Equivariant Neural Tangent Kernels

by Philipp Misof

Department of Mathematical Sciences, Division of Algebra and Geometry

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UNIVERSITY OF GOTHENBURG

CHALMERS
UNIVERSITY OF TECHNOLOGY

WASP | WALLENBERG AI, AUTONOMOUS SYSTEMS AND SOFTWARE PROGRAM

Joint work with

Jan Gerken
(Chalmers)

Pan Kessel
(Prescient Design, Switzerland)

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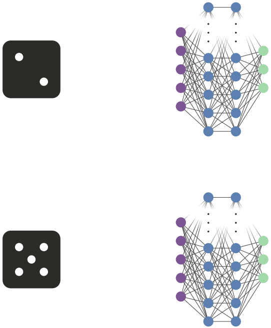

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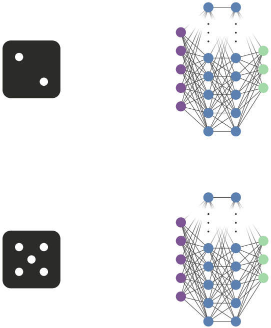
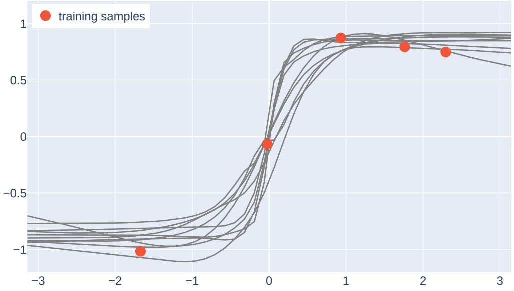


Let's learn $\sin(x)$

3-layer MLP with widths 8



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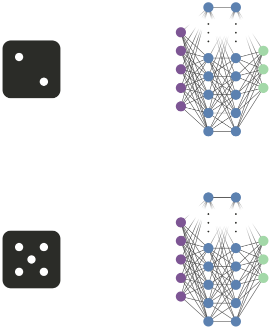

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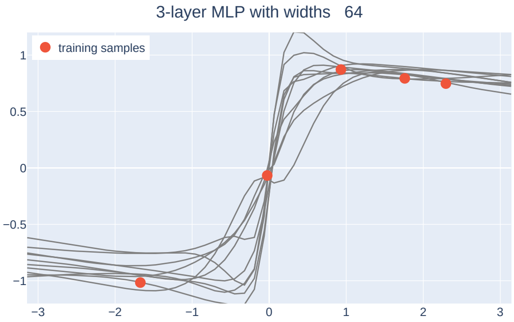

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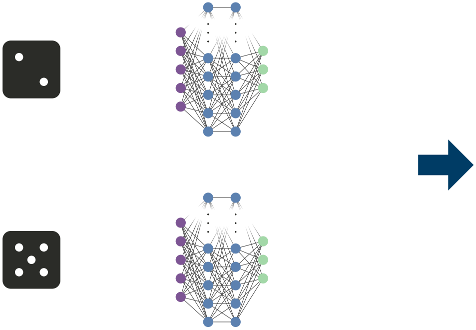

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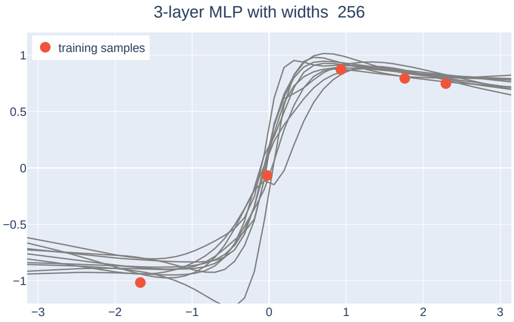

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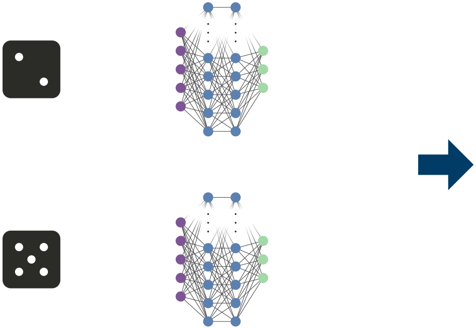

