

The Neural Tangent Kernel

Equivariance, Data Augmentation and Corrections from
Feynman Diagrams

Philipp Misof

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August 28, 2025



UNIVERSITY OF
GOTHENBURG



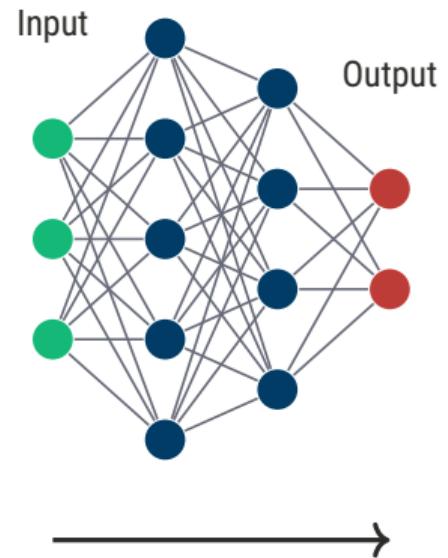
- 1 The Neural Tangent Kernel
- 2 Equivariance and Data Augmentation
- 3 Beyond the strict limit with Feynman diagrams
- 4 Conclusion and Outlook

Feedforward Neural Network (NN)

alias *Multi-layer Perceptron* (MLP)

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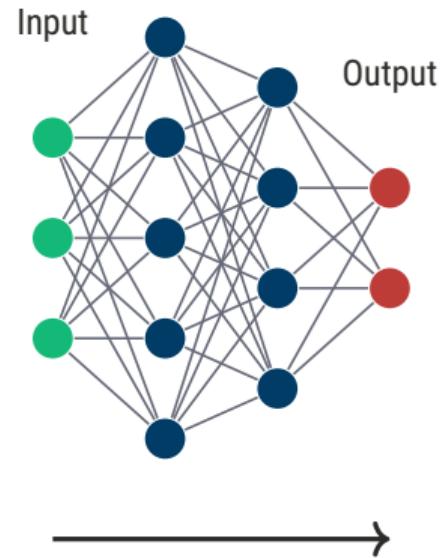
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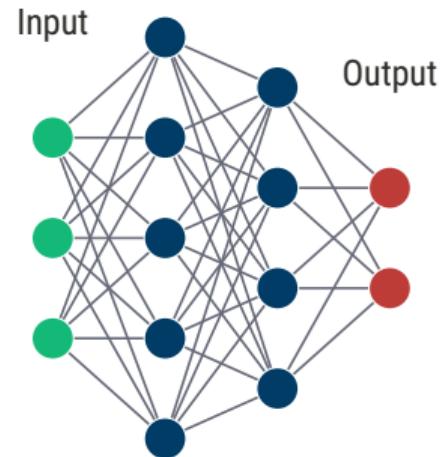
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- Recursively defined via **layers** $\mathcal{N}^{(\ell)}$

Activation function

$$\mathcal{N}^{(\ell)}(x) = \sigma \left(\frac{1}{\sqrt{n_{\ell-1}}} W^{(\ell)} \mathcal{N}^{(\ell-1)}(x) + b^{(\ell)} \right),$$

↑
weights ↑
 biases

for $\ell < L$, $\mathcal{N}^{(L)}(x) = W^{(L)} \mathcal{N}^{(L-1)}(x)$.



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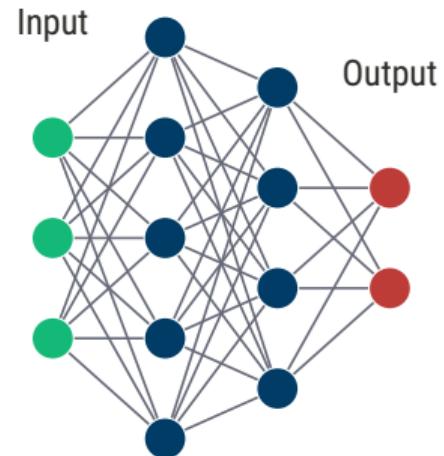
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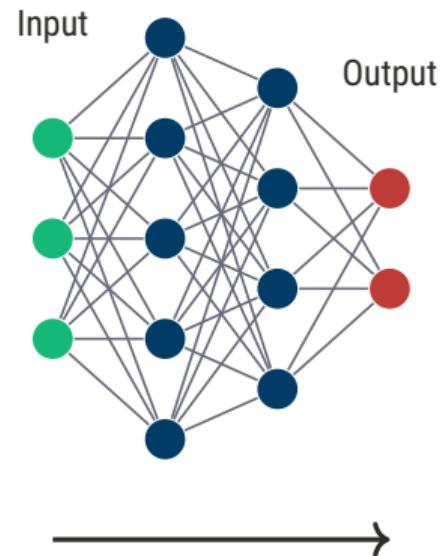
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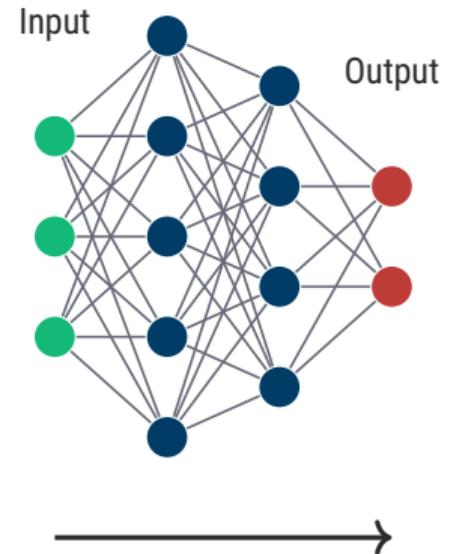
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parameters sampled **iid**

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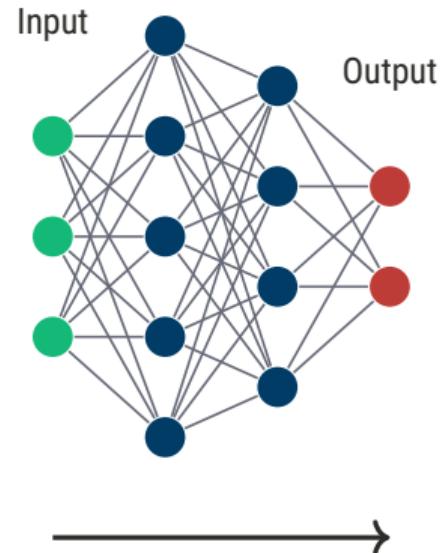
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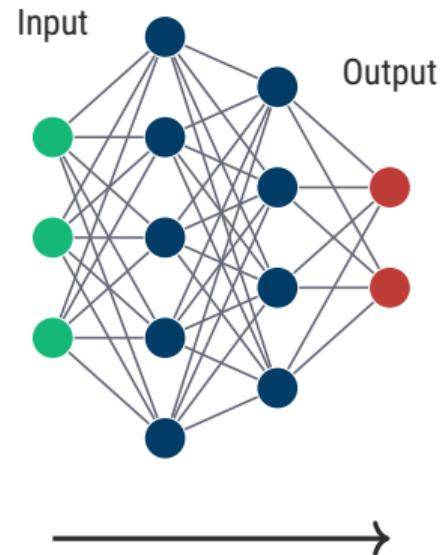
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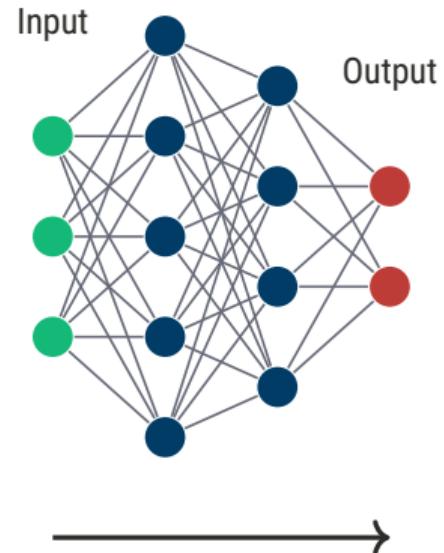
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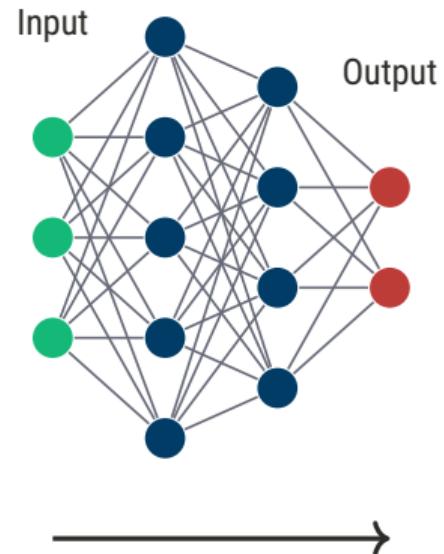
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- Almost always **Gradient Descent** (GD) based.



