Neural Tangent Kernels for Equivariant Neural Networks

Talk at the GeUmetric Deep Learning Workshop @Umeå

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

Pan Kessel

arXiv:2406.06504

Outline

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Neural Tangent Kernel (NTK) encodes training dynamics

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- Assuming **Gradient Flow** of a NN $\mathcal{N} : \mathbb{R}^{n_{\text{in}}} \to \mathbb{R}^{n_{\text{out}}}$

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

  - $\mathcal{N} \ldots$ Neural Network (NN)
  - $\Theta_t(x, x_i) \ldots$ NTK
  - $\mathcal{L} \ldots$ loss function
  - $\eta \ldots$ learning rate

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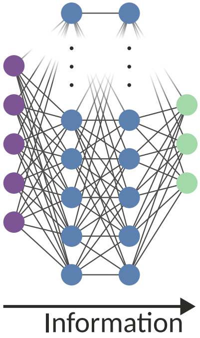

- **Infinite width limit** $\to \Theta_t(x, x_i)$ becomes
  - deterministic
  - time-independent
- Combine with **MSE loss** $\to$ linear ODE with **analytical solution**

What do we gain?

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- Analytical **study of training** independent of particular initialization
  - Influence of **hyperparameters** *(Geiger et al. 2020)*
  - Impact of **data augmentation** *(Gerken and Kessel 2024)*
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$\longrightarrow$ Let's extend this to **equivariant neural networks**!

The empirical NTK

Empirical NTK

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- **time-dependent**

NNs become Gaussian processes

- At $t = 0$, all parameters $\theta_i(0)$ are *iid*
- **law of large numbers**

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Neural Network Gaussian Process (Lee et al. 2018)

Gaussian process with zero mean and deterministic covariance

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

. . . **NNGP kernel**

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- Only dependent on distribution of parameters θ_0
- Can be computed recursively

$$K^{(\ell+1)} = f(K^{(\ell)})$$
$$\Theta^{(\ell+1)} = g(\Theta^{(\ell)}, K^{(\ell+1)}, \dot{K}^{(\ell+1)})$$

where

$$\dot{K}^{(\ell+1)}(x, x') = \mathbb{E}[\sigma'(\mathcal{N}^{(\ell)}(x))\sigma'(\mathcal{N}^{(\ell)}(x'))],$$

$\sigma \ldots$ non-linearity

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Frozen NTK *(Jacot, Gabriel, and Hongler 2018)*

$$\Theta_t(x, x') \to \Theta(x, x')$$

uniformly in t when taking the limit layer by layer

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NTK as a kernel method

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Kernel $\Phi(x, x') : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ similarity measure
Kernel regression:

$$f(x) = \alpha(\mathcal{Y})\Phi(x, \mathcal{X})$$

with $(\mathcal{X}, \mathcal{Y}) \ldots$ whole training set, $\alpha(\mathcal{X}, \mathcal{Y}) \ldots$ coefficients of the regression

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Take **infinite width infinite time limit** and **MSE** loss $\to$ Mean of Gaussian process is

$$\mu(x) = \Theta(x, \mathcal{X})\Theta(\mathcal{X}, \mathcal{X})^{-1}\mathcal{Y}$$

$\to$ NTK yields kernel method

Ingredients for Equivariant Neural Networks

Equivariance under group G

$$\mathcal{N}(\rho_{\text{reg}}(g)f) = \rho_{\text{reg}}(g)\mathcal{N}(f)\,, \qquad g \in G$$

$\rightarrow$ **group convolutional neural networks** (GCNN)

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$\rightarrow$ **group convolutional neural networks** (GCNN)

- Group convolutional layers
- Lifting layer
- elementwise non-linearity σ
- group pooling layer (to achieve **invariance**)

$\rightarrow$ Need recursive relations for the NTK for all of them

Group Convolution (GCNN)

- Data given in form of feature maps $f : X \to \mathbb{R}^{n_{\text{in}}}$
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$$[\mathcal{N}^{(1)}(f)](g) = [\kappa * f](g) = \frac{1}{\sqrt{n_{\text{in}} \text{vol}(S_\kappa)}} \int_X \mathrm{d}x \, \kappa\big(\rho(g^{-1})x\big) f(x)$$

$\kappa : X \to \mathbb{R}^{n_{\text{in}} \times n_1}$ . . . filter with support S_κ

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- consecutive **group convolutional layer**

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

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- **infinite width limit:** channels $n_1, \ldots n_{L-1} \to \infty$

Equivariant NTK

GCNN layers

At each layer ℓ

$$K^{(\ell)}_{g,g'}(f,f') = \mathbb{E}\Big[[\mathcal{N}^{(\ell)}(f)](g)\ [\mathcal{N}^{(\ell)}(f')](g')^{\mathsf{T}}\Big]$$

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Recursion for GCNN layer

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

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

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If first layer $\rightarrow$

$$K^{(0)}_{x,x'}(f,f') = f(x)f'(x')\,, \qquad \Theta^{(0)}_{x,x'}(f,f') = 0$$

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$$\Lambda^{(\ell)}(f,f') = \begin{pmatrix} K^{(\ell)}(f,f) & K^{(\ell)}(f,f') \\ K^{(\ell)}(f',f) & K^{(\ell)}(f',f') \end{pmatrix}$$

$$K^{(\ell+1)}(f,f') = \mathbb{E}_{(u,v)\sim\mathcal{N}(0,\Lambda^{(\ell)}(f,f'))}[\sigma(u)\sigma(v)]$$

$$\dot{K}^{(\ell+1)}(f,f') = \mathbb{E}_{(u,v)\sim\mathcal{N}(0,\Lambda^{(\ell)}(f,f'))}[\sigma'(u)\sigma'(v)]$$