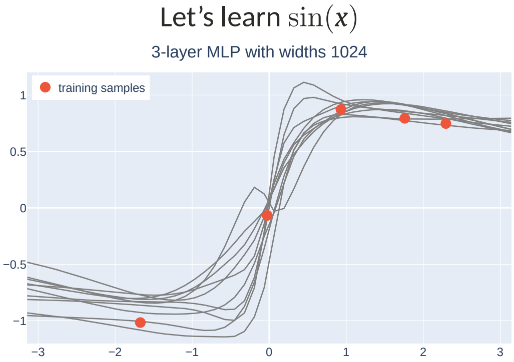

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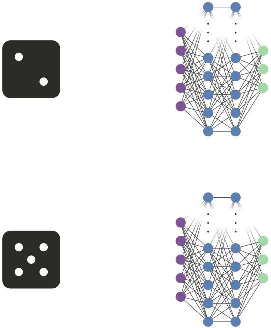

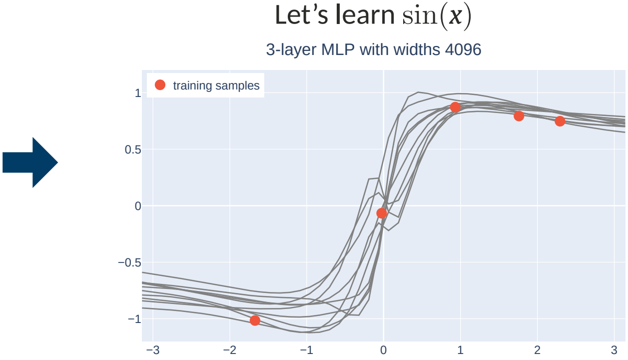

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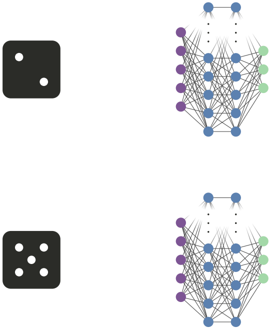

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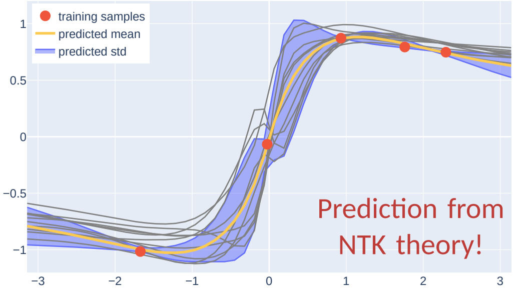
3-layer MLP with widths 4096



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(Jacot, Gabriel, and Hongler 2018)

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Assume **Gradient Flow** instead of discrete Gradient Descent

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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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Neural Network output

Learning rate

Loss

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(empirical) Neural Tangent Kernel

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

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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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layer-specific NNGP map

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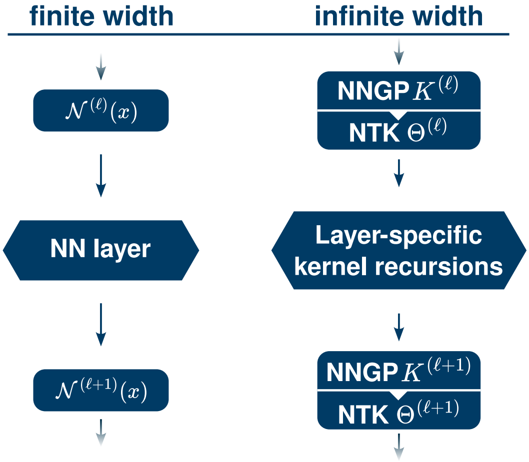
layer-specific NTK map