Training Dynamics

Assume **Gradient Flow**

$$\frac{d\theta_\mu(t)}{dt} = -\eta \frac{d\mathcal{L}}{d\theta_\mu}$$

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Intuition: Similarity measure of gradients at different inputs

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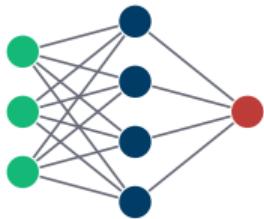
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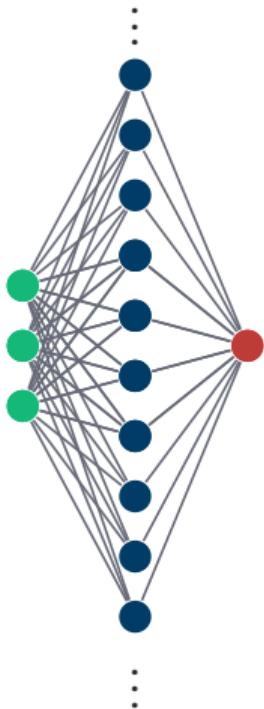
Intuition: Similarity measure of gradients at different inputs

Θ_t is **time-dependent** and **stochastic**.

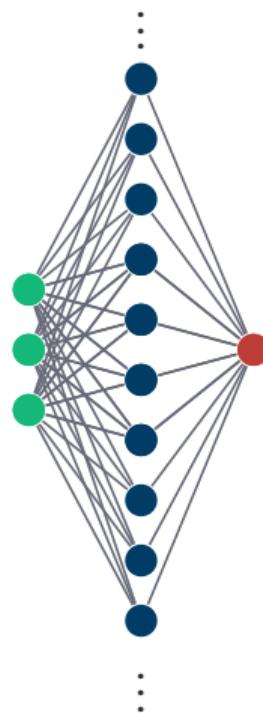
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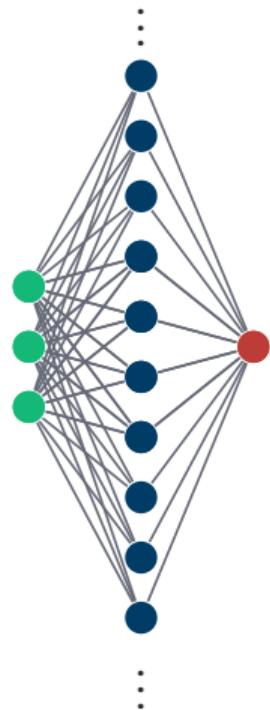
- Obtain a centered **Gaussian process**
- With covariance (**NNGP**) kernel

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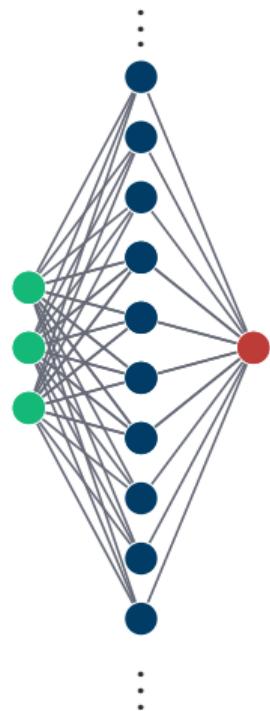


Due to the *Law of Large Numbers*.

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Similarly

Due to the *Law of Large Numbers*.

Freezing of the NTK

(Jacot, Gabriel, and Hongler 2018)

$$\Theta_t(x, x') \rightarrow \mathbb{E} [\Theta_t(x, x')] = \Theta(x, x') \mathbb{I}_{n_L}$$

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is now deterministic and time-independent

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Analytic solution

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

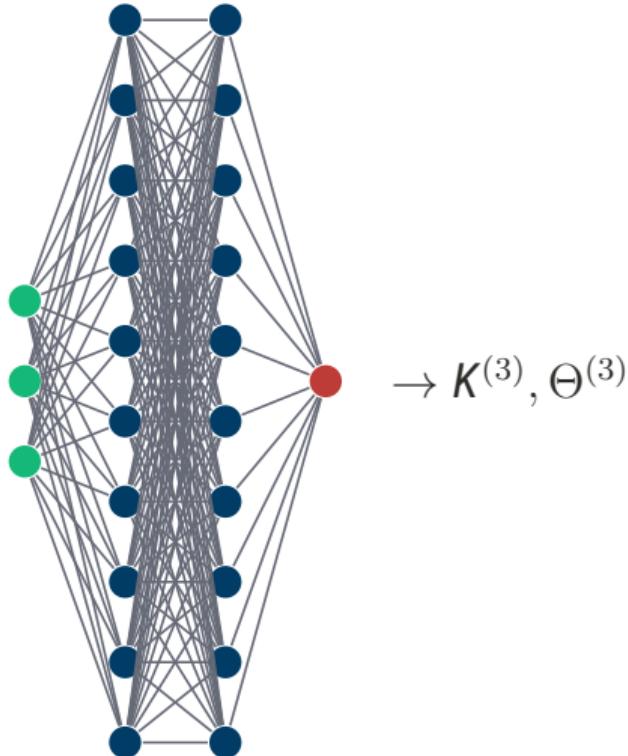
↑
Train inputs

↑
Train labels

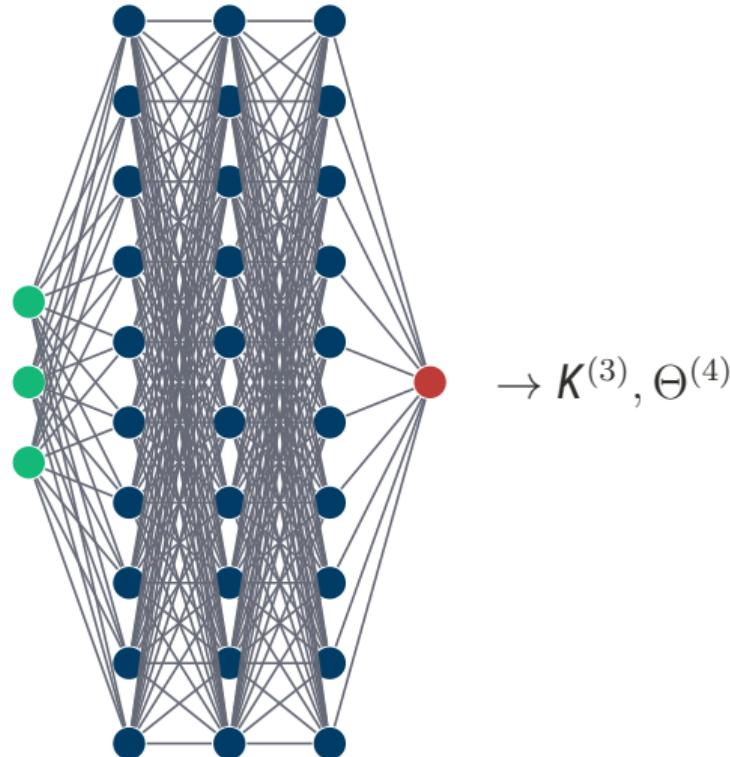
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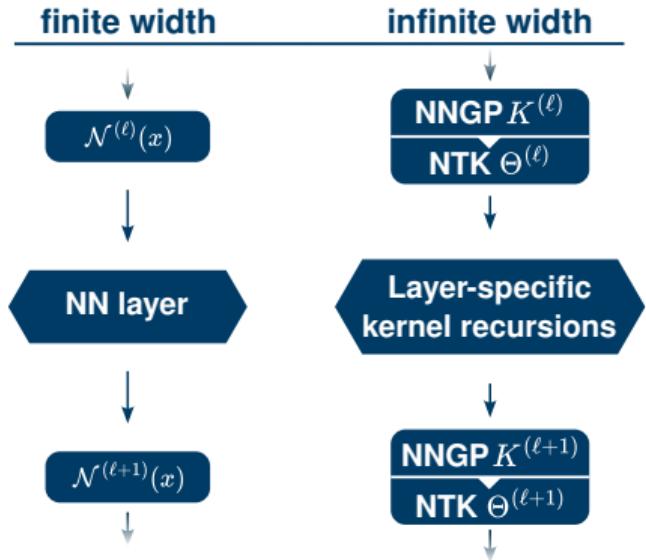
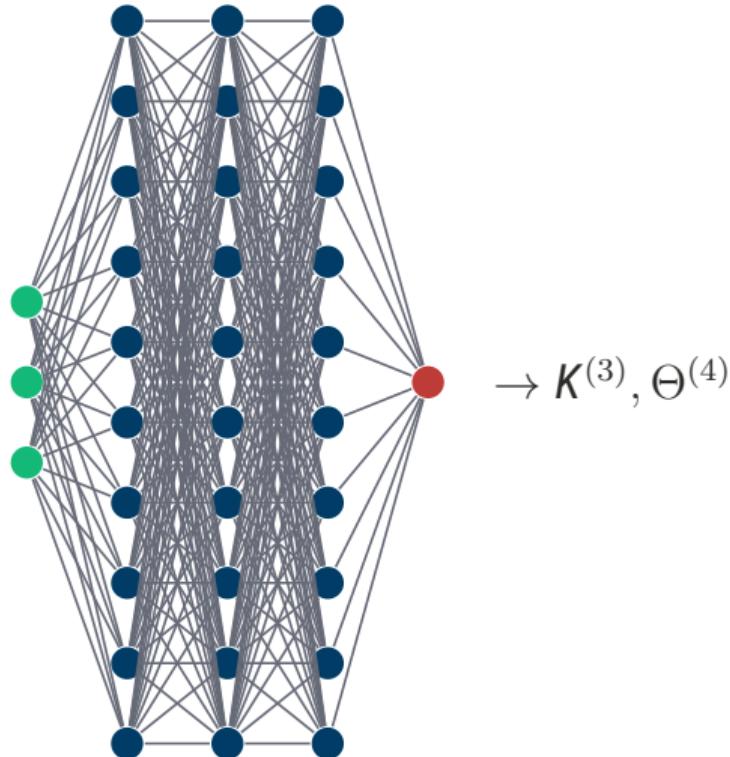


