On the Inductive Bias of Neural Tangent Kernels

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Generalization and Inductive Bias

Goal of supervised learning:
Given $(x_1, y_1), \ldots, (x_N, y_N) \sim \mathcal{D}$, find $f \in \mathcal{F}$ with small *expected loss*:

$$\mathbb{E}_{(x,y)\sim\mathcal{D}}[\ell(y_i, f(x_i))]$$

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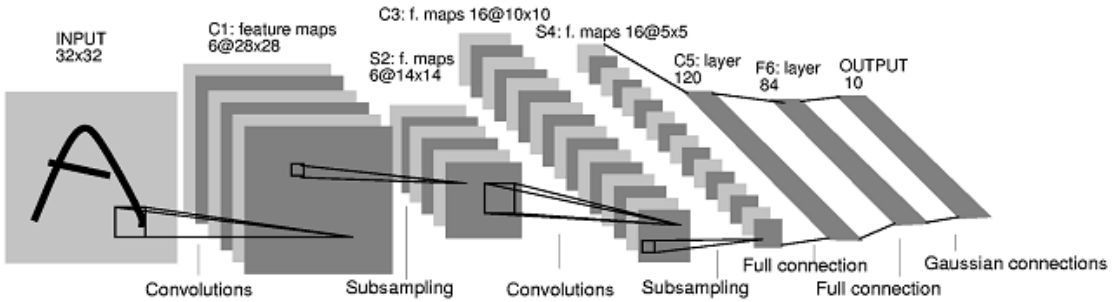
Inductive bias:

- Cannot generalize if $\mathcal{F}$ too large
  - all functions: "no free lunch theorem"
  - Lipschitz functions: "curse of dimensionality" (need $O(1/\epsilon^p)$ samples)
- Need for prior knowledge or *inductive bias* in the choice of $\mathcal{F}$

Generalization in deep learning



$$f_\theta(x) = W^n \sigma(W^{n-1} \cdots \sigma(W^1 x) \cdots)$$

- Heavily over-parameterized (millions/billions of parameters)
- Trained to fit the training data (almost) perfectly
- Often specific choices of architectures (convolutions, recurrent, attention)

Generalization in deep learning: complexity

What controls the "complexity" of the hypothesis class $\mathcal{F}$?

- Number of parameters is a poor measure of complexity!

For valid generalization, the size of the weights is more important than the size of the network

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- Some kind of norm of the weights? (*e.g.*, spectral norms)
  - often too large in practice

From Bartlett et al. (2017):

$$R_{\mathcal{A}} := \left(\prod_{i=1}^{L} \rho_i \|A_i\|_\sigma \right) \left(\sum_{i=1}^{L} \frac{\|A_i - M_i\|_1^{2/3}}{\|A_i\|_\sigma^{2/3}} \right)^{3/2}$$

Generalization in deep learning: complexity

What controls the "complexity" of the hypothesis class $\mathcal{F}$?

- Number of parameters is a poor measure of complexity!
- Some kind of norm of the weights? (*e.g.*, spectral norms)
  - often too large in practice
- Norm of the corresponding function in a functional space? $\|f_\theta\|_{\mathcal{H}}$ instead of $\|\theta\|$
  - Question: what is an appropriate functional space?

Generalization in deep learning: role of optimization

- Optimization of deep models often framed as the (non-convex) problem:

$$\min_{\theta} \frac{1}{N} \sum_{i=1}^{N} \ell(y_i, f_\theta(x_i)) \tag{1}$$

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- $\implies$ **optimization algorithm** selects the better, "simpler" models
- **Implicit bias** of (stochastic) gradient descent: for which norm $\|\cdot\|$ does (S)GD lead to the solution of

$$\begin{aligned} \min \quad & \|\theta\| \quad \text{or} \quad \|f_\theta\| \\ s.t. \quad & f_\theta(x_i) = y_i, \quad i = 1, \ldots, N \end{aligned}$$

Kernels for deep learning

Kernels?

- Map data x to high-dimensional space, $\Phi(x) \in \mathcal{H}$ ($\mathcal{H}$: "RKHS")
- Non-linear $f \in \mathcal{H}$ takes linear form: $f(x) = \langle f, \Phi(x) \rangle$
- Learning with a positive definite kernel $K(x, x') = \langle \Phi(x), \Phi(x') \rangle$
- Convex optimization problem (tractable)
- Statistical and approximation properties well understood
- Costly (kernel matrix of size N^2) but approximations are possible

Kernels for deep learning

Kernels from deep architectures

- Can construct *hierarchical kernels* following a given architecture
  - *e.g.*, convolutional kernels (Mairal, 2016)
- Arise naturally from infinite-width networks at initialization
- Recent work shows that similar kernels arise for *optimization* of over-parameterized networks: **neural tangent kernels** (NTKs, Jacot et al., 2018)
- Leads to **tractable** functional spaces to study deep networks

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This work:

- What are properties of the functional space for NTKs? (approximation, smoothness, stability to deformations for CNNs)
- How do they compare to previous deep kernels?

Outline

Warmup: random features

Two-layer ReLU network, with fixed first layer (a.k.a. random features):

$$f_\theta(x) = \frac{1}{\sqrt{m}} \sum_{i=1}^{m} v_i \sigma(w_i^\top x),$$

- $w_i \sim N(0, I)$ fixed
- $\theta = v \in \mathbb{R}^m$ optimized ($1/\sqrt{m}$ scaling is standard in initializations of v_i)
- $\sigma(u) = \max(0, u)$ (ReLU)
- Optimize loss with gradient descent on θ (convex problem here)

Warmup: random features

- Same as linear model $f_\theta(x) = \langle \theta, \phi(x) \rangle$ with random features

$$\phi(x) = \frac{1}{\sqrt{m}}(\sigma(w_1^\top x), \ldots, \sigma(w_m^\top x))$$

- Limiting kernel:

$$\begin{aligned} K_1(x, x') &= \lim_{m \to \infty} \langle \phi(x), \phi(x') \rangle \\ &= \mathbb{E}_{w \sim N(0,I)}[\sigma(w^\top x)\sigma(w^\top x')] \\ &= \|x\|\|x'\|\kappa_1\left(\frac{x^\top x'}{\|x\|\|x'\|}\right), \end{aligned}$$

with $\kappa_1(u) = \frac{1}{\pi}\left(u \cdot (\pi - \arccos(u)) + \sqrt{1-u^2}\right)$.

