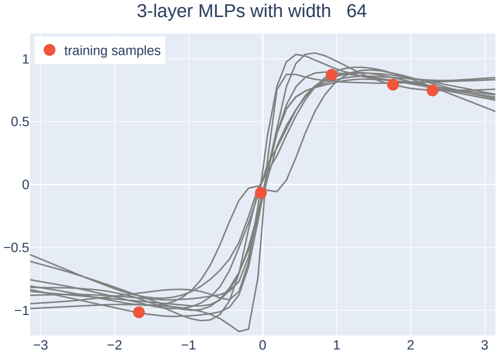

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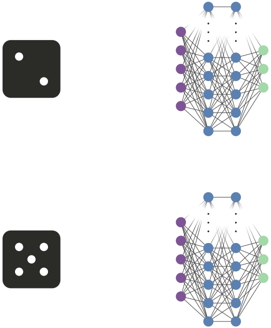

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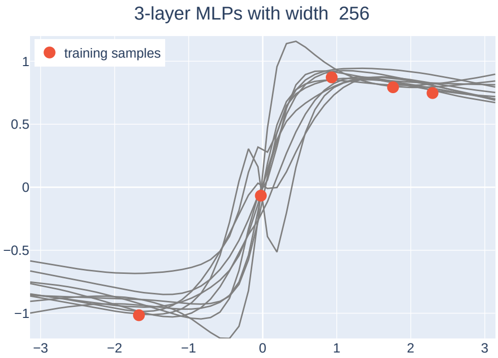

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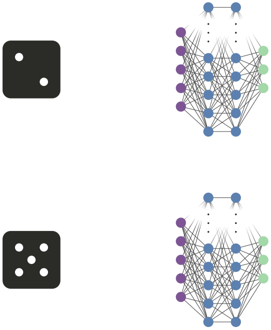

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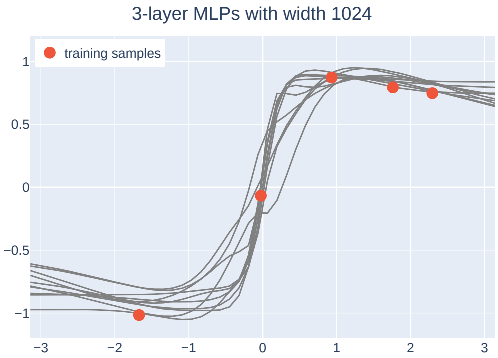

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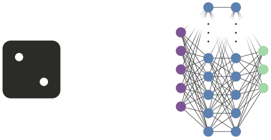

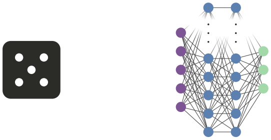

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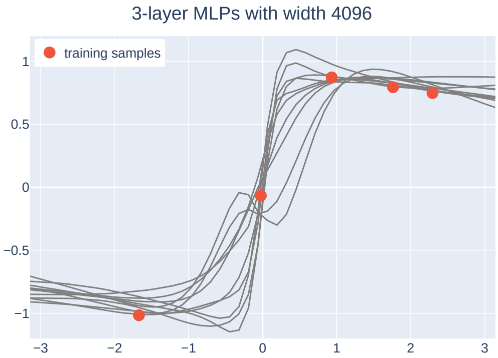

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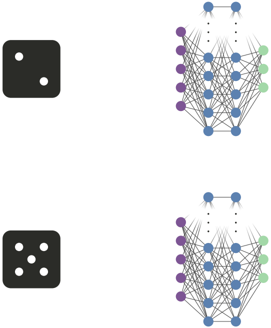

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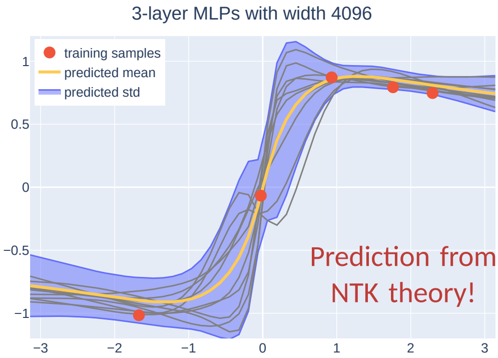