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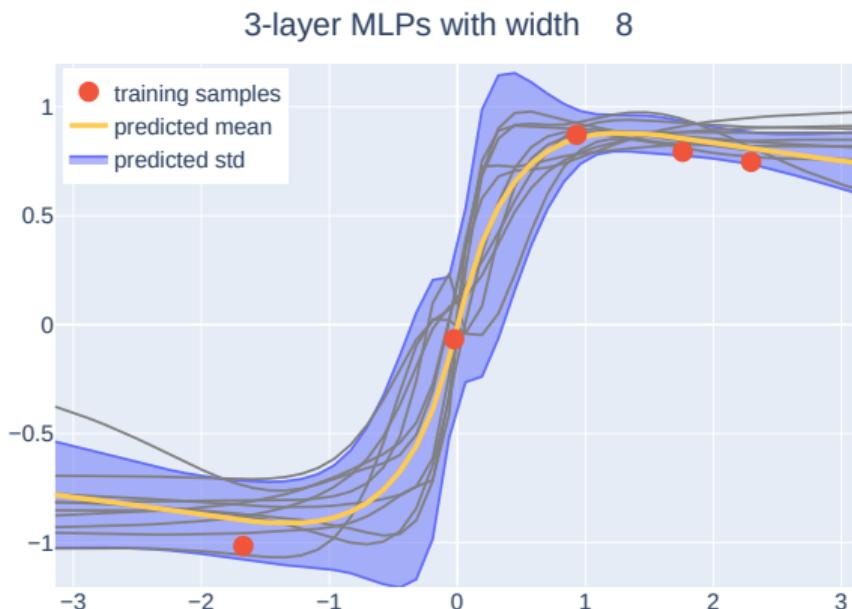
$$\rightarrow K^{(3)}, \Theta^{(4)}$$

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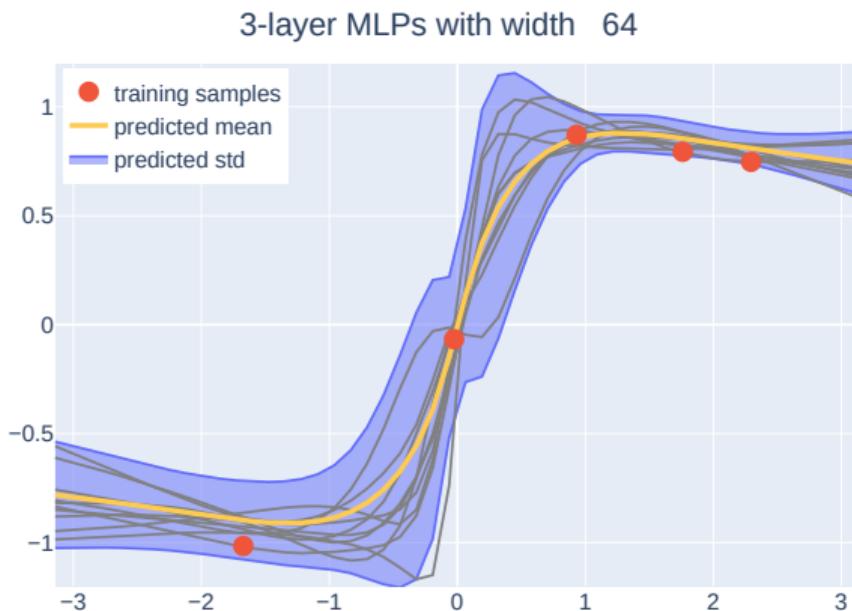


Toy example: Learning $\sin(x)$

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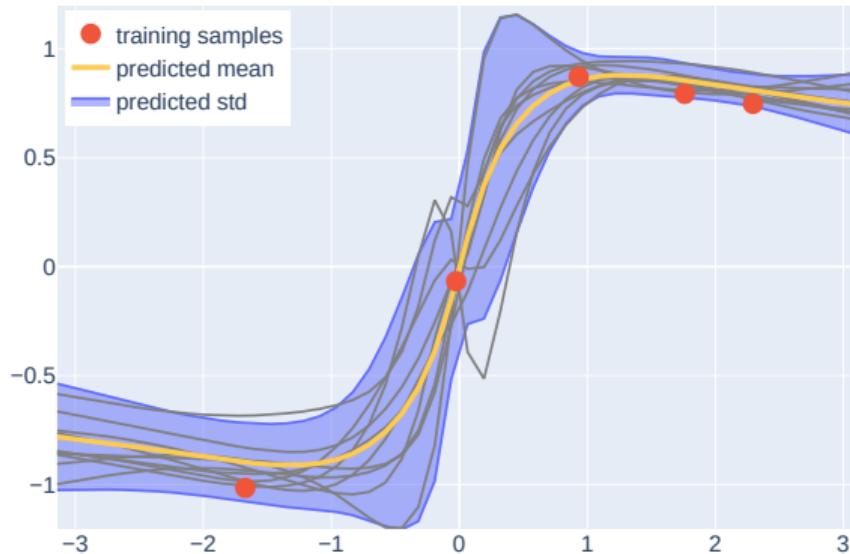


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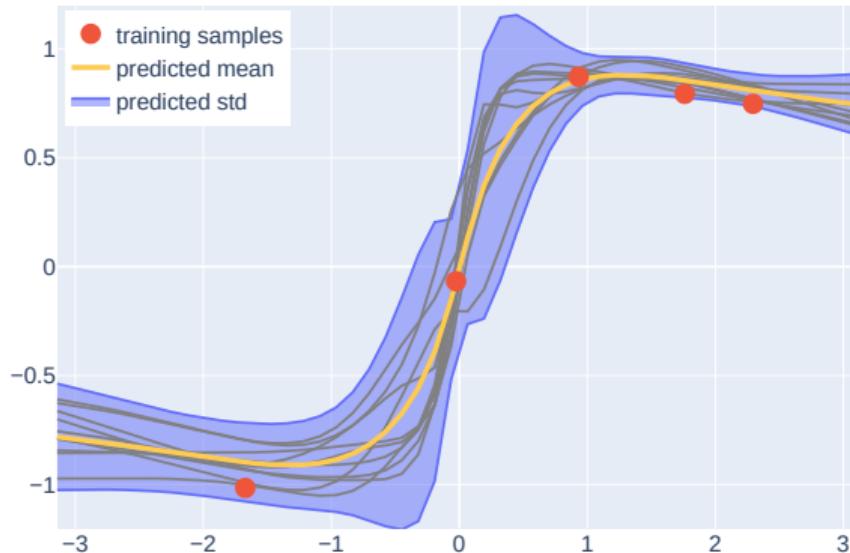
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3-layer MLPs with width 256



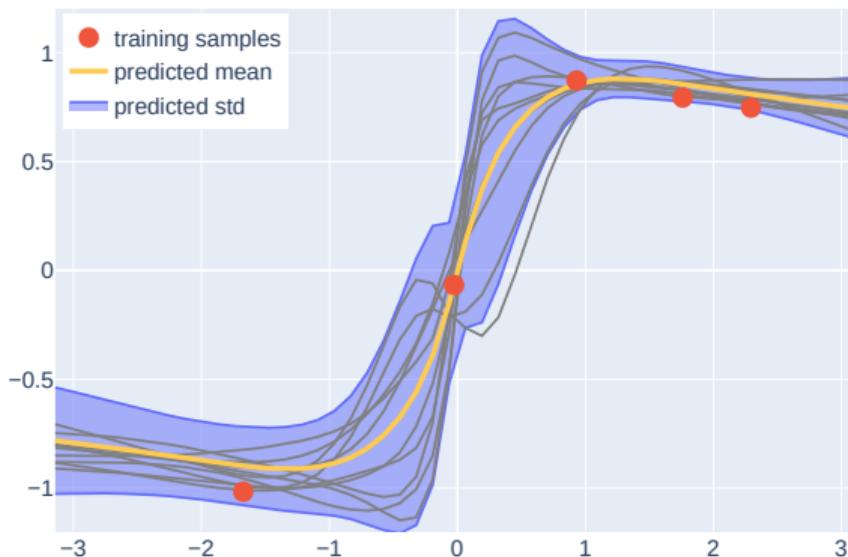
Toy example: Learning $\sin(x)$

3-layer MLPs with width 1024



Toy example: Learning $\sin(x)$

3-layer MLPs with width 4096



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Philipp Misof¹ Pan Kessel² Jan E. Gerken¹

Abstract

Little is known about the training dynamics of equivariant neural networks, in particular how it compares to data augmented training of their non-equivariant counterparts. Recently, neural tangent kernels (NTKs) have emerged as a powerful tool to analytically study the training dynamics of wide neural networks. In this work, we take an important step towards a theoretical understanding of training dynamics of equivariant models by deriving neural tangent kernels for a broad class of equivariant architectures based on group convolutions. As a demonstration of the capabilities of our framework, we show an interesting relationship between data augmentation and group convolutional networks. Specifically, we prove that they share the same expected pre-

Schut et al., 2021; Unke et al., 2021). Other application areas include particle physics (Bogatskiy et al., 2020), cosmology (Perraudin et al., 2019) and even fairness in large language models (Basu et al., 2023).