Warmup: random features

- Gradient descent implicitly acts as an ℓ^2 regularizer on θ
- For $m \to \infty$ and square loss, GD is implicitly solving a **regularized** version of the problem

$$\min_{f \in \mathcal{H}} \frac{1}{N} \sum_{i=1}^{N} \ell(y_i, f(x_i)),$$

  - $t \to \infty$ leads to **minimum-norm** interpolating solution
  - smaller t (**early stopping**) has a stronger regularization effect
- For finite but large enough m, similar generalization properties as full kernel (Bach, 2017b; Rudi and Rosasco, 2017).

Training both layers: lazy training

$$f_\theta(x) = \frac{1}{\sqrt{m}} \sum_{i=1}^{m} v_i \sigma(w_i^\top x),$$

What happens when training both layers? (or even multiple layers)

- $\theta = (v, w)$, initialization θ_0, i.i.d. $N(0, 1)$ params
- If m is (very) large, many results from past year essentially show that model stays close to **linearization** throughout training:

$$f_\theta(x) \approx f_{\theta_0}(x) + \langle \theta - \theta_0, \nabla_\theta f_\theta(x)|_{\theta=\theta_0} \rangle.$$

- weights move very little ("lazy training", Chizat et al., 2019)
  - tldr: 2nd order Taylor term remains negligible due to $1/\sqrt{m}$ scaling
  - not really what happens in practice... (for later)

Training both layers: neural tangent kernel (NTK)

$$f_\theta(x) \approx f_{\theta_0}(x) + \langle \theta - \theta_0, \nabla_\theta f_\theta(x)|_{\theta=\theta_0} \rangle.$$

- When $m \to \infty$, $f_{\theta_0}(x) \approx 0$
- Again, linear model on random features $\psi(x) = \nabla_\theta f_\theta(x)|_{\theta=\theta_0}$
- Limiting kernel:

$$\begin{aligned} K_{NTK}(x, x') &= \lim_{m\to\infty} \langle \psi(x), \psi(x') \rangle \\ &= (x^\top x')\, \mathbb{E}_{w\sim\mathcal{N}(0,I)}[1\{w^\top x \geq 0\} 1\{w^\top x' \geq 0\}] \\ &\quad + \mathbb{E}_{w\sim\mathcal{N}(0,I)}[(w^\top x)_+ (w^\top x')_+] \\ &= \|x\|\|x'\| \kappa_{NTK}\left(\frac{x^\top x'}{\|x\|\|x'\|}\right), \end{aligned}$$

with $\kappa_{NTK}(u) = u\kappa_0(u) + \kappa_1(u)$ ($\kappa_{1/0}$ are arc-cosine kernels for different activations, ReLU and threshold)

Outline

K_1 vs K_{NTK}

Training top layer vs both layers?

- Both kernels are *homogeneous dot-product kernels* of the form

$$K(x, x') = \|x\|\|x'\|\kappa\left(\frac{x^\top x'}{\|x\|\|x'\|}\right).$$

- For RF, $\kappa(u) = \kappa_1(u)$
- For NTK, $\kappa(u) = u\kappa_0(u) + \kappa_1(u)$
- How do the RKHSs differ?
- $\implies$ spectral description through Mercer decomposition

Mercer's theorem (*e.g.*, Schölkopf and Smola, 2001)

Define integral operator: $T_K f(x) = \int K(x, y) d\nu(y)$ for some $d\nu$

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Theorem (Mercer)

If $\mathcal{X}$ is compact and K is continuous, then there exists an orthonormal basis $(\phi_i)_{i \in \mathbb{N}}$ of $L^2(\mathcal{X}, d\nu)$, and non-negative eigenvalues $(\mu_i)_{i \in \mathbb{N}}$ such that

$$T_K \phi_i = \mu_i \phi_i, \quad i = 1, 2, \ldots$$

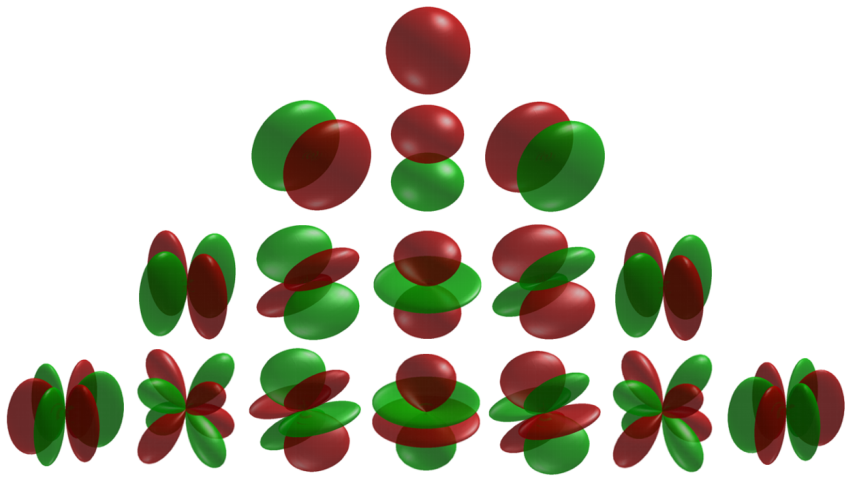
$$K(x, y) = \sum_{i=1}^{\infty} \mu_i \phi_i(x) \phi_i(y)$$

$$\mathcal{H} = \left\{ f = \sum_{i : \mu_i \neq 0} a_i \phi_i : a_i \in \mathbb{R}, \sum_{i : \mu_i \neq 0} \frac{a_i^2}{\mu_i} < \infty \right\},$$

where the norm of $f = \sum_{i:\mu_i \neq 0} a_i \phi_i$ is given by $\|f\|_{\mathcal{H}}^2 = \sum_{i:\mu_i \neq 0} \frac{a_i^2}{\mu_i}$.

