

Foundations of Deep Convolutional Models through Kernel Methods

Alberto Bietti

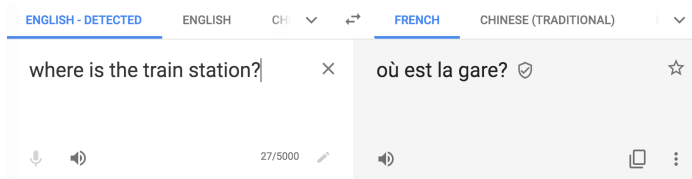
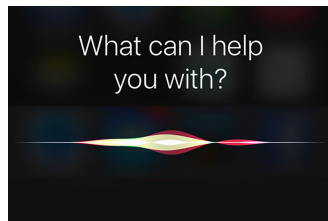
NYU

MaLGa Seminar. Feb. 16, 2021.



Success of deep learning

State-of-the-art models in various domains (images, speech, text, ...)



Success of deep learning

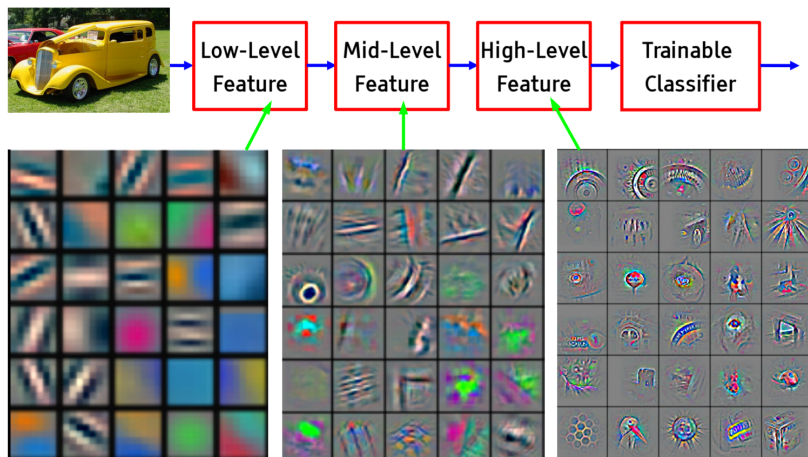
State-of-the-art models in various domains (images, speech, text, ...)

$$f(x) = W_n \sigma(W_{n-1} \cdots \sigma(W_1 x) \cdots)$$

Recipe: **huge models** + **lots of data** + **compute** + **simple algorithms**

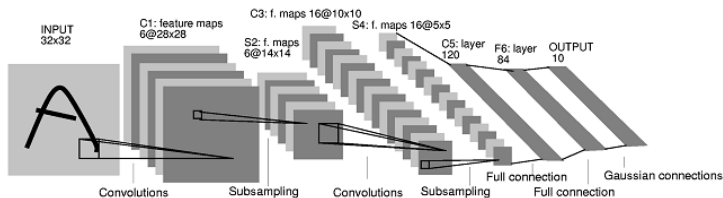
Convolutional networks

Exploiting structure of natural images (LeCun et al., 1989)



Feature visualization of convolutional net trained on ImageNet from [Zeiler & Fergus 2013]

Convolutional networks

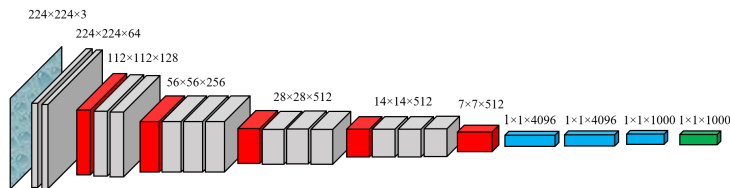


(LeCun et al., 1998)

Convolutional networks

- Model local neighborhoods at different scales
- Provide some invariance through pooling
- Useful **inductive bias** for learning efficiently on natural images

Convolutional networks



(Simonyan and Zisserman, 2014)

Convolutional networks

- Model local neighborhoods at different scales
- Provide some invariance through pooling
- Useful **inductive bias** for learning efficiently on natural images

Understanding deep learning

The challenge of deep learning theory

- **Over-parameterized** (millions of parameters)
- **Expressive** (can approximate any function)
- Complex **architectures** for exploiting problem structure
- Yet, **easy to optimize** with (stochastic) gradient descent!