Recently, there has been a number of works which avoid equivariant architectures but rely on data augmentation to approximately learn equivariance, most notably AlphaFold3 (Abramson et al., 2024). This has the potential advantage that non-equivariant architectures may offer better training dynamics, for example favorable scaling capabilities. There has been a vigorous debate on this subject with some empirical works claiming superiority of equivariant architectures (Gerken et al., 2022; Brehmer et al., 2024) while others suggest the opposite (Wang et al., 2024; Abramson et al., 2024). One challenging aspect to conclusively settle the matter is that there is no good theoretical understanding of how the equivariant and the purely augmentation-based

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**Presented at the ICML
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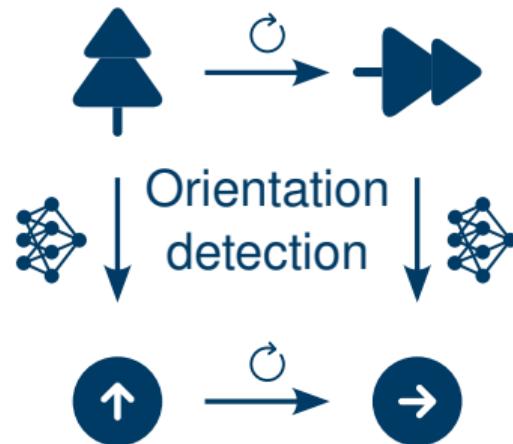


Symmetries in Machine Learning

Want to enforce symmetry w.r.t a group G acting on the input signal $f : X \rightarrow \mathbb{R}^d$

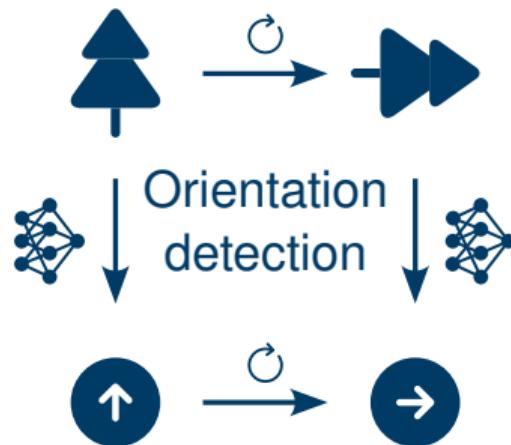
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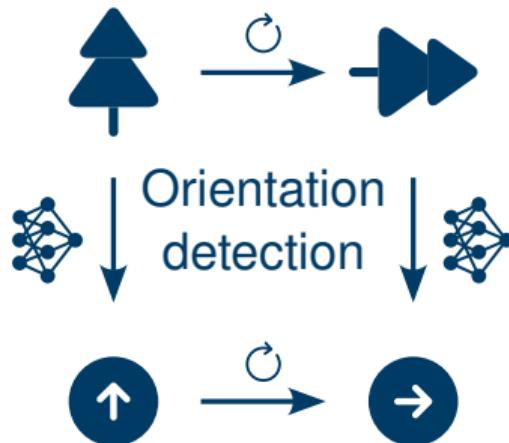
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$$\begin{array}{ccc} f & \xrightarrow{\rho_{\text{in}}(g)} & \rho_{\text{in}}(g)(f) \\ \downarrow \mathcal{N} & & \downarrow \mathcal{N} \\ \mathcal{N}(f) & \xrightarrow{\rho_{\text{out}}(g)} & \rho_{\text{out}}(g)[\mathcal{N}(f)] \\ & & \forall g \in G \end{array}$$

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This is called **equivariance**

Convolutional Neural Networks (CNNs)

Single Channel Padded Image

0	0	0	0	0	0	0	0	0	0
0	5	0	8	7	8	1	0	0	0
0	1	9	5	0	7	7	0	0	0
0	6	0	2	4	6	6	0	0	0
0	9	7	6	6	8	4	0	0	0
0	8	3	8	5	1	3	0	0	0
0	7	2	7	0	1	0	0	0	0
0	0	0	0	0	0	0	0	0	0

*

Filter

0	1	0
1	-4	1
0	1	0

II

Result

-19	22	-20	-12	-17	11	
16	-30	-1	23	-7	-14	
-14	24	7	-2	1	-7	
-15	-10	-1	-1	-15	1	
-13	13	-11	-5	13	-7	
-18	9	-18	13	-3	4	

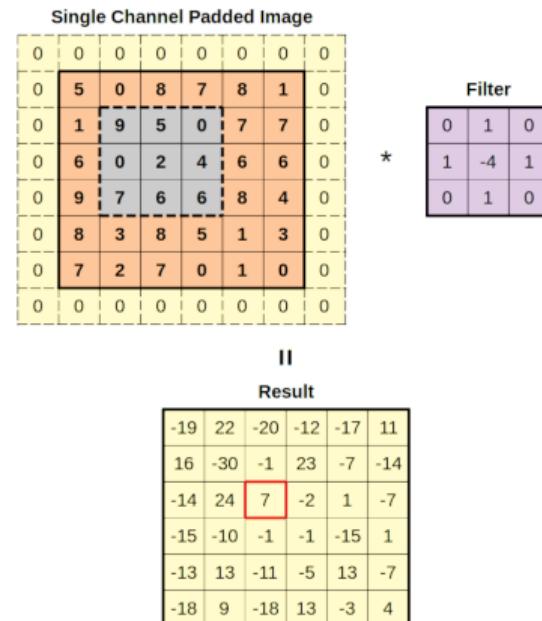
(https://en.wikipedia.org/wiki/Convolutional_neural_network)

Convolutional Neural Networks (CNNs)

Classic convolution layer

$$[\mathcal{N}^{(1)}(f)](y) = \frac{1}{\sqrt{|S_\kappa|}} \int_{\mathbb{R}^d} dx \kappa(x - y) f(x)$$

filter
filter support ↗ ↖ domain of input signal



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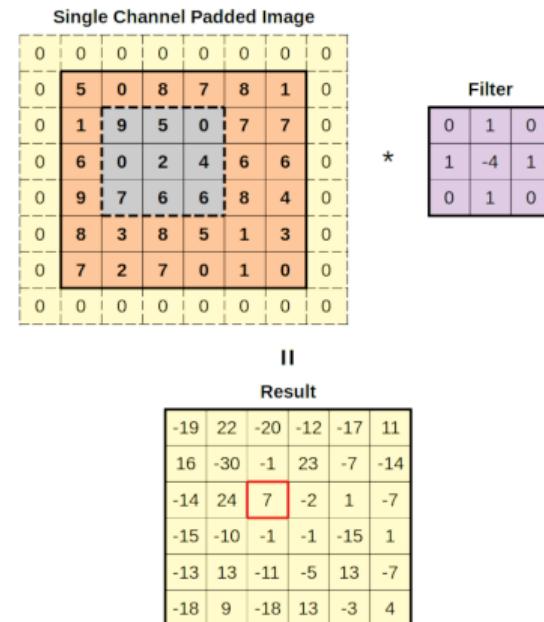
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Equivariant w.r.t. translation group $G = \mathbb{R}^d$



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Generalization of a CNN to other groups G acting on a homogeneous space X .

$$[\mathcal{N}^{(1)}(f)](\textcolor{red}{y}) = \frac{1}{\sqrt{|S_\kappa|}} \int_{\mathbb{R}^d} d\textcolor{red}{x} \, \kappa(\textcolor{red}{x} - \textcolor{red}{y}) f(\textcolor{red}{x})$$

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$$[\mathcal{N}^{(1)}(f)](\textcolor{red}{g}) = \frac{1}{\sqrt{|S_\kappa|}} \int_X d\textcolor{red}{h} \, \kappa(\textcolor{red}{g}^{-1}\textcolor{red}{h}) [(\textcolor{red}{f})](\textcolor{red}{h})$$

group element 

Remark: Subtle difference between the first (*lifting*) layer and subsequent layers

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Equivariant w.r.t. the regular representation

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group element 

Remark: Subtle difference between the first (*lifting*) layer and subsequent layers

Equivariant w.r.t. the regular representation

Group pooling

$$\mathcal{N}^{(\ell+1)}(f) = \frac{1}{\text{vol}(G)} \int_G dg [\mathcal{N}^{(\ell)}(f)](g)$$

The Equivariant NTK

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$$\mathbb{E} \left[\sum_{\mu} \frac{\partial [\mathcal{N}^{(\ell)}(f)](g)}{\partial \theta_{\mu}} \left(\frac{\partial [\mathcal{N}^{(\ell)}(f')](g')}{\partial \theta_{\mu}} \right)^T \right]$$

The Equivariant NTK

$$\Theta_{g,g'}^{(\ell)}(f, f') = \mathbb{E} \left[\sum_{\mu} \frac{\partial[\mathcal{N}^{(\ell)}(f)](g)}{\partial \theta_{\mu}} \left(\frac{\partial[\mathcal{N}^{(\ell)}(f')](g')}{\partial \theta_{\mu}} \right)^T \right]$$

Evaluation point in group space

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∞ -width limit: # channels $\rightarrow \infty$

Kernel Recursions of the Group Convolutional Layer

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$$K_{g,g'}^{(\ell+1)}(f, f') = \frac{1}{\text{vol}(S_\kappa)} \int_{S_\kappa} dh K_{gh, g'h}^{(\ell)}(f, f')$$

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How to implement this depends on the group G and the space X .