Dot-product kernels on the sphere

- When $x, s' \in \mathbb{S}^{p-1}$, K_1 and K_{NTK} are dot-product kernels $K(x, x') = \kappa(x^\top x')$
- Such kernels are invariant to rotations (orthogonal matrices)
- Integral operator is diagonalized in the basis of **spherical harmonics**



Dot-product kernels on the sphere

We have

$$\kappa(x^\top y) = \sum_{k=0}^{\infty} \mu_k \sum_{j=1}^{N(p,k)} Y_{k,j}(x) Y_{k,j}(y) = \sum_{k=0}^{\infty} \mu_k N(p,k) P_k(x^\top y)$$

- $Y_{k,j}$, $j = 1, \ldots, N(p,k)$ are spherical harmonic polynomials of degree k
- P_k is the corresponding Legendre polynomials of degree k
- μ_k eigenvalue associated to spherical harmonics of degree k, given by

$$\mu_k = \frac{\omega_{p-2}}{\omega_{p-1}} \int_{-1}^{1} \kappa(t) P_k(t) (1-t^2)^{(p-3)/2} dt.$$

Decay of μ_k

- "Size" of the RKHS governed by the eigenvalue decay
- For κ_0 and κ_1, the μ_k follow from decompositions of positively homogeneous activations by Bach (2017a); slower decay for κ_0
- For κ_{NTK}, can use recurrence on Legendre polynomials: slower decay similar to $\kappa_0 \implies$ **larger** RKHS compared to κ_1

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- We have (for fixed dimension p)

	κ_1	κ_{NTK}
μ_k	$O(k^{-p-2})$	$O(k^{-p})$

Approximation properties

- As in Fourier, decay of coefficients $\leftrightarrow$ regularity
- Leads to approximation properties similar to Sobolev spaces, following Bach (2017a)

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- For κ_1, $p/2$ is replaced by $p/2+1$ (need more regularity)

Corollary (Sufficient condition for $f \in \mathcal{H}_{NTK}$)

Let $f : \mathbb{S}^{p-1} \to \mathbb{R}$ be an even function such that all i-th order derivatives exist and are bounded by η for $0 \leq i \leq s$, with $s \geq p/2$. Then $f \in \mathcal{H}$ with $\|f\|_{\mathcal{H}} \leq C(p)\eta$, where $C(p)$ is a constant that only depends on p.

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Corollary (Approximation of Lipschitz functions)

Let $f : \mathbb{S}^{p-1} \to \mathbb{R}$ be an even function such that $f(x) \leq \eta$ and $|f(x) - f(y)| \leq \eta \|x - y\|$, for all $x, y \in \mathbb{S}^{p-1}$. There is a function $g \in \mathcal{H}$ with $\|g\|_{\mathcal{H}} \leq \delta$, where δ is larger than a constant depending only on p, such that

$$\sup_{x \in \mathbb{S}^{p-1}} |f(x) - g(x)| \leq C(p)\eta \left(\frac{\delta}{\eta}\right)^{-1/(p/2-1)} \log\left(\frac{\delta}{\eta}\right).$$

Outline

Interlude: infinite width beyond two-layers

- **Deep network**: define "pre-activations" $\tilde{a}^1 = W^1 x$ and

$$\tilde{a}^k = \frac{1}{\sqrt{m_{k-1}}} W^k \sigma(\tilde{a}^{k-1})$$

- For inputs x, x' on the sphere and infinite width, $\tilde{a}_i^k, \tilde{a}_i'^k$ are Gaussian
- Covariance follows recurrence $\Sigma_1(x, x') = x^\top x'$

$$B_k = \begin{pmatrix} 1 & \Sigma_{k-1}(x, x') \\ \Sigma_{k-1}(x, x') & 1 \end{pmatrix}$$

$$\begin{aligned} \Sigma_k(x, x') &= \mathbb{E}_{(u,v)\sim N(0, B_k)}[\sigma(u)\sigma(v)] \\ &= \kappa_1(\Sigma_{k-1}(x, x')). \end{aligned}$$