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Group pooling layer

Making equivariant network **invariant** $\rightarrow$ **group pooling**

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$$K^{(\ell+1)}(f,f') = \frac{1}{\mathrm{vol}(G)} \int_G \mathrm{d}g \, \mathrm{d}g' \; K^{(\ell)}_{g,g'}(f,f')$$
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Symmetries of the NTK

$$K^{(\ell)}_{g,g'}(\rho_{\text{reg}}(h)f, \rho_{\text{reg}}(h')f') = K^{(\ell)}_{h^{-1}g,h'^{-1}g'}(f,f')$$

$$\Theta^{(\ell)}_{g,g'}(\rho_{\text{reg}}(h)f, \rho_{\text{reg}}(h')f') = \Theta^{(\ell)}_{h^{-1}g,h'^{-1}g'}(f,f')$$

$C_n \ltimes \mathbb{R}^2$

Discrete roto-translations in the plane

- $g = tr$, where $t \in \mathbb{R}^2$ and $r \in C_n$

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- Keep t as spatial indices, for r extend to nn_ℓ channel indices in layer $\ell \rightarrow$

$$K_{g=tr,g'=t'r'}(f,f') = [K_{rr}(f,f')](t,t')\,, \quad \Theta_{g=tr,g'=t'r'}(f,f') = [\Theta_{rr'}(f,f')](t,t')$$

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- For CNN, `neural-tangents` library provides the following highly optimized operator

$$[\mathcal{A}_{S_\kappa}(K)](t,t') = \frac{1}{S_\kappa}\int_{S_\kappa} \mathrm{d}\tilde{t}\; K(t+\tilde{t}, t'+\tilde{t})$$

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- Can this be exploited for $C_n \ltimes \mathbb{R}^2$ as well?

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$\rightarrow$ **Yes!**

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Kernel convergence

- Comparing limit kernels with mean of finite-width kernels
- $G = C_4 \ltimes \mathbb{R}^2$ and random input data
- Relative error averaged over all components of the Gram matrix
- Implemented in the `JAX`-based `neural-tangents` library[1]

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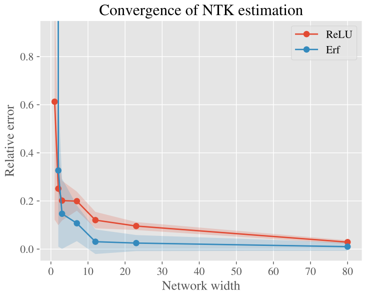

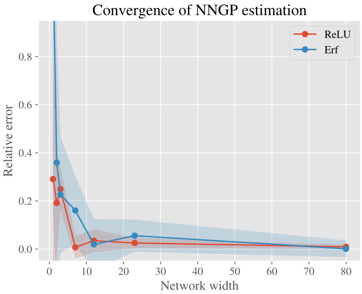

Histological image classification

The data set

NCT-CRC-HE-100K *(Kather, Halama, and Marx 2018)*

- $100\,000$ histological images of human colorectal cancer (CRC) and normal tissue
- 9 classes, 2 are cancerous
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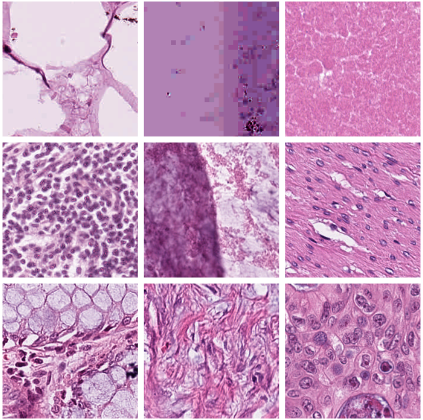
Here:

- downsampled to 32×32 pixels
- Only up to 1000 training samples used



Histological image classification

Performance for small training sets

- NTK kernel method
- Corresponds to training with MSE loss
- Comparison
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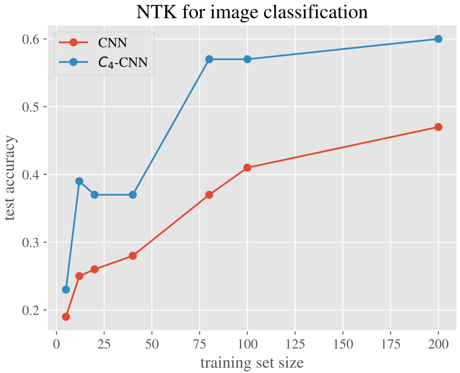

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- Trainability and generalization regimes of equivariant NNs *(Xiao, Pennington, and Schoenholz 2020)*

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- equivariant graph NNs
- Trainability and generalization regimes of equivariant NNs *(Xiao, Pennington, and Schoenholz 2020)*
- Relations to Quantum Field Theory *(Banta et al. 2023)*

Thanks for your attention!

arXiv:2406.06504