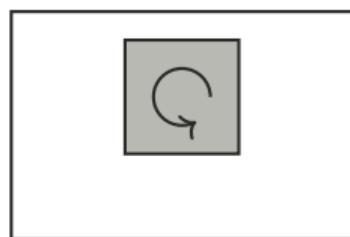
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We cover

Roto-translations in the plane

$$G = \mathbb{C}^4 \ltimes \mathbb{Z}^2$$

$$X = \mathbb{Z}^2$$



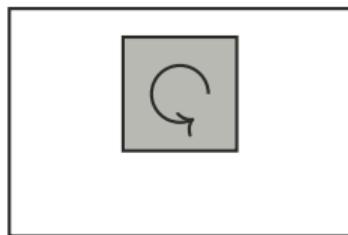
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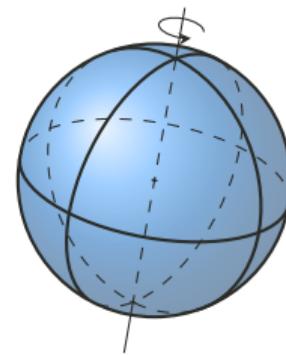
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Rotations on $\text{SO}(3)$

$$G = \text{SO}(3)$$

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SO(3) Implementation

$$K_{R,R'}^{(\ell+1)}(f, f') = \frac{1}{8\pi^2} \int_{\text{SO}(3)} dS K_{RS,R'S}^{(\ell)}(f, f')$$

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(Wigner transform on SO(3))

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- D_{mn}^I are the **Wigner D-matrices**, irreps of SO(3)
- $I \in \mathbb{N}_0, m, n \in \{-I, \dots, I\}$
- for the first layer $\ell = 1$, **spherical harmonics** Y_I^m are used instead of Wigner D-matrices

Fourier Recursion

Fourier Recursion

Kernel recursion in Fourier space

$$[\widehat{K^{(\ell+1)}(f, f')}]_{mn, m'n'}^{l,l'} = \frac{1}{2l+1} \delta_{ll'} \delta_{n, -n'} \sum_{p=-l}^l (-1)^{n-p} [\widehat{K^\ell(f, f')}]_{mp, m'(-p)}^{l,l'}$$

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Straightforward to implement . . . right?

Goal: Integrate it in the neural-tangents library (written in JAX).

The screenshot shows the GitHub repository page for `neural-tangents`. The repository is owned by `google`. The main tab is selected, showing 62 issues, 7 pull requests, and 234 forks. The repository was archived by the owner on May 6, 2025, and is now read-only. The commit history lists 650 commits from `romanngg`, starting with a fix for GitHub action versioning. Other contributors include `c17e770` and `61`. The repository has 2.4k stars and 61 watchers. The sidebar includes links for Readme, Apache-2.0 license, Code of conduct, Contributing, Security policy, Cite this repository, Activity, Custom properties, 2.4k stars, 61 watching, and 234 forks.

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Code Issues 62 Pull requests 7 Discussions Actions Projects Wiki Security Insights

neural-tangents Public archive

main 5 Branches 17 Tags

romannngg Fix github action version (missed in previous commit) c17e770 · last year 650 Commits

.github/workflows Fix github action version (missed in previous commit) last year

docs Update requirements.txt 2 years ago

examples No-op refactoring: use the modern jnp/mp aliases convention... 2 years ago

neural_tangents Avoid deprecated ad.config & ad.source_info util last year

notebooks Updated jax.config import 2 years ago

presentation Add paper 3 years ago

tests Remove tests for zeros_like and add_any primitives from ne... last year

.readthedocs.yml Update readthedocs python version 2 years ago

CITATION Deflake tests; update citation file 3 years ago

CONTRIBUTING.md Project import generated by Copybara. 6 years ago

LICENSE Refactoring: a long awaited refactor that splits the huge sta... 3 years ago

LICENSE_SHORT Add paper 3 years ago

README.md No-op refactoring: use the modern jnp/mp aliases convention... 2 years ago

About

Fast and Easy Infinite Neural Networks in Python

iclr.cc/virtual_2020/poster_SKID9yrFP...

kernel neural-networks gradient-descent bayesian-inference gaussian-processes bayesian-networks deep-networks gradient-flow jax infinite-networks training-dynamics neural-tangents kernel-computation

Readme Apache-2.0 license Code of conduct Contributing Security policy Cite this repository Activity Custom properties 2.4k stars 61 watching 234 forks

Fortunately, Fast Fourier Transforms (FFT) on $SO(3)$ and S^2 provided by s2fft.

The screenshot shows the GitHub repository page for `s2fft`. The repository is owned by `astro-informatics` and has 45 issues, 3 pull requests, 10 forks, and 201 stars. The repository is public and has 8 branches and 10 tags. The code tab is selected. The repository's description is "S2FFT: Differentiable and accelerated spherical transforms". The repository has 1,007 commits. The commit history includes:

- Bump pypa/cibuildwheel from 3.1.3 to 3.1.4 (#323) - b239a11 - 8 hours ago
- Update python_requires and test matrix to support Python ... - last month
- Clean-up unused files (#271) - 5 months ago
- Add headers with attributions / license details - 11 months ago
- Update Torch notebook cell outputs (#301) - 4 months ago
- Update custom_ops.py (#315) - 2 weeks ago
- Factor out torch.autograd checks into separate tests and skip ... - 3 months ago
- docs: add mdavezac as a contributor for infra (#297) - 4 months ago
- clang format - last year
- .coveragerc: Exclude CUDA functions from test coverage - 10 months ago
- .gitignore: merge with main - 11 months ago
- .pre-commit-config.yaml: Add pre-commit config - 10 months ago
- Update CITATION.cff - 6 months ago

The repository has 201 stars, 10 watching, 13 forks, and a latest release at v1.3.0.

Fortunately, Fast Fourier Transforms (FFT) on $\text{SO}(3)$ and S^2 provided by s2fft.

The screenshot shows the GitHub repository page for `astro-informatics / s2fft`. The main content is a "Contributors" section featuring 13 contributors with their GitHub profiles and an emoji key indicating their roles. Below this is a timeline of recent commits and a releases section for version 1.3.0.

Contributors:

- Matt Price
- Jason McEwen
- Matt Graham
- srmig
- Devaraj Gopinathan
- François Larusse
- Ikko Etooclear Ashimine
- Kevin Mulder
- Philipp Misof
- Elis Roberts
- Wassim KABALAN
- Mayeul d'Avezac

Recent Activity:

- merge with main (11 months ago)
- Add pre-commit config (10 months ago)
- Update CITATION.cff (#270) (6 months ago)

Releases:

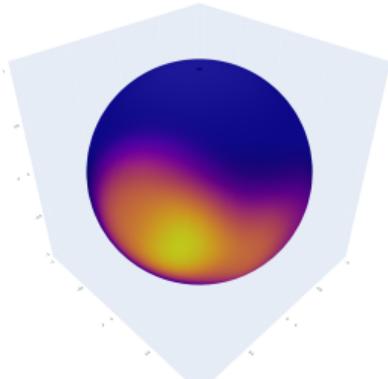
- v1.3.0 (Latest)

Testing the $\text{SO}(3)$ NTK on molecular data (QM9)

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

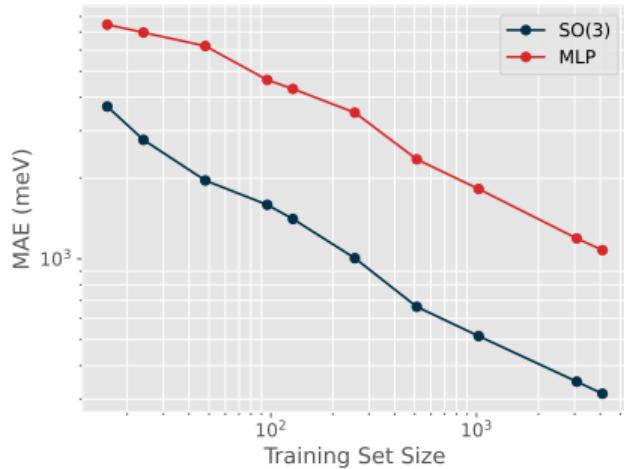
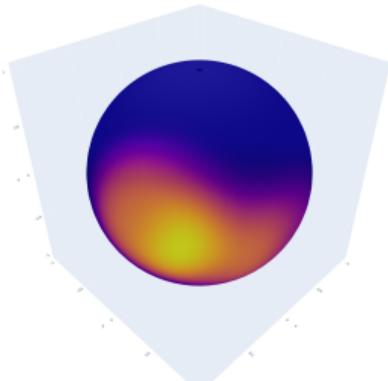
$$f_{i,z,p}(x) = \sum_{j:z_j=z} \frac{z_i z}{\|r_{ij}\|^p} e^{-\frac{1}{\beta} \left(\frac{r_{ij}}{\|r_{ij}\|} \cdot x - 1 \right)^2}$$