Interlude: infinite width beyond two-layers

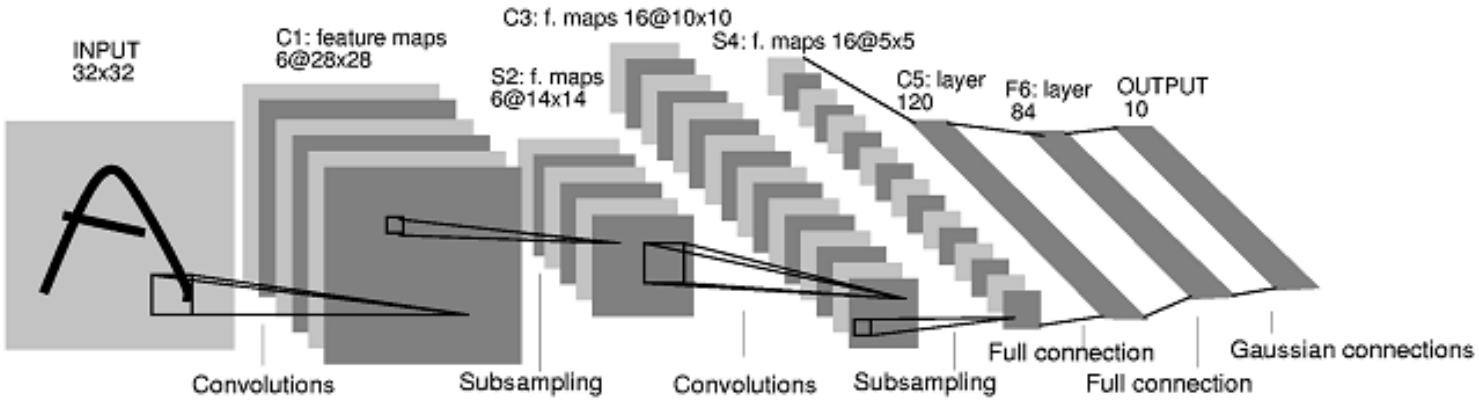
$$\Sigma_k(x, x') = \kappa_1(\Sigma_{k-1}(x, x'))$$

- Defines **hierarchical kernels**
- If $\kappa_1(x^\top x') = \langle \varphi_1(x), \varphi_1(x') \rangle$, then Σ_k has feature map

$$\Phi_k(x) = \underbrace{\varphi_1 \circ \cdots \circ \varphi_1}_{k \text{ times}}(x)$$

- Corresponds to training only last layer
- Similar for the NTK, but a sum of such kernels, one for each layer

Kernels for deep convolutional networks (CNNs)



Convolutional Neural Networks (CNNs):

- Capture **multi-scale** and **compositional** structure in natural signals
- Provide some **invariance**
- Model **local stationarity**
- **State-of-the-art** in many applications

Smoothness and stability with kernels

Study geometry of the kernel mapping $f(x) = \langle f, \Phi(x) \rangle$

$$|f(x) - f(x')| \leq \|f\|_{\mathcal{H}} \cdot \|\Phi(x) - \Phi(x')\|_{\mathcal{H}}$$

- $\|f\|_{\mathcal{H}}$ controls **smoothness** and **complexity** of the model
- $\Phi(x)$ encodes CNN **architecture** independently of the model (smoothness, invariance, stability to deformations)

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- $\|f\|_{\mathcal{H}}$ controls **smoothness** and **complexity** of the model
- $\Phi(x)$ encodes CNN **architecture** independently of the model (smoothness, invariance, stability to deformations)
- Training last layer of infinite-width CNN leads to a special case of **convolutional kernel networks** (CKNs, Mairal, 2016; Bietti and Mairal, 2019a)
- NTK (all layers) similar but more involved

Convolutional kernel network (CKN)

- $x_0 : \Omega \to \mathcal{H}_0$: initial (**continuous**) signal
  - $u \in \Omega = \mathbb{R}^d$: location ($d = 2$ for images)
  - $x_0(u) \in \mathcal{H}_0$: value ($\mathcal{H}_0 = \mathbb{R}^3$ for RGB images)

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- $x_k : \Omega \to \mathcal{H}_k$: *feature map* at layer k

$$P_k x_{k-1}$$

  - P_k: **patch extraction** operator, extract small patch of feature map x_{k-1} around each point u

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$$x_k = A_k M_k P_k x_{k-1}$$