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(Jacot, Gabriel, and Hongler 2018)

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$$\frac{\mathrm{d}\mathcal{N}}{\mathrm{d}t}(x) = -\eta \sum_{i=1}^{n_{\text{train}}} \Theta_t(x, x_i) \frac{\partial \mathcal{L}}{\partial \mathcal{N}(x_i)}$$

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Learning rate

Loss

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- Tool for **dataset distillation** *(Nguyen, Chen, and Lee 2021)*

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$$K^{(\ell)}(x, x') = \mathbb{E}\left[\mathcal{N}^{(\ell)}(x)\left(\mathcal{N}^{(\ell)}(x')\right)^{\mathsf{T}}\right]$$

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Each NN layer then corresponds to a particular **recursion**

$$\begin{aligned} K^{(\ell+1)}(x, x') &= A^{(\ell)}(K^{(\ell)}(x, x')), \\ \Theta^{(\ell+1)}(x, x') &= B^{(\ell)}(\Theta^{(\ell)}(x, x'), K^{(\ell+1)}(x, x')) \end{aligned}$$

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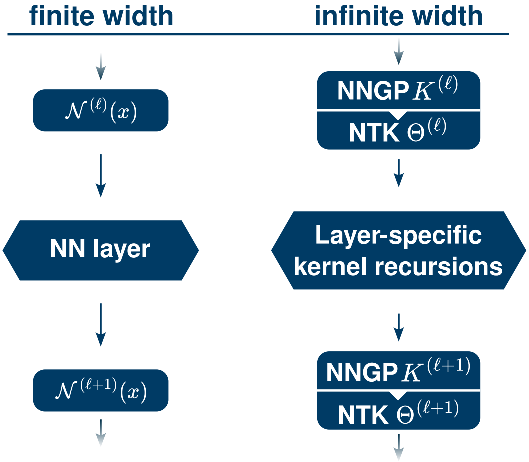
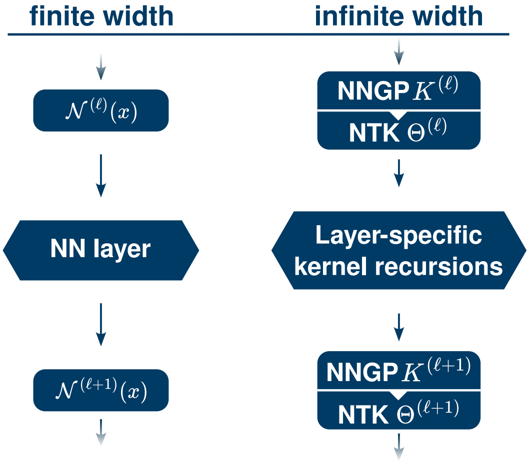
$$\begin{aligned}
K^{(\ell+1)}(x, x') &= \overbrace{A^{(\ell)}}^{\text{layer-specific NNGP map}}(K^{(\ell)}(x, x')), \\
\Theta^{(\ell+1)}(x, x') &= \underbrace{B^{(\ell)}}_{\text{layer-specific NTK map}}(\Theta^{(\ell)}(x, x'), K^{(\ell+1)}(x, x'))
\end{aligned}$$


finite width
infinite width
$\mathcal{N}^{(\ell)}(x)$
NN layer
$\mathcal{N}^{(\ell+1)}(x)$
NNGP $K^{(\ell)}$
NTK $\Theta^{(\ell)}$
Layer-specific kernel recursions
NNGP $K^{(\ell+1)}$
NTK $\Theta^{(\ell+1)}$



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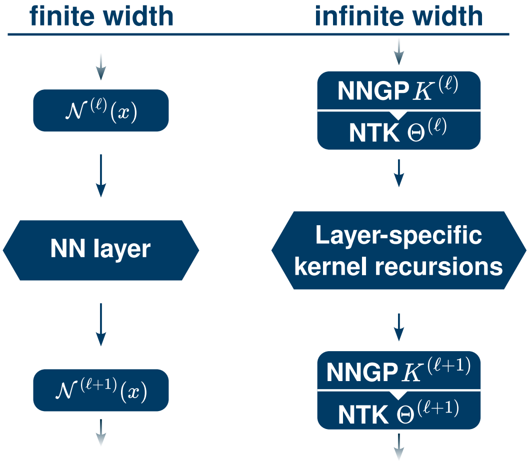

