On the Inductive Bias of Neural Tangent Kernels

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Inductive Bias and Over-Parameterization

Optimization and Inductive Bias:

- Over-parameterized deep networks are very expressive
- Optimization algorithm is plays a crucial role for generalization

Lazy Training: In certain regimes (over-parameterization, particular initialization), neural networks behave like their **linearization** near initialization

$$f(x;\theta) \approx f(x;\theta_0) + \langle \theta - \theta_0, \nabla_\theta f(x;\theta_0)\rangle$$

Neural Tangent Kernels (NTK): In this regime, generalization properties are controlled by the **limiting kernel** [Jacot et al., 2018]

$$\langle \nabla_\theta f(x;\theta_0), \nabla_\theta f(x';\theta_0)\rangle \to K(x,x').$$

In particular, with squared loss and infinite width, we get the interpolating solution with minimum RKHS norm.

Contributions:

- Derivation of NTK for **convolutional networks** with generic linear patch extraction/pooling operators;
- Study of **smoothness, stability, and approximation** properties of functions with finite RKHS norm;
- Comparison to other ReLU kernels (e.g. training only last layer with random weights): the NTK has **weaker smoothness** properties but **better approximation**.

Approximation Properties (two layers)

Q: How rich is the RKHS for the NTK κ_{NTK} versus the simpler kernel κ_1 obtained by training just the second layer (random features)?

Mercer decomposition with spherical harmonics:

Proposition (Mercer decomposition)

For any $x, y \in \mathbb{S}^{p-1}$, we have the following decomposition of the NTK κ_{NTK}:

$$\kappa_{NTK}(\langle x,y\rangle) = \sum_{k=0}^{\infty} \mu_k \sum_{j=1}^{N(p,k)} Y_{k,j}(x) Y_{k,j}(y), \qquad (1)$$

*where $Y_{k,j}$ are **spherical harmonic** polynomials of degree k, and the non-negative eigenvalues μ_k satisfy $\mu_0, \mu_1 > 0$, $\mu_k = 0$ if $k = 2j+1$ with $j \geq 1$, and otherwise $\mu_k \sim C(p)k^{-p}$ as $k \to \infty$.*

This gives an explicit characterization of the RKHS norm of a function.

Approximation results: (following [Bach 2017])

- The RKHS is "**larger**": **slower decay** compared to κ_1, for which $\mu_k = O(k^{-p-2})$;
- f with $p/2$ η-bounded derivatives $\implies$ $f \in \mathcal{H}$ with $\|f\| \leq O(\eta)$;
- Weaker requirement compared to κ_1 (need $p/2+1$ derivatives);
- Better rates for approximating Lipschitz functions on the sphere.

Neural Tangent Kernels for CNNs

Two-layer ReLU Networks: $f(x;\theta) = \sqrt{\frac{2}{m}} \sum_{j=1}^m v_j \sigma(w_j^\top x)$, NTK given by

$$K(x,x') = \|x\|\|x'\| \kappa_{NTK}\left(\frac{\langle x,x'\rangle}{\|x\|\|x'\|}\right),$$

where $\kappa_{NTK}(u) := u\kappa_0(u) + \kappa_1(u)$, $\kappa_{0/1}$ arccos kernels of degree 0/1

Convolutional networks:

- Signals $x[u]$ in $\ell^2(\mathbb{Z}^d)$
- **Patch extraction** operators $P^k x[u] = |S_k|^{-1/2}(x[u+v])_{v \in S_k} \in \mathcal{H}^{|S_k|}$
- Linear **pooling** operators $A^k x[u] = \sum_{v \in \mathbb{Z}^d} h_k[u-v] x[v]$

Network: $f(x;\theta) = \sqrt{\frac{2}{m_n}} \langle w^{n+1}, a^n\rangle_{\ell^2}$, with

$$\tilde{a}^k[u] = \sqrt{2/m_{k-1}}\, W^k P^k a^{k-1}[u],$$
$$a^k[u] = A^k \sigma(\tilde{a}^k)[u], \quad k = 1, \ldots, n,$$

NTK: Consider the non-linear operator

$$M(x,y)[u] = \begin{pmatrix} \varphi_0(x[u]) \otimes y[u] \\ \varphi_1(x[u]) \end{pmatrix},$$

where φ_0, φ_1 are kernel mappings for kernels κ_0 and κ_1.