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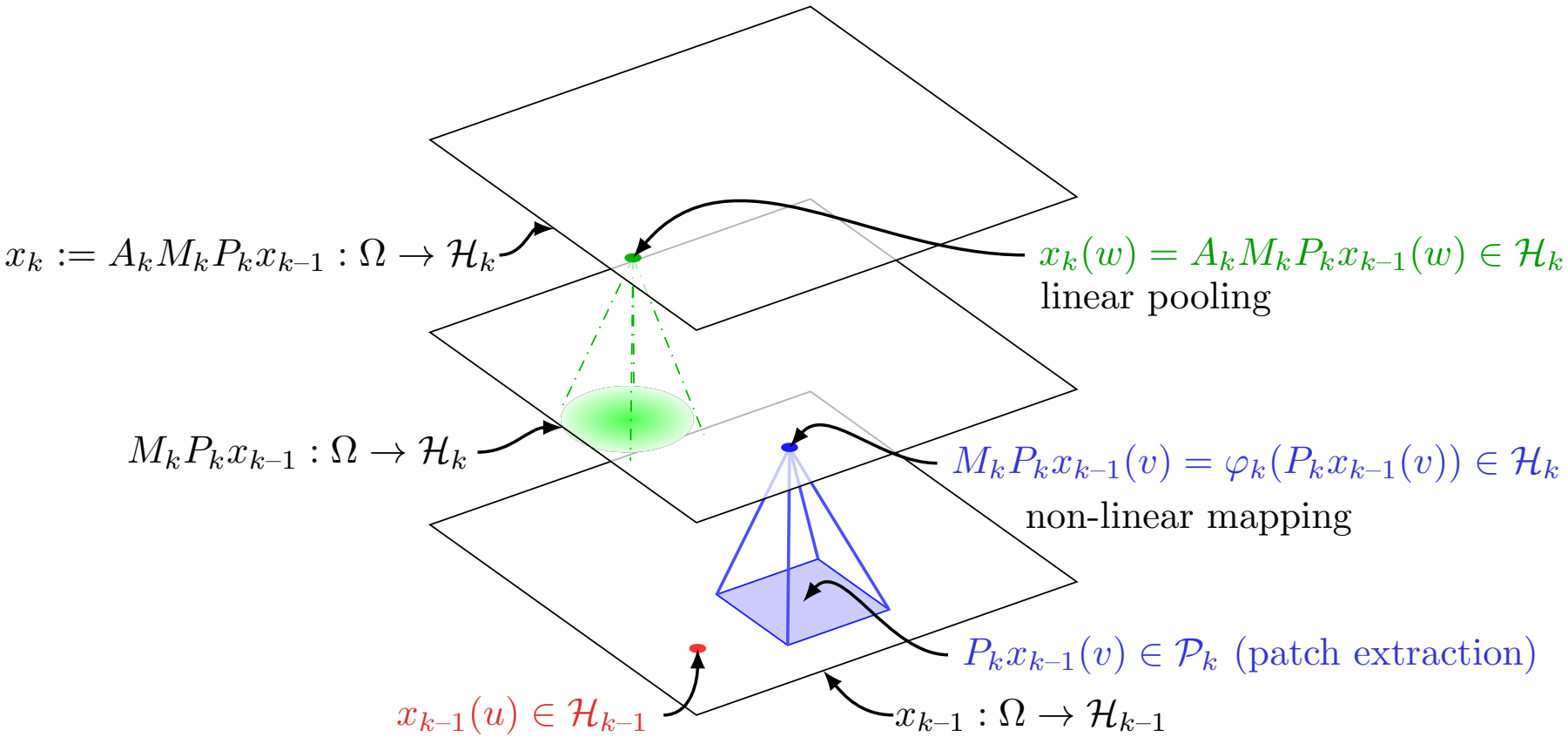
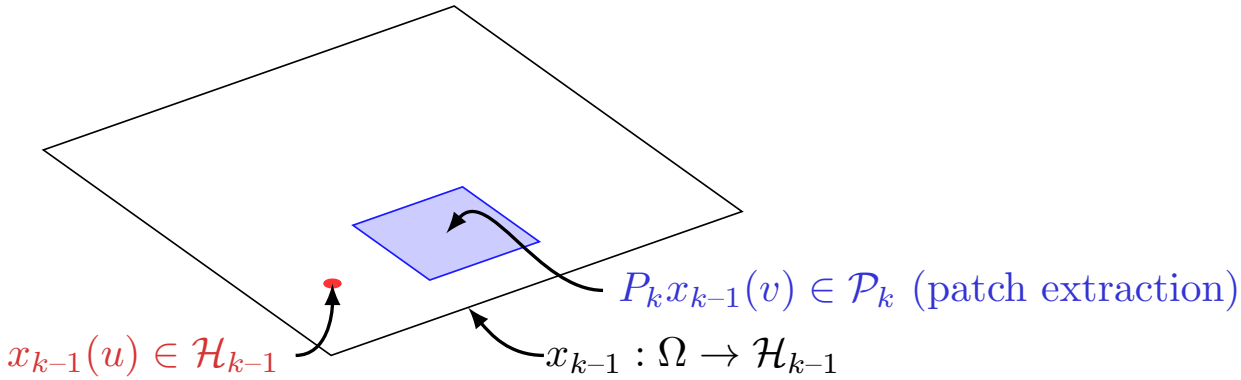
  - A_k: (linear, Gaussian) **pooling** operator at scale σ_k

CKN construction



Patch extraction operator P_k

$$P_k x_{k-1}(u) := (v \in S_k \mapsto x_{k-1}(u+v)) \in \mathcal{P}_k = \mathcal{H}_{k-1}^{S_k}$$



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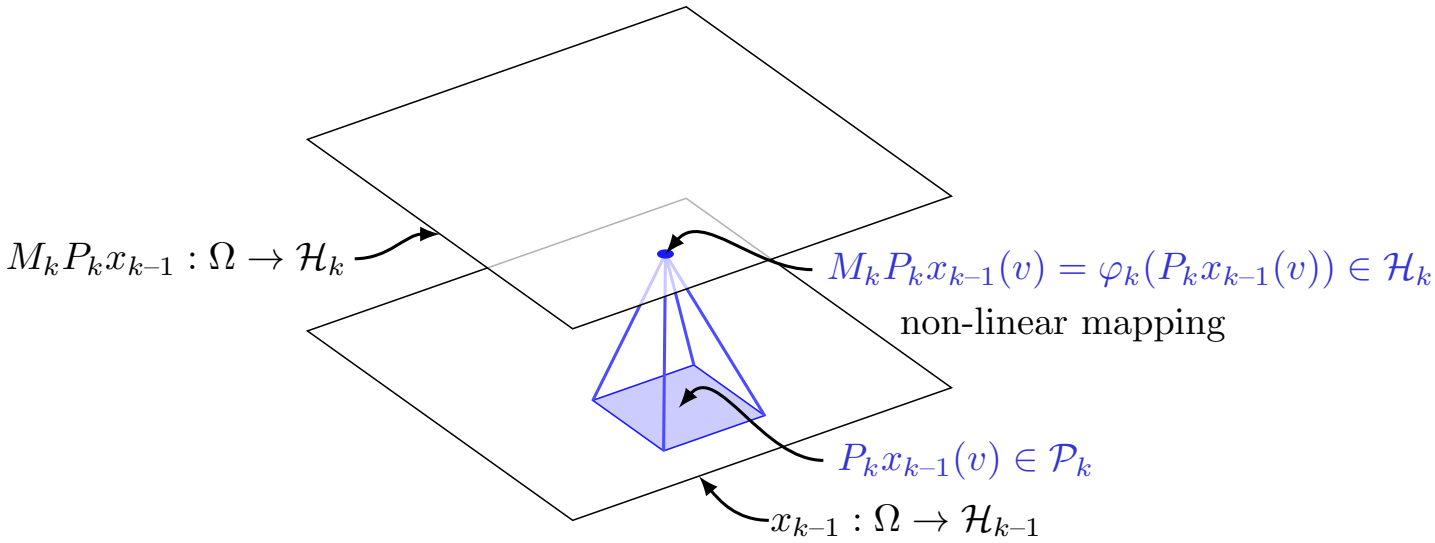
- S_k: patch shape, e.g. box
- P_k is **linear**, and **preserves the L^2 norm**: $\|P_k x_{k-1}\| = \|x_{k-1}\|$