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Convention: We treat nonlinearities σ as individual layers

We extend the NTK to equivariant NNs

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We cover

Group Convolution

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Elementwise Non-linearity

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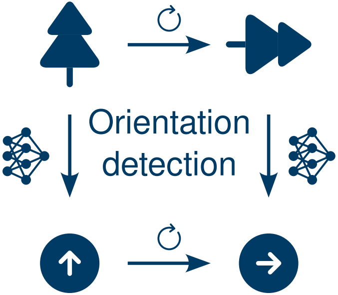

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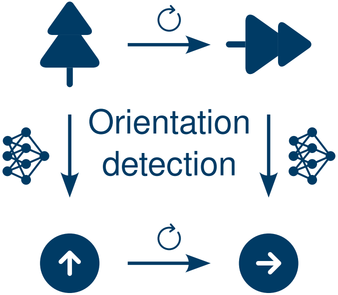

$$\begin{tikzcd} f \arrow[r, "\rho_{\text{in}}(g)"] \arrow[d, "\mathcal{N}"] & \rho_{\text{in}}(g)(f) \arrow[d, "\mathcal{N}"] \\ \mathcal{N}(f) \arrow[r, "\rho_{\text{out}}(g)"] & \rho_{\text{out}}(g)[\mathcal{N}(f)] \end{tikzcd}$$

$$\forall g \in G$$

Recap on Group Convolutional Neural Networks (GCNNs)

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Group convolutional layer

$$[\mathcal{N}^{(\ell+1)}(f)](g) = \frac{1}{\sqrt{n_\ell |S_\kappa|}} \int_G \mathrm{d}h \, \kappa\big(g^{-1}h\big) [\mathcal{N}^{(\ell)}(f)](h)$$

Recap on Group Convolutional Neural Networks (GCNNs)

Group convolutional layer

filter

input signal

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group element

group

\# channels

filter support

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Elementwise non-linearity σ

$$[\mathcal{N}^{(\ell+1)}(f)](g) = \sigma\big([\mathcal{N}^{(\ell)}(f)](g)\big), \qquad \sigma : \mathbb{R} \to \mathbb{R} \text{ elementwise}$$

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∞-width limit:

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∞**-width limit:** # channels $\to \infty$

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- Obtain **equivariant Kernel methods**

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Provide **implementations** in the `neural-tangents` library *(Novak et al. 2020)*

∞-width limit in practice: Histological image classification

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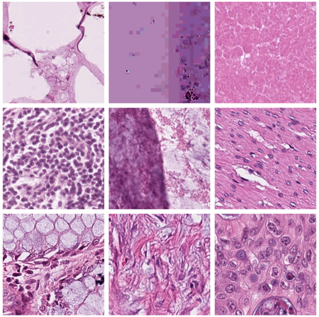

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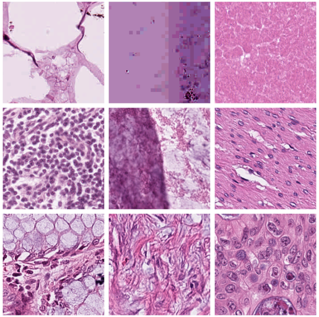

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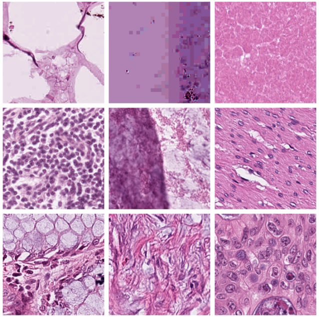

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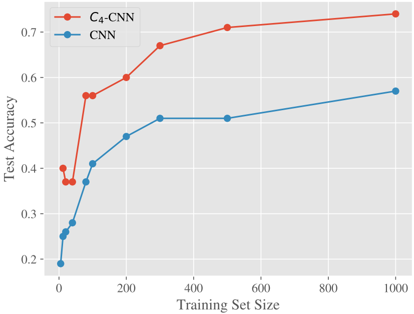