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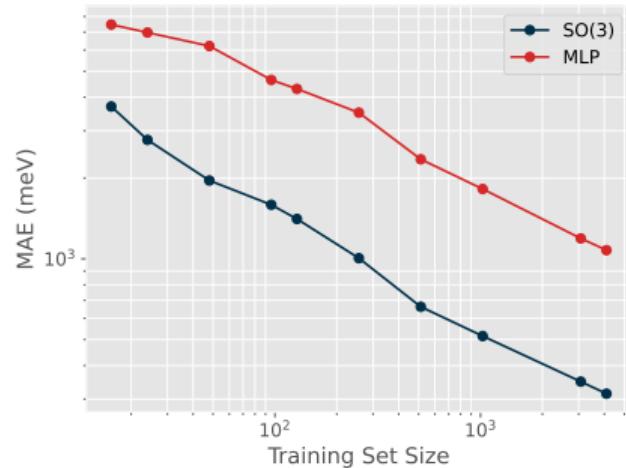
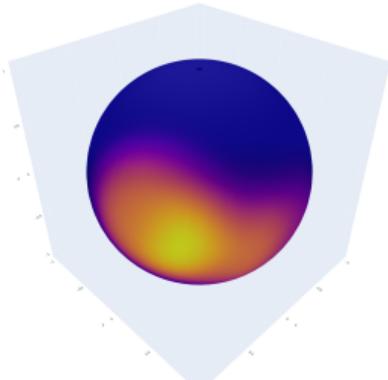
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→ Performance boost due to 3d-rotation invariance extends to the ∞ -width limit

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Can we **compare the two approaches** theoretically?

NTK under data augmentation

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- Full data augmentation

$$\mathcal{D}^{\text{aug}} = \bigcup_{i=1}^{n_{\text{train}}} \bigcup_{g \in \mathcal{G}} \{(\rho_{\text{reg}}(g)f_i, \tilde{\rho}_{\text{reg}}(g)y_i)\},$$

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- μ_t^{aug} evolves like a non-augmented NN mean μ_t with NTK

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

Data Augmentation \leftrightarrow Group Convolutional (GC) NNs

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For a given MLP, we can **construct a GCNN** s.t.

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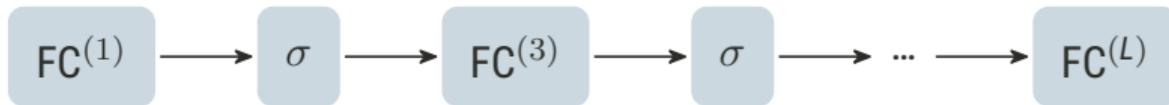
At ∞ -width and quadratic \mathcal{L} :



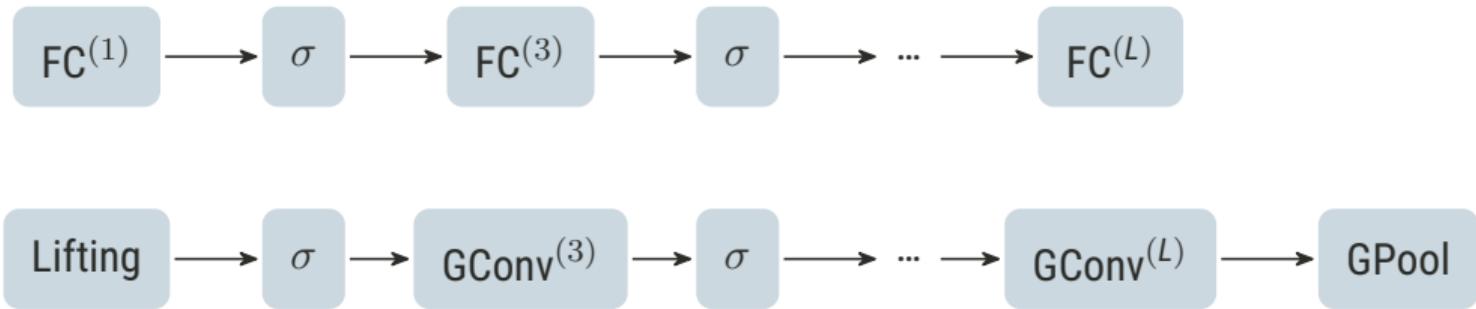
Expectation of a data augmented MLP equals the **expectation** of an GCNN **at all training times t** .

Architecture correspondence

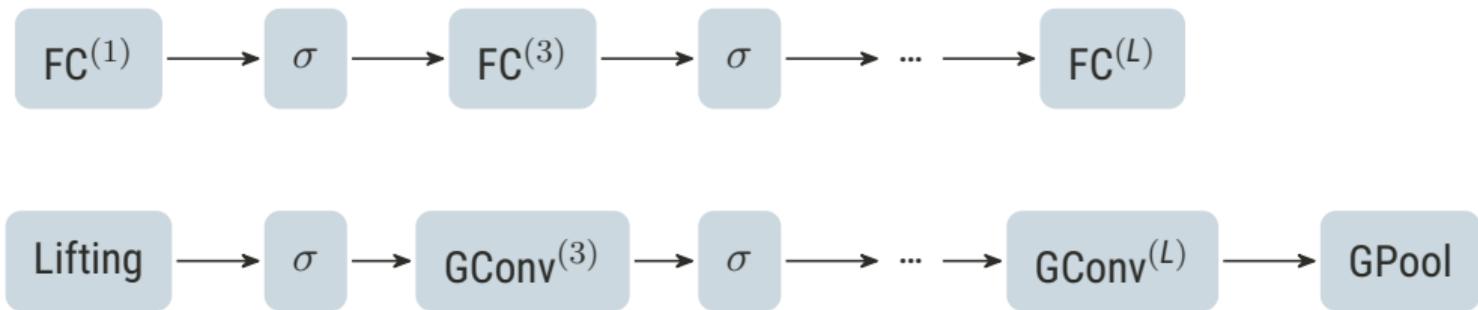
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Architecture correspondence



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

Data Augmentation vs. Group Convolutions at finite width

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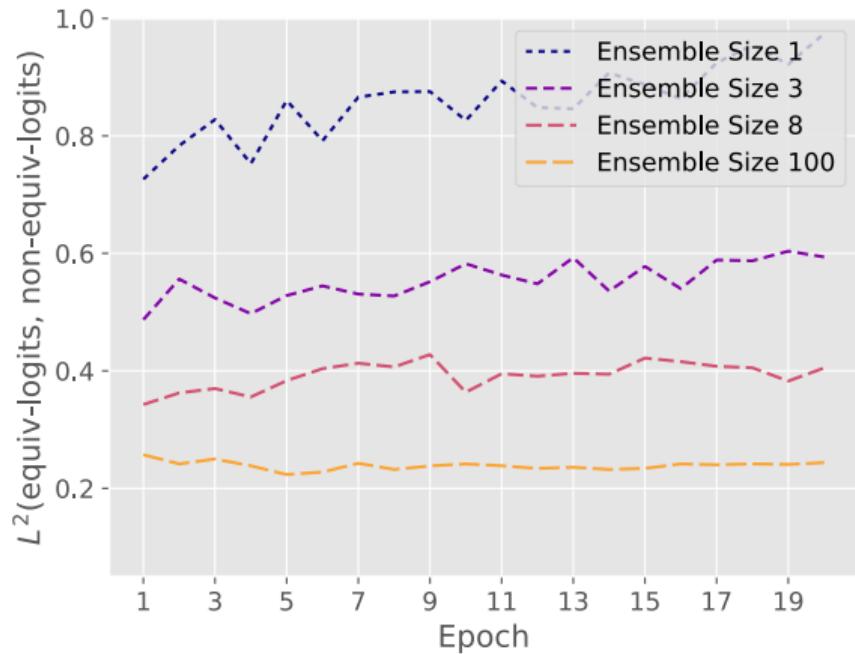
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GCNN on **MNIST**

Data Augmentation vs. Group Convolutions at finite width

- Data augmented CNN vs $C_4 \times \mathbb{R}^2$
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- 1 The Neural Tangent Kernel
- 2 Equivariance and Data Augmentation
- 3 Beyond the strict limit with Feynman diagrams
- 4 Conclusion and Outlook

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IOP Publishing *Mach. Learn.: Sci. Technol.* 2 (2021) 035002 <https://doi.org/10.1088/2632-2153/abeca3>

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James Halverson , **Anindita Maiti***  and **Keegan Stoner** 

Department of Physics, Northeastern University, Boston, MA 02115, United States of America
* Author to whom any correspondence should be addressed.