Non-linear mapping operator M_k

$$M_k P_k x_{k-1}(u) := \varphi(P_k x_{k-1}(u)) \in \mathcal{H}_k$$



Non-linear mapping operator M_k

$$M_k P_k x_{k-1}(u) := \varphi(P_k x_{k-1}(u)) \in \mathcal{H}_k$$

- $\varphi : \mathcal{P}_k \to \mathcal{H}_k$ pointwise non-linearity on patches (kernel map)
- For ReLU, we use φ_1 from arc-cosine kernel, but other kernels are possible
- We assume **non-expansivity**: for $z, z' \in \mathcal{P}_k$

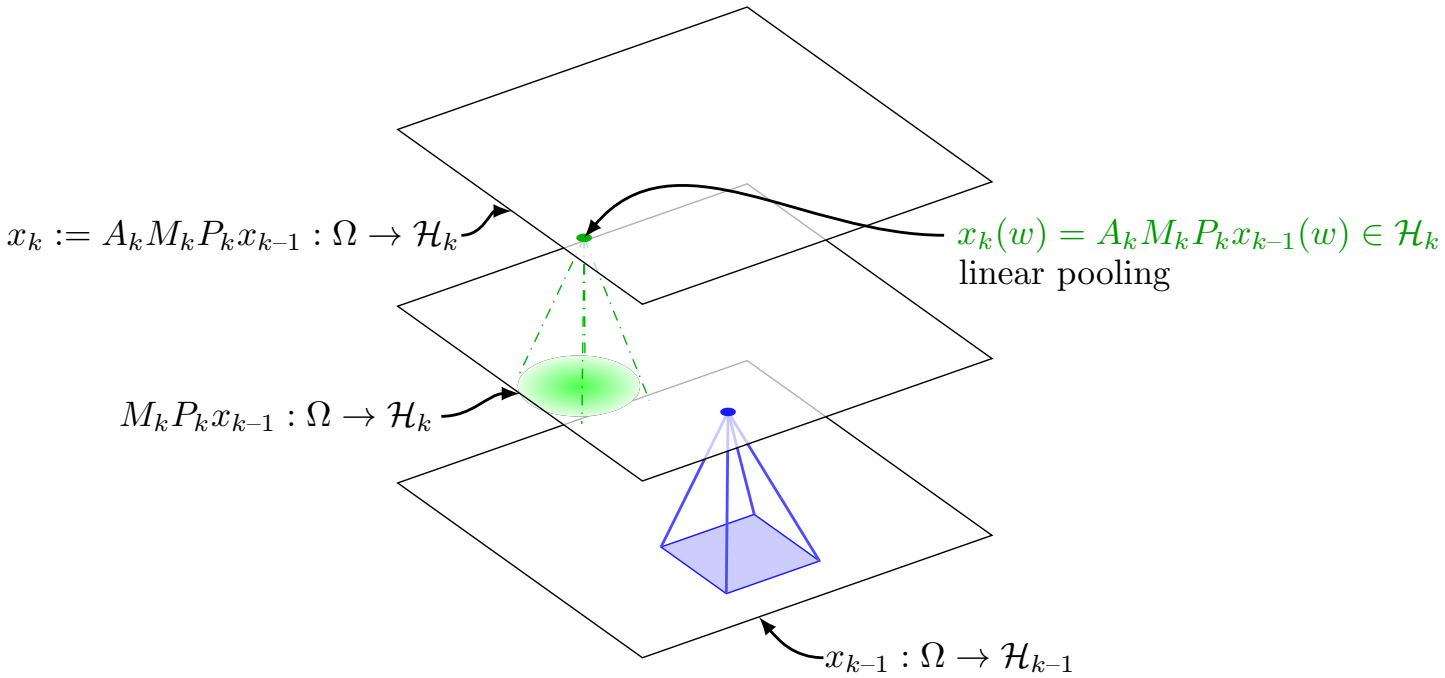
$$\|\varphi(z)\| \leq \|z\| \quad \text{and} \quad \|\varphi(z) - \varphi(z')\| \leq \|z - z'\|$$

- M_k then satisfies, for $x, x' \in L^2(\Omega, \mathcal{P}_k)$

$$\|M_k x\| \leq \|x\| \quad \text{and} \quad \|M_k x - M_k x'\| \leq \|x - x'\|$$

Pooling operator A_k

$$x_k(u) = A_k M_k P_k x_{k-1}(u) = \int_{\mathbb{R}^d} h_{\sigma_k}(u-v) M_k P_k x_{k-1}(v) dv \in \mathcal{H}_k$$