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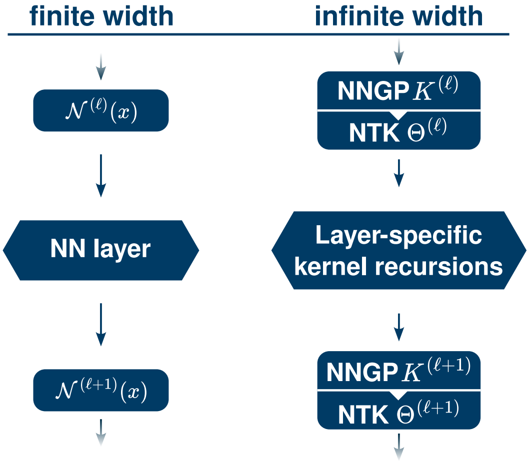

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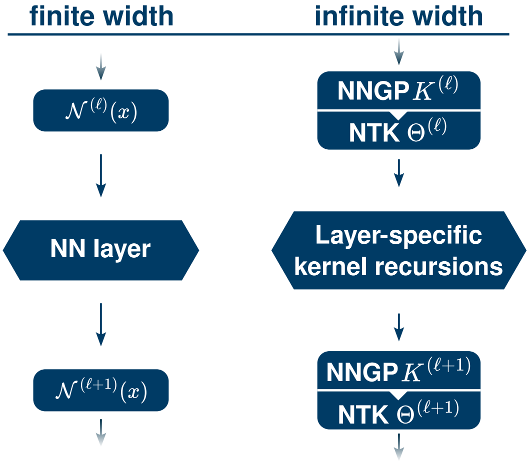

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Convention: We treat nonlinearities σ as individual layers

We extend the NTK to equivariant NNs

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We cover

Group Convolution

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Group Pooling

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Elementwise Non-linearity

Recap on equivariant NNs

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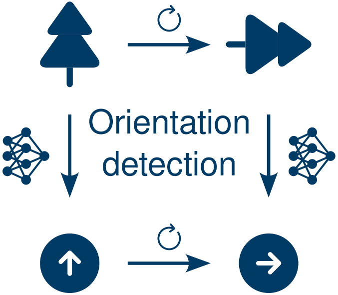

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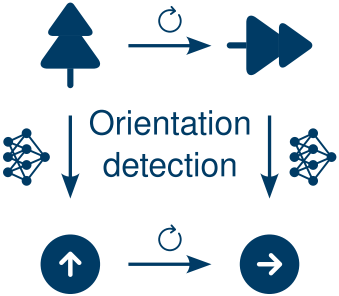

$$\begin{tikzcd}
f \arrow[r, "\rho_{\text{in}}(g)"] \arrow[d, "\mathcal{N}"] & \rho_{\text{in}}(g)(f) \arrow[d, "\mathcal{N}"] \\
\mathcal{N}(f) \arrow[r, "\rho_{\text{out}}(g)"] & \rho_{\text{out}}(g)[\mathcal{N}(f)]
\end{tikzcd}$$

$$\forall g \in G$$

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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Evaluation point in group space

∞**-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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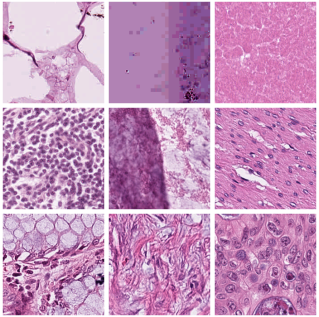

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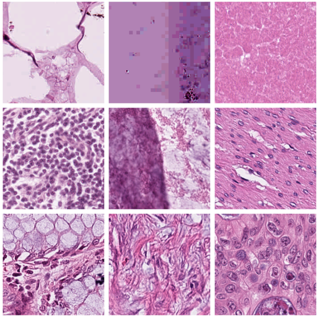

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vs.