E-mail: maiti.a@northeastern.edu

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Idea: Derive finite-width corrections with techniques from quantum field theory (QFT)

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The Setup

We now focus on **preactivations**

$$z_i^{(\ell)}(x) = \frac{1}{\sqrt{n_{\ell-1}}} \sum_{j=1}^{n_{\ell-1}} W_{ij}^{(\ell)} \underbrace{\sigma(z_j^{(\ell-1)}(x))}_{\mathcal{N}^{(\ell-1)} \text{ before}} + b_i^{(\ell)}$$

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Decompose it **layer by layer**

Notation: $z_{i;\alpha}^{(\ell)} = z_i^{(\ell)}(x_\alpha)$

$$p(z^{(\ell+1)} | \mathcal{D}) = \int \prod_{i,\alpha} dz_{i;\alpha}^{(\ell)} \underbrace{p(z^{(\ell+1)} | z^{(\ell)})}_{\text{Normal dist.}} p(z^{(\ell)} | \mathcal{D})$$

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We know that $p(z^{(\ell)}|\mathcal{D})$ **becomes a Normal distribution** as $n \rightarrow \infty$.

$$p(z^{(\ell+1)}|\mathcal{D}) = \int \prod_{i,\alpha} dz_{i;\alpha}^{(\ell)} p(z^{(\ell+1)}|z^{(\ell)}) \textcolor{red}{p(z^{(\ell)}|\mathcal{D})}$$

We know that $p(z^{(\ell)}|\mathcal{D})$ **becomes a Normal distribution** as $n \rightarrow \infty$.

Instead of a Normal distribution with probability density function

$$p(z) = \frac{1}{Z} \exp\left(-\frac{1}{2} z^T K^{-1} z\right) = e^{-S[z]}$$

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where $V^{(\alpha_1 \alpha_2)(\alpha_3 \alpha_4)} = \mathbb{E}^c[z_{\alpha_1}, z_{\alpha_2}, z_{\alpha_3}, z_{\alpha_4}]$ is the **4th cumulant**.

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$$K^{(\ell)}, V_4^{(\ell)}, A^{(\ell)}, B^{(\ell)}, D^{(\ell)}, F^{(\ell)}$$

$$\longrightarrow K^{(\ell+1)}, \Theta^{(\ell)}, V_4^{(\ell+1)}, A^{(\ell+1)}, B^{(\ell+1)}, D^{(\ell+1)}, F^{(\ell+1)} + \mathcal{O}\left(\frac{1}{n^2}\right)$$

Recursions

- have been used to find optimal initialization hyperparameters (**Criticality**)

Recursions

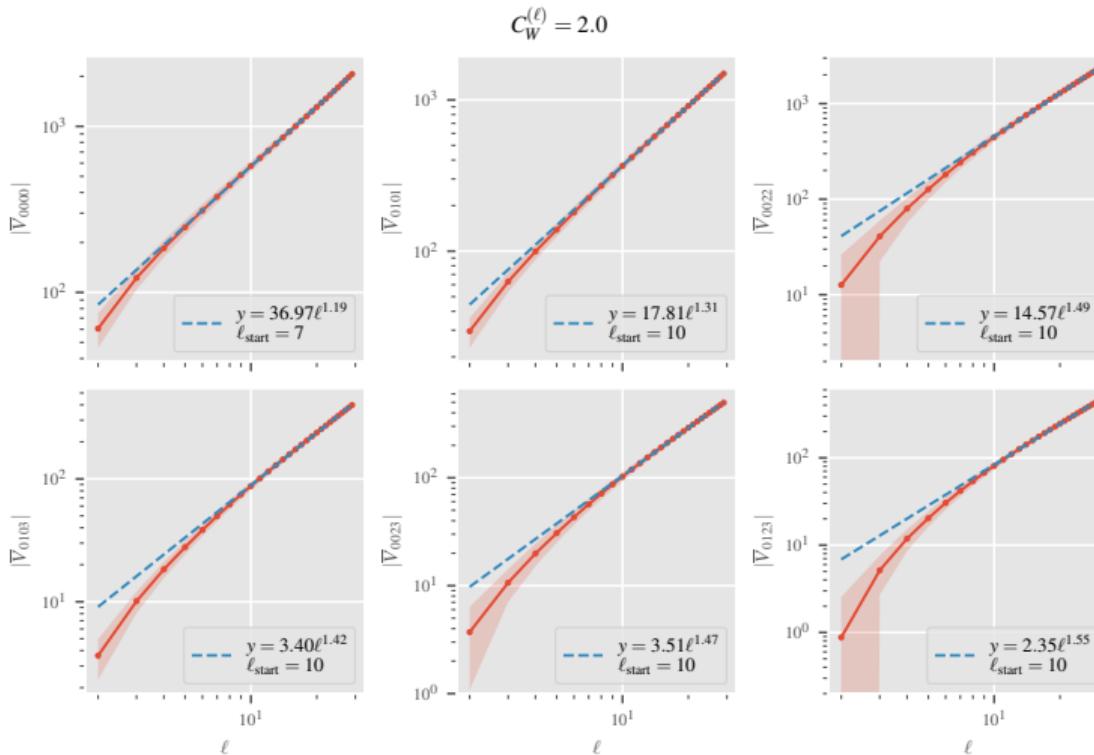
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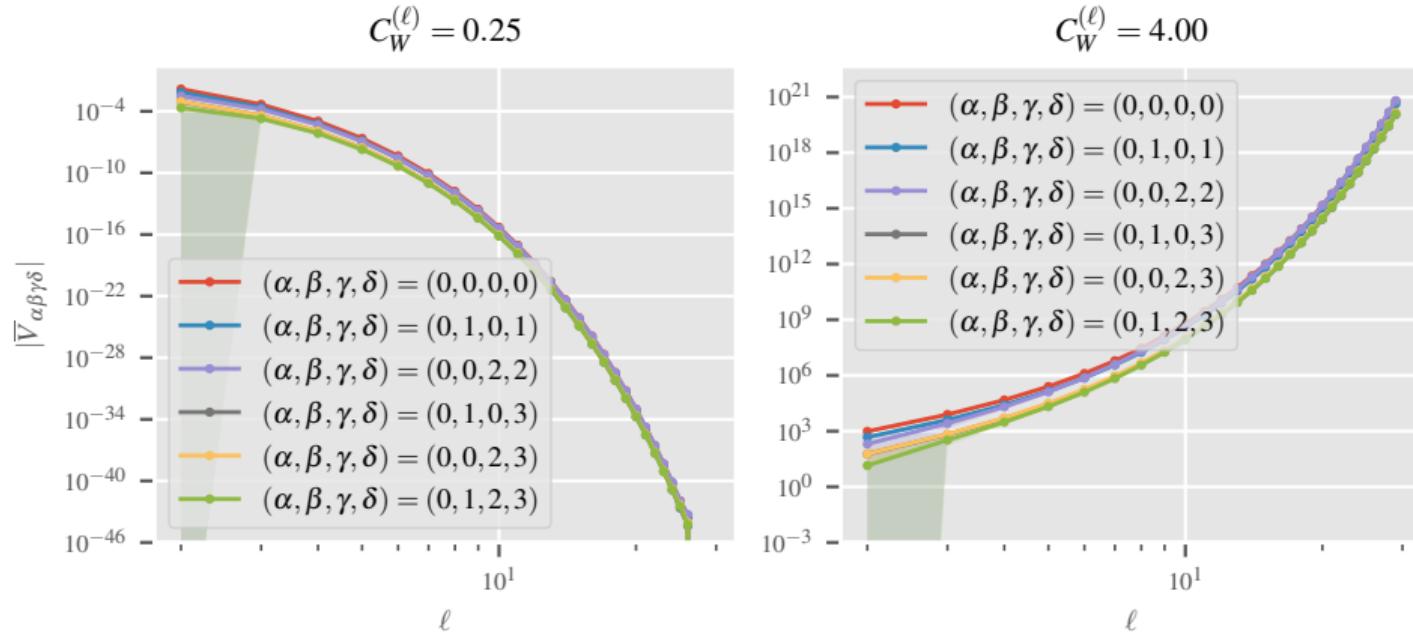
Empirical V_4 evolution at criticality

for a ReLU network



for a ReLU network

Empirical V_4 evolution away from criticality



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This is done with **Feynman diagrams**

- **Diagrammatic representation** of algebraic expressions
- Careful rules specify what diagrams are allowed
- Each diagram corresponds to a term at a certain order

Finite-Width Neural Tangent Kernels from Feynman Diagrams

Max Guillen^{*a}

Philipp Misof^{*a}

Jan E. Gerken^a

Abstract

Neural tangent kernels (NTKs) are a powerful tool for analyzing deep, non-linear neural networks. In the infinite-width limit, NTKs can easily be computed for most common architectures, yielding full analytic control over the training dynamics. However, at infinite width, important properties of training such as NTK evolution or feature learning are absent. Nevertheless, finite width effects can be included by computing corrections to the Gaussian statistics at infinite width. We introduce Feynman diagrams for computing finite-width corrections to NTK statistics. These dramatically simplify the

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Example: F recursion

$$\text{Diagram with 4 external lines (1, 2, 3, 4) and 1 internal loop} = \sum_j \text{Diagram with 4 external lines (1, 2, 3, 4), 1 internal line labeled } \sigma_j \sigma'_j, \text{ and 1 loop labeled } \sigma_j \sigma'_j + \sum_{j_1, j_2} \text{Diagram with 4 external lines (1, 2, 3, 4), 2 internal lines labeled } \sigma_{j_1} \sigma'_{j_1}, \sigma_{j_2} \sigma'_{j_2}, \text{ and 2 loops labeled } z_{j_1}, z_{j_2} \text{ with a factor } \frac{1}{n_{\ell-1}} F_4^{(\ell)}$$