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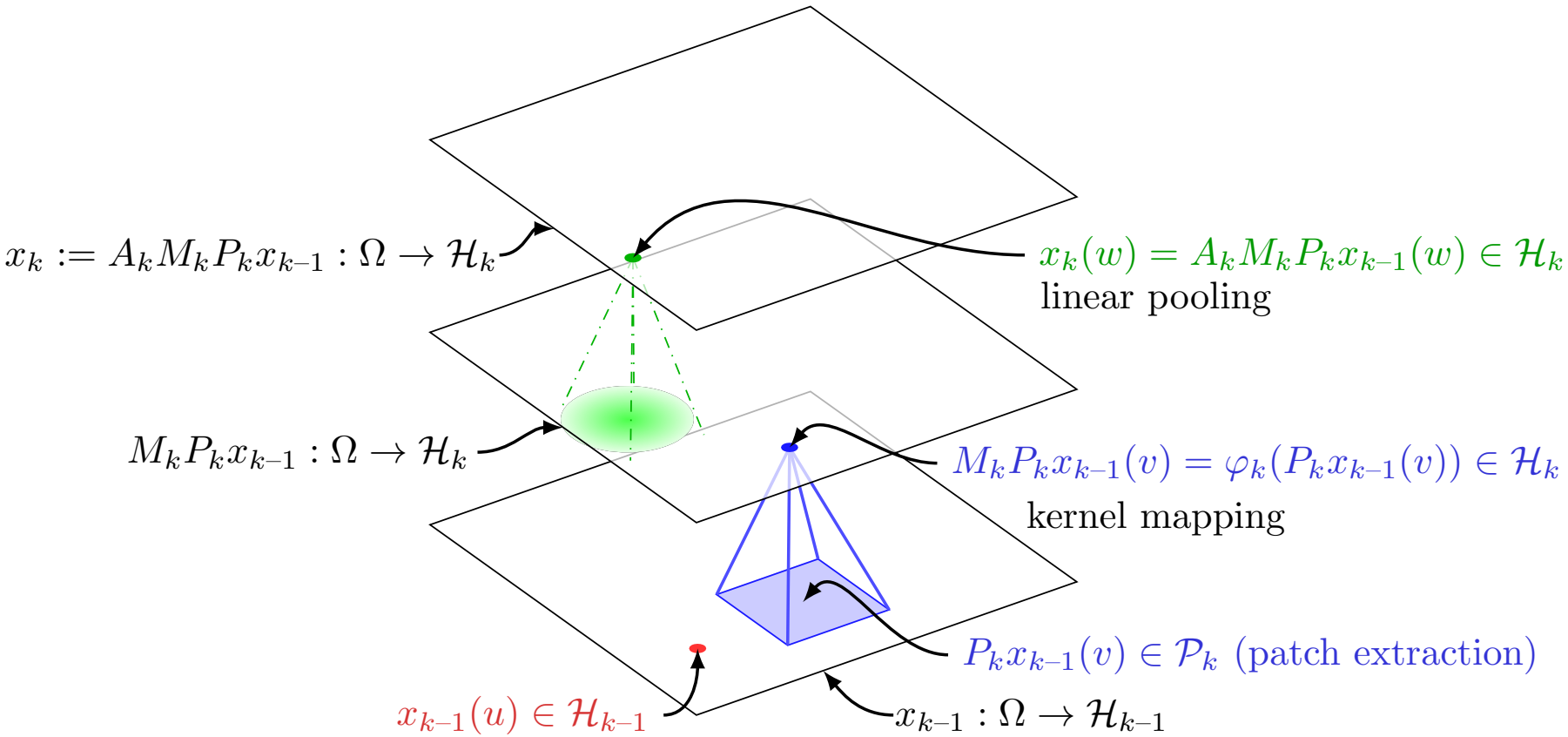
- h_{σ_k}: pooling filter at scale σ_k
- $h_{\sigma_k}(u) := \sigma_k^{-d} h(u/\sigma_k)$ with $h(u)$ **Gaussian**
- **linear, non-expansive operator**: $\|A_k\| \leq 1$

Recap: P_k, M_k, A_k



Final CKN kernel mapping

Assumption on x_0

- x_0 is typically a **discrete** signal aquired with physical device.
- Natural assumption: $x_0 = A_0 x$, with x the original continuous signal, A_0 local integrator with scale σ_0 (**anti-aliasing**).

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- x_0 is typically a **discrete** signal aquired with physical device.
- Natural assumption: $x_0 = A_0 x$, with x the original continuous signal, A_0 local integrator with scale σ_0 (**anti-aliasing**).

Multilayer representation

$$\Phi(x) = A_n M_n P_n A_{n-1} M_{n-1} P_{n-1} \cdots A_1 M_1 P_1 x_0 \ \in \ L^2(\Omega, \mathcal{H}_n).$$

- S_k, σ_k grow exponentially in practice (i.e., fixed with subsampling).

Final CKN kernel mapping

Assumption on x_0

- x_0 is typically a **discrete** signal aquired with physical device.
- Natural assumption: $x_0 = A_0 x$, with x the original continuous signal, A_0 local integrator with scale σ_0 (**anti-aliasing**).

Multilayer representation

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Final kernel

$$K_{CKN}(x, x') = \langle \Phi_n(x), \Phi_n(x') \rangle_{L^2(\Omega)} = \int_\Omega \langle x_n(u), x'_n(u) \rangle du$$

Convolutional NTK kernel mapping

Define

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

Theorem (NTK feature map for CNN)

$$K_{NTK}(x, x') = \langle \Phi(x), \Phi(x') \rangle_{L^2(\Omega)},$$

with $\Phi(x)(u) = A_n M(x_n, y_n)(u)$, *where* $y_1(u) = x_1(u) = P_1 x(u)$ *and*

$$x_k(u) = P_k A_{k-1} \varphi_1(x_{k-1})(u)$$
$$y_k(u) = P_k A_{k-1} M(x_{k-1}, y_{k-1})(u).$$

Smoothness: CKN vs NTK

Weaker smoothness for NTK!