Understanding deep learning

The challenge of deep learning theory

- **Over-parameterized** (millions of parameters)
- **Expressive** (can approximate any function)
- Complex **architectures** for exploiting problem structure
- Yet, **easy to optimize** with (stochastic) gradient descent!

A functional space viewpoint

- View deep networks as functions in some functional space
- Non-parametric models, natural measures of complexity (e.g., norms)

Understanding deep learning

The challenge of deep learning theory

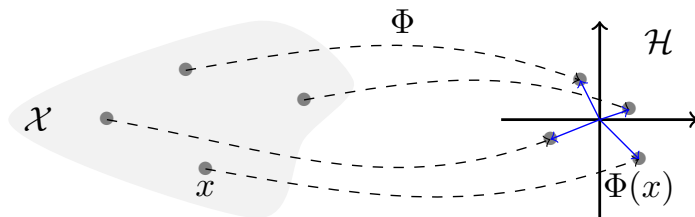
- **Over-parameterized** (millions of parameters)
- **Expressive** (can approximate any function)
- Complex **architectures** for exploiting problem structure
- Yet, **easy to optimize** with (stochastic) gradient descent!

A functional space viewpoint

- View deep networks as functions in some functional space
- Non-parametric models, natural measures of complexity (e.g., norms)

What is an appropriate functional space?

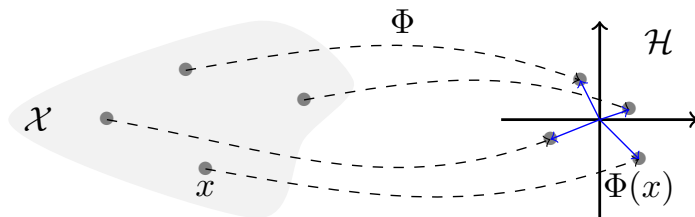
Kernels to the rescue



Kernels?

- Map data x to high-dimensional space, $\Phi(x) \in \mathcal{H}$ (\mathcal{H} : “RKHS”)
- Functions $f \in \mathcal{H}$ are linear in features: $f(x) = \langle f, \Phi(x) \rangle$ (f can be non-linear in x !)
- Learning with a positive definite kernel $K(x, x') = \langle \Phi(x), \Phi(x') \rangle$
 - ▶ \mathcal{H} can be infinite-dimensional! (*kernel trick*)
 - ▶ Need to compute kernel matrix $K = [K(x_i, x_j)]_{ij} \in \mathbb{R}^{N \times N}$

Kernels to the rescue



Clean and well-developed theory

- Tractable methods (convex optimization)
- Statistical and approximation properties well understood for many kernels
- Costly (kernel matrix of size N^2) but approximations are possible

Kernels for deep models: deep kernel machines

Hierarchical kernels (Cho and Saul, 2009)

- Kernels can be constructed **hierarchically**

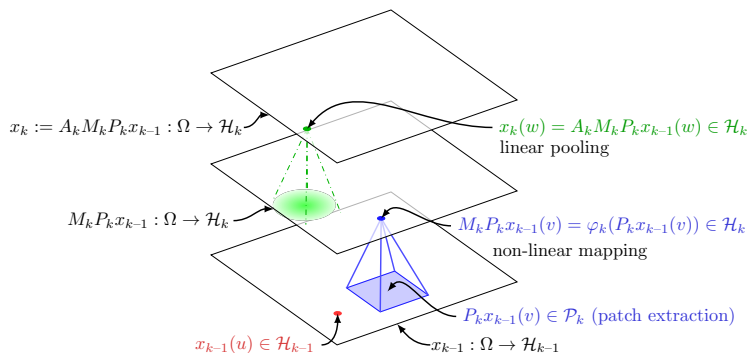
$$K(x, x') = \langle \Phi(x), \Phi(x') \rangle \text{ with } \Phi(x) = \varphi_2(\varphi_1(x))$$