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Example: F recursion

$$\text{Diagram with 4 external nodes (1, 2, 3, 4) connected to a central gray circle.} = \sum_j \text{Diagram with 4 external nodes (1, 2, 3, 4) connected to a sequence of nodes: a blue dashed circle, a white circle, and a blue dashed circle. The first and last nodes have labels } \sigma_j \sigma'_j \text{ above them.} + \sum_{j_1, j_2} \text{Diagram with 4 external nodes (1, 2, 3, 4) connected to a sequence of nodes: a blue dashed circle, a white circle, a blue dashed circle, and a white circle. The first node has label } \sigma_{j_1} \sigma'_{j_1} \text{ above it, and the second blue dashed circle has label } \frac{1}{n_{\ell-1}} F_4^{(\ell)} \text{ below it. The third white circle has labels } z_{j_1} \text{ and } z_{j_2} \text{ above it.}$$

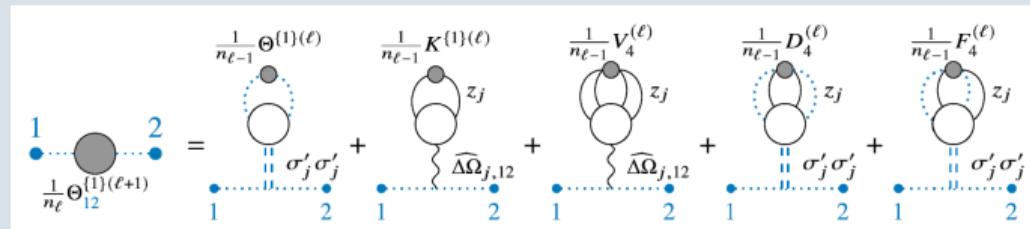
Generalization to higher orders follows the same principles.

Recursions from Feynman diagrams

New Recursion: First order correction $\Theta^{(1)(\ell)}$ to the infinite width NTK $\Theta^{(0)(\ell)}$

$$\frac{1}{n_{\ell-1}} \Theta_{12}^{(1)(\ell+1)} = \frac{1}{n_{\ell-1}} \Theta^{(1)(\ell)} + \frac{1}{n_{\ell-1}} K^{(1)(\ell)} z_j + \frac{1}{n_{\ell-1}} V_4^{(\ell)} z_j + \frac{1}{n_{\ell-1}} D_4^{(\ell)} z_j + \frac{1}{n_{\ell-1}} F_4^{(\ell)} z_j$$

where $\Theta^{(1)(\ell)}$ is a grey circle with two external lines labeled 1 and 2, and $K^{(1)(\ell)}$, $V_4^{(\ell)}$, $D_4^{(\ell)}$, and $F_4^{(\ell)}$ are Feynman diagrams involving loops and vertices.



The diagram shows the decomposition of the first-order correction $\Theta_{12}^{(1)(\ell+1)}$ into five terms. The first term is the first-order correction $\Theta^{(1)(\ell)}$. The second term is $K^{(1)(\ell)} z_j$, which consists of a circle with a vertical line through it, with a loop attached to the top. The third term is $V_4^{(\ell)} z_j$, which consists of a circle with a vertical line through it, with a loop attached to the right. The fourth term is $D_4^{(\ell)} z_j$, which consists of a circle with a vertical line through it, with a loop attached to the left. The fifth term is $F_4^{(\ell)} z_j$, which consists of a circle with a vertical line through it, with a loop attached to the bottom. All terms have a factor of $\frac{1}{n_{\ell-1}}$.

Solving the V_4 recursion [WIP]

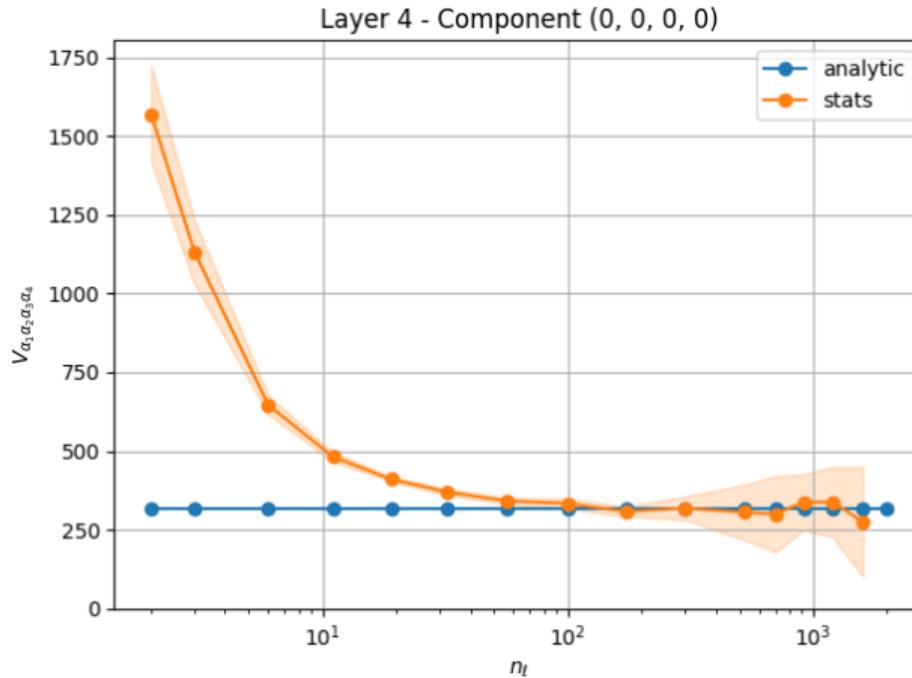
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$$\begin{aligned} \frac{1}{n_\ell} V_{(\alpha_1\alpha_2)(\alpha_3\alpha_4)}^{(\ell+1)} &= \frac{1}{n_\ell} \left(C_W^{(\ell+1)} \right)^2 [\langle \sigma_{\alpha_1} \sigma_{\alpha_2} \sigma_{\alpha_3} \sigma_{\alpha_4} \rangle_{G^{(\ell)}} - \langle \sigma_{\alpha_1} \sigma_{\alpha_2} \rangle_{G^{(\ell)}} \langle \sigma_{\alpha_3} \sigma_{\alpha_4} \rangle_{G^{(\ell)}}] \\ &\quad + \frac{1}{n_{\ell-1}} \frac{\left(C_W^{(\ell+1)} \right)^2}{4} \sum_{\beta_1, \dots, \beta_4 \in D} V_{(\ell)}^{(\beta_1\beta_2)(\beta_3\beta_4)} \langle \sigma_{\alpha_1} \sigma_{\alpha_2} (z_{\beta_1} z_{\beta_2} - g_{\beta_1\beta_2}) \rangle_{G^{(\ell)}} \\ &\quad \times \langle \sigma_{\alpha_3} \sigma_{\alpha_4} (z_{\beta_3} z_{\beta_4} - g_{\beta_3\beta_4}) \rangle_{G^{(\ell)}} + \mathcal{O}\left(\frac{1}{n^2}\right) \end{aligned}$$

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- **Numerically cheaper**, but **number of terms explodes** fast.
- **Solution:** Do IBP symbolically and create numeric functions from that.

```
GaussExpec(sig(z[a1])*sig(z[a2]))*K[b1, b3]*K[b2, b4] +GaussExpec(sig(z[a1])*sig(z[a2]))*K[b1, b4]*K[b2, b3] +GaussExpec(Derivative(sig(z[a1]), z[a1])*Derivative(sig(z[a2]), z[a2]))*K[b1, a1]*K[b2, b3]*K[b4, a2] +GaussExpec(Derivative(sig(z[a1]), z[a1])*Derivative(sig(z[a2]), z[a2]))*K[b1, a1]*K[b2, b4]*K[b3, a2] +GaussExpec(Derivative(sig(z[a1]), z[a1])*Derivative(sig(z[a2]), z[a2]))*K[b1, a2]*K[b2, b3]*K[b4, a1] +GaussExpec(Derivative(sig(z[a1]), z[a1])*Derivative(sig(z[a2]), z[a2]))*K[b1, a2]*K[b2, b4]*K[b3, a1] +GaussExpec(Derivative(sig(z[a1]), z[a1])*Derivative(sig(z[a2]), z[a2]))*K[b1, b3]*K[b2, a1]*K[b4, a2] +GaussExpec(Derivative(sig(z[a1]), z[a1])*Derivative(sig(z[a2]), z[a2]))*K[b1, b3]*K[b2, a2]*K[b4, a1] +GaussExpec(Derivative(sig(z[a1]), z[a1])*Derivative(sig(z[a2]), z[a2]))*K[b1, b4]*K[b2, a1]*K[b3, a2] +GaussExpec(Derivative(sig(z[a1]), z[a1])*Derivative(sig(z[a2]), z[a2]))*K[b1, b4]*K[b2, a2]*K[b3, a1] +GaussExpec(sig(z[a2])*Derivative(sig(z[a1]), (z[a1], 2)))*K[b1, a1]*K[b2, b3]*K[b4, a1] +GaussExpec(sig(z[a2])*Derivative(sig(z[a1]), (z[a1], 2)))*K[b1, b3]*K[b2, a1]*K[b4, a1]
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- We implement solutions to the governing recursions

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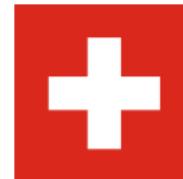
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But first

- **Internship** in Switzerland at **Genentech (Roche)** with Pan Kessel
- 10 months
- About **generative models** for protein design



Genentech

Thank you for the last two years!