Proposition (NTK feature map for CNN)

The NTK is given by

$$K(x,x') = \langle \Phi(x), \Phi(x')\rangle_{\ell^2(\mathbb{Z}^d)},$$

with $\Phi(x)[u] = A^n M(x_n, y_n)[u]$, $y_1[u] = x_1[u] = P^1 x[u]$ and

$$x_k[u] = P^k A^{k-1} \varphi_1(x_{k-1})[u]$$
$$y_k[u] = P^k A^{k-1} M(x_{k-1}, y_{k-1})[u],$$

with the notation $\varphi_1(x)[u] = \varphi_1(x[u])$ for a signal x.

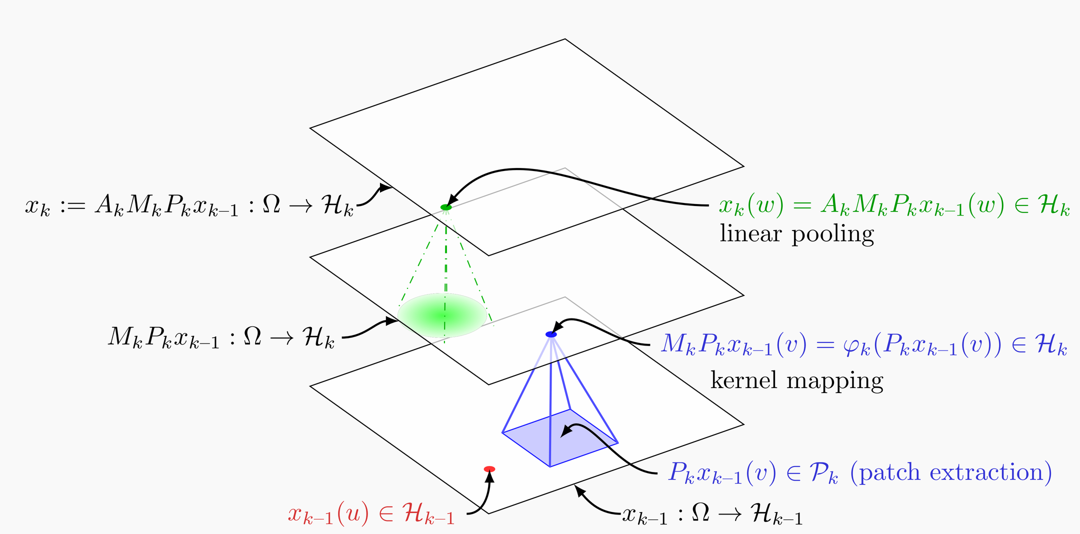


Illustration of feature maps construction for x_k.

Relevant References

- F. Bach (2017). Breaking the curse of dimensionality with convex neural networks.
- A. Bietti and J. Mairal (2019). Invariance and stability of deep convolutional representations.
- A. Jacot, F. Gabriel and C. Hongler (2018). Neural Tangent Kernel: convergence and generalization in neural networks.

Smoothness and Deformation Stability

Two-layer ReLU networks: The NTK (when training both layers) has **weaker smoothness** compared to training only the second layer.

Proposition (Non-Lipschitzness)

The kernel mapping $\Phi(\cdot)$ of the two-layer NTK is not Lipschitz:

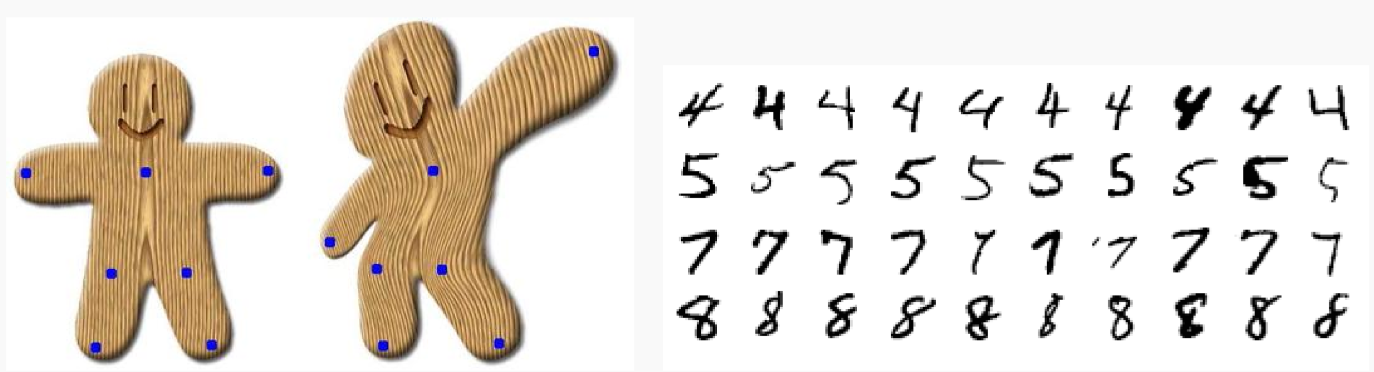
$$\sup_{x,y} \frac{\|\Phi(x) - \Phi(y)\|_{\mathcal{H}}}{\|x-y\|} \to +\infty.$$