- e.g., dot-product kernels on the sphere

$$K(x, x') = \kappa_2(\langle \varphi_1(x), \varphi_1(x') \rangle) = \kappa_2(\kappa_1(x^\top x'))$$

Kernels for deep models: deep kernel machines

Convolutional kernels networks (CKNs) for images (Mairal et al., 2014; Mairal, 2016)



- Good empirical performance with tractable approximations (Nyström)

Kernels for deep models: infinite-width networks

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

Random feature kernels (RF, Neal, 1996; Rahimi and Recht, 2007)

- $\theta = (v_i)_i$, fixed random weights $w_i \sim N(0, I)$

$$K_{RF}(x, x') = \mathbb{E}_{w \sim N(0, I)} [\sigma(w^{\top} x) \sigma(w^{\top} x')]$$

Kernels for deep models: infinite-width networks

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

Random feature kernels (RF, Neal, 1996; Rahimi and Recht, 2007)

- $\theta = (v_i)_i$, fixed random weights $w_i \sim N(0, I)$

$$K_{RF}(x, x') = \mathbb{E}_{w \sim N(0, I)} [\sigma(w^{\top} x) \sigma(w^{\top} x')]$$

Neural tangent kernels (NTK, Jacot et al., 2018)

- $\theta = (v_i, w_i)_i$, initialization $\theta_0 \sim N(0, I)$
- **Lazy training** (Chizat et al., 2019): θ stays close to θ_0 when training with large m

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

Kernels for deep models: infinite-width networks

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

Random feature kernels (RF, Neal, 1996; Rahimi and Recht, 2007)

- $\theta = (v_i)_i$, fixed random weights $w_i \sim N(0, I)$

$$K_{RF}(x, x') = \mathbb{E}_{w \sim N(0, I)} [\sigma(w^{\top} x) \sigma(w^{\top} x')]$$

Neural tangent kernels (NTK, Jacot et al., 2018)

- $\theta = (v_i, w_i)_i$, initialization $\theta_0 \sim N(0, I)$
- **Lazy training** (Chizat et al., 2019): θ stays close to θ_0 when training with large m

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

- Gradient descent for $m \rightarrow \infty \approx$ kernel ridge regression with **neural tangent kernel**

$$K_{NTK}(x, x') = \lim_{m \rightarrow \infty} \langle \nabla_{\theta} f_{\theta_0}(x), \nabla_{\theta} f_{\theta_0}(x') \rangle$$

Kernels for deep models: infinite-width networks

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

Random feature kernels (RF, Neal, 1996; Rahimi and Recht, 2007)

- $\theta = (v_i)_i$, fixed random weights $w_i \sim N(0, I)$

$$K_{RF}(x, x') = \mathbb{E}_{w \sim N(0, I)} [\sigma(w^{\top} x) \sigma(w^{\top} x')]$$

Neural tangent kernels (NTK, Jacot et al., 2018)

- $\theta = (v_i, w_i)_i$, initialization $\theta_0 \sim N(0, I)$
- **Lazy training** (Chizat et al., 2019): θ stays close to θ_0 when training with large m

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

- Gradient descent for $m \rightarrow \infty \approx$ kernel ridge regression with **neural tangent kernel**

$$K_{NTK}(x, x') = \lim_{m \rightarrow \infty} \langle \nabla_{\theta} f_{\theta_0}(x), \nabla_{\theta} f_{\theta_0}(x') \rangle$$