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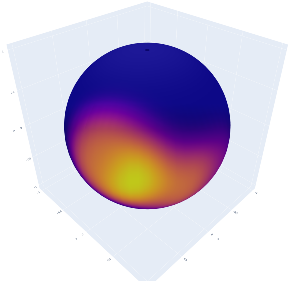
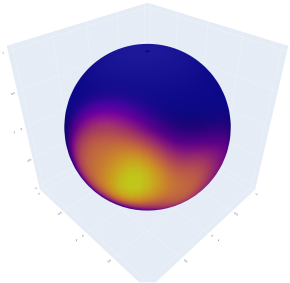


Atoms' environments are represented as signals on the sphere *(Esteves, Slotine, and Makadia 2023)*

∞-width limit in practice: Molecular Energy Prediction on QM9



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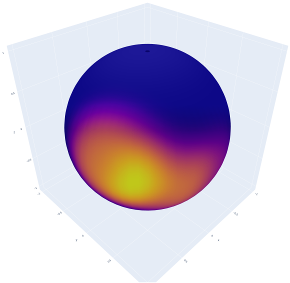

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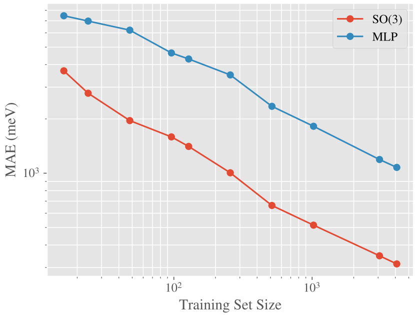

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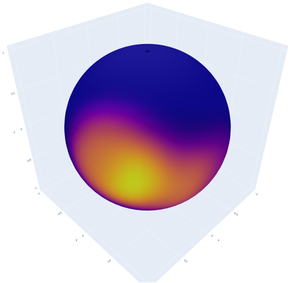

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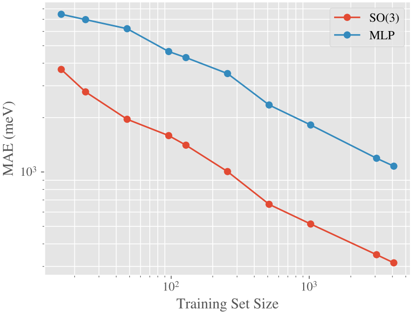

➡ Performance boost due to 3d-rotation invariance extends to the ∞-width limit

Data Augmentation $\leftrightarrow$ Group Convolutional (GC) NNs

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Similar result for data augmented CNN $\leftrightarrow$ $C_4 \ltimes \mathbb{R}^2$ GCNN

Architecture correspondence

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$$\mathrm{FC}^{(1)} \longrightarrow \sigma \longrightarrow \mathrm{FC}^{(3)} \longrightarrow \sigma \longrightarrow \cdots \longrightarrow \mathrm{FC}^{(L)}$$

$$\mathrm{Lifting} \longrightarrow \sigma \longrightarrow \mathrm{GConv}^{(3)} \longrightarrow \sigma \longrightarrow \cdots \longrightarrow \mathrm{GConv}^{(L)} \longrightarrow \mathrm{GPool}$$

All group convolutions with global filter support $S_\kappa^\ell = G$ or $S_\kappa^1 = X$ for the lifting layer.

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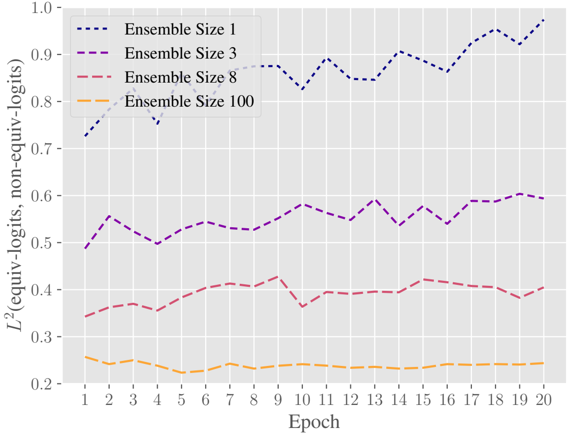

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Do you want to know more?