It follows that the RKHS $\mathcal{H}$ contains unit-norm functions with arbitrarily large Lipschitz constant.

Proposition (Smoothness for ReLU NTK)

The kernel mapping Φ satisfies

$$\|\Phi(x) - \Phi(y)\| \leq \sqrt{\min(\|x\|, \|y\|)\|x-y\|} + 2\|x-y\|.$$



Deformation stability for deep ReLU CNNs: Similar assumptions to [Bietti and Mairal, 2019]

- **Continuous** signals $x(u)$ in $L^2(\mathbb{R}^d)$, $t: \mathbb{R}^d \to \mathbb{R}^d$, C^1, deformations $L_\tau x(u) = x(u - \tau(u))$
- **Anti-aliasing** of the original signal: $A_0 x$ instead of x
- **Patch sizes** controlled at current resolution: $\sup_{v \in S_k} |v| \leq \beta \sigma_{k-1}$

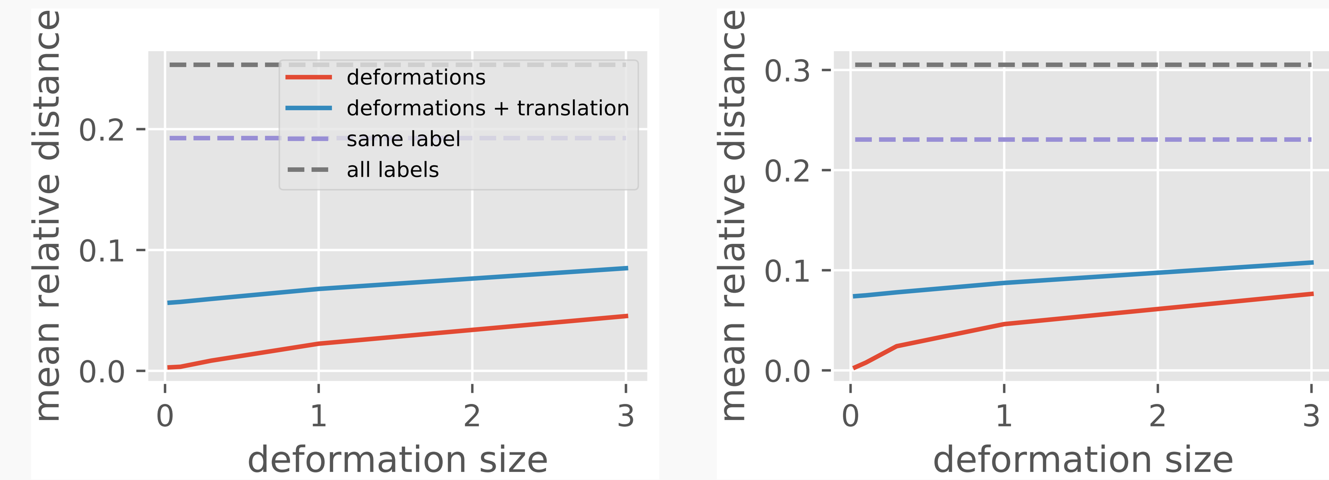
Proposition (Stability of NTK)

Let $\Phi_n(x) = \Phi(A_0 x)$, and assume $\|\nabla \tau\|_\infty \leq 1/2$. We have:

$$\|\Phi_n(L_\tau x) - \Phi_n(x)\| \leq \left(C_{\beta,n} \|\nabla\tau\|_\infty^{1/2} + C'_{\beta,n}\|\nabla\tau\|_\infty + \frac{C''_n}{\sigma_n}\|\tau\|_\infty\right)\|x\|.$$

Worse dependence on $\|\nabla\tau\|_\infty$ for small deformations compared to CKN/random feature kernel obtained when training just the last layer!

Comparison for MNIST digits + deformations



CKN/RF   NTK