CKN: Lipschitz

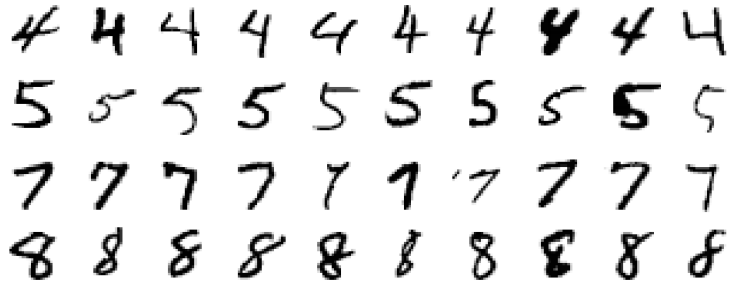
$$\|\Phi(x) - \Phi(x')\| \leq \|x - x'\|$$

NTK: $\approx$ Hölder

$$\|\Phi(x) - \Phi(x')\| \leq (n+1)\|x - x'\| + O(n^{5/4})\sqrt{\|\mathbf{x}\|\|\mathbf{x} - \mathbf{x}'\|}.$$

Stability to deformations: definitions

- $\tau : \Omega \to \Omega$: C^1-diffeomorphism
- $L_\tau x(u) = x(u - \tau(u))$: action operator
- Much richer group of transformations than translations



- Studied for wavelet-based scattering transform (Mallat, 2012; Bruna and Mallat, 2013)

Stability to deformations: definitions

- Representation $\Phi(\cdot)$ is **stable** (Mallat, 2012) if:

$$\|\Phi(L_\tau x) - \Phi(x)\| \leq (C_1 \|\nabla \tau\|_\infty + C_2 \|\tau\|_\infty) \|x\|$$

- $\|\nabla \tau\|_\infty = \sup_u \|\nabla \tau(u)\|$ controls deformation
- $\|\tau\|_\infty = \sup_u |\tau(u)|$ controls translation
- $C_2 \to 0$: translation invariance

Stability to deformations: CKN (Bietti and Mairal, 2019a)

Theorem

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

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

- translation invariance: large σ_n
- stability: small patch sizes ($\beta \approx$ patch size, $C_\beta = O(\beta^3)$ for images)
- signal preservation: subsampling factor $\approx$ patch size
- $\Longrightarrow$ **needs several layers**

Stability to deformations: NTK (Bietti and Mairal, 2019b)

Theorem (Stability of NTK)

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

$$\|\Phi_n(L_\tau x) - \Phi_n(x)\| \leq \left(C_\beta n^{7/4} \|\nabla\tau\|_\infty^{1/2} + C'_\beta n^2 \|\nabla\tau\|_\infty + \sqrt{n+1}\frac{C}{\sigma_n}\|\tau\|_\infty \right) \|x\|,$$

Stability to deformations: NTK (Bietti and Mairal, 2019b)

Theorem (Stability of NTK)

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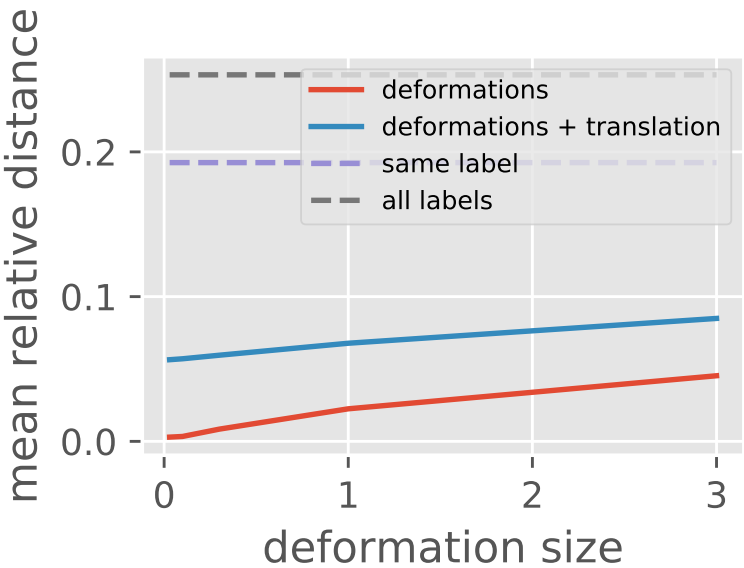
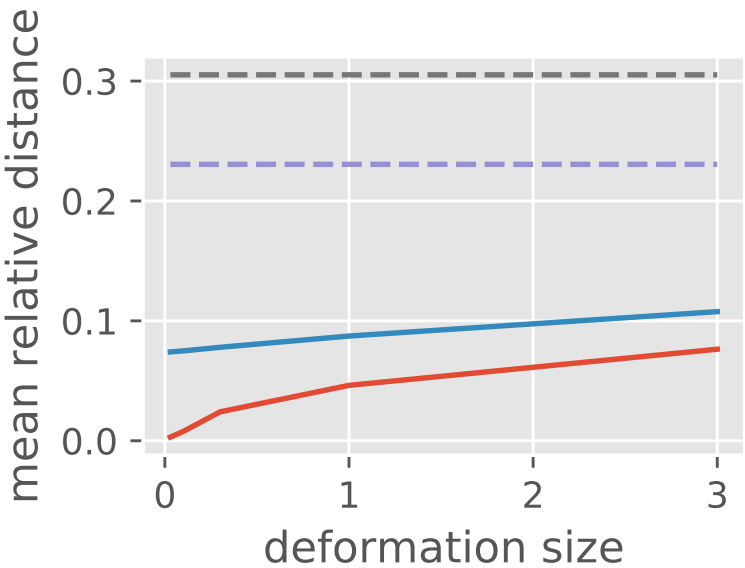


CKN



NTK

Conclusion

CKN vs NTK, last layer vs all layers

- NTK leads to a "larger" RKHS, better approximation
- NTK functions for CNNs are less smooth/stable

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- need huge number of neurons for NTK regime
- functions with finite neurons are not smooth! (*e.g.*, adversarial examples?)
- lazy training is limited (*e.g.*, cannot explain learning Gabor filters)

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Future directions

- approximation properties for deep networks / CNNs
- a "less lazy" regime? (*e.g.*, only first layers move)

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