$C_4 \ltimes \mathbb{R}^2$ GCNN

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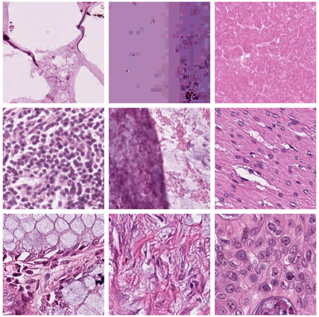

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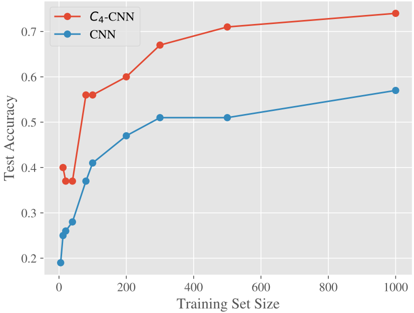

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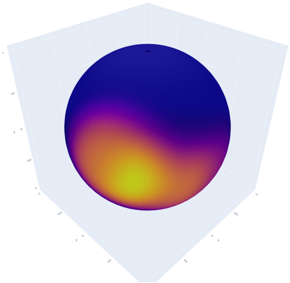

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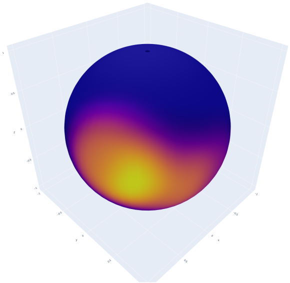

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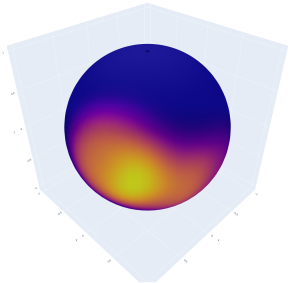
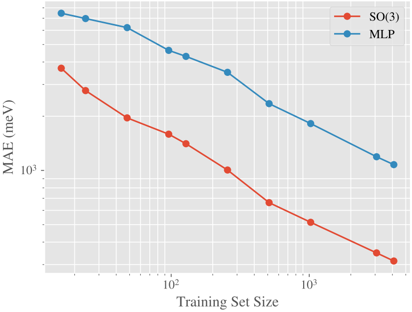


Atoms' environments are represented as signals on the sphere *(Esteves, Slotine, and Makadia 2023)*

MLP

vs.

$\mathrm{SO}(3)$ **GCNN**



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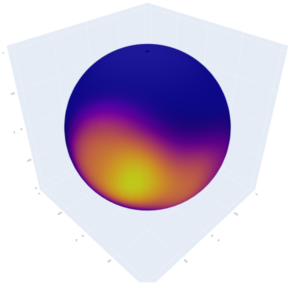

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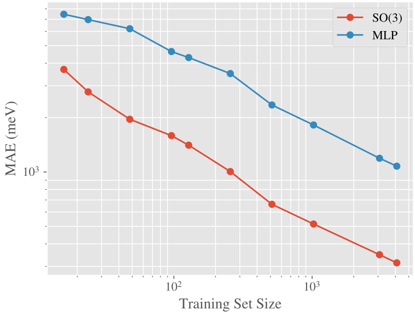

Performance boost due to 3d-rotation invariance extends to the ∞-width limit

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

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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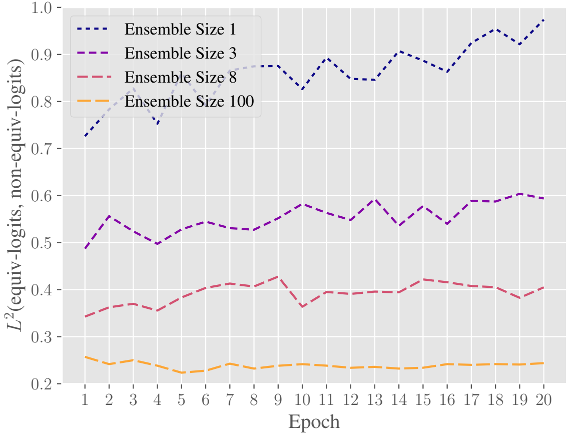

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Do you want to know more?

arXiv:2406.06504