RF and NTK extend to deep architectures

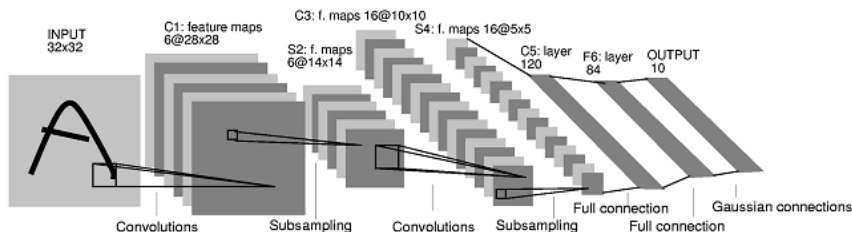
Outline

- 1 Convolutional kernels and their stability
- 2 Approximation and regularization properties

Outline

- 1 Convolutional kernels and their stability
- 2 Approximation and regularization properties

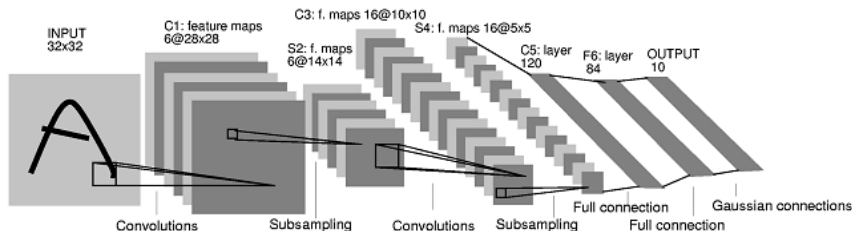
Folklore properties of convolutional models



Convolutional architectures:

- Capture **multi-scale** and **compositional** structure in natural signals
- Model **local stationarity**
- Provide some **translation invariance**

Folklore properties of convolutional models



Convolutional architectures:

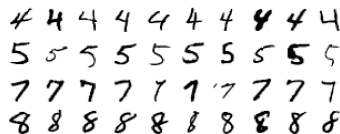
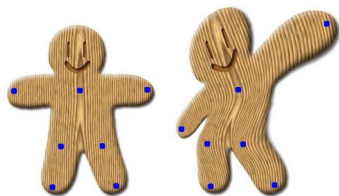
- Capture **multi-scale** and **compositional** structure in natural signals
- Model **local stationarity**
- Provide some **translation invariance**

Beyond translation invariance?

Stability to deformations

Deformations

- $\tau : \Omega \rightarrow \Omega$: 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

Deformations

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

Definition of stability

- 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
- $C_2 \rightarrow 0$: translation invariance

Smoothness and stability with kernels

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 **complexity** of the model
- $\Phi(x)$ encodes CNN **architecture** independently of the model (smoothness, invariance, stability to deformations)

Smoothness and stability with kernels

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 **complexity** of the model
- $\Phi(x)$ encodes CNN **architecture** independently of the model (smoothness, invariance, stability to deformations)

Useful kernels in practice:

- Convolutional kernel networks (**CKNs**, Mairal, 2016) with efficient approximations
- Extends to neural tangent kernels (**NTKs**, Jacot et al., 2018) of infinitely wide CNNs (Bietti and Mairal, 2019b)

Construction of convolutional kernels

Construct a sequence of feature maps x_1, \dots, x_n

- $x_0 : \Omega \rightarrow \mathcal{H}_0$: 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)

Construction of convolutional kernels

Construct a sequence of feature maps x_1, \dots, x_n

- $x_0 : \Omega \rightarrow \mathcal{H}_0$: 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)
- $x_k : \Omega \rightarrow \mathcal{H}_k$: **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

Construction of convolutional kernels

Construct a sequence of feature maps x_1, \dots, x_n

- $x_0 : \Omega \rightarrow \mathcal{H}_0$: 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)
- $x_k : \Omega \rightarrow \mathcal{H}_k$: **feature map** at layer k

$$M_k P_k x_{k-1}$$

- ▶ P_k : **patch extraction** operator, extract small patch of feature map x_{k-1} around each point u
- ▶ M_k : **non-linear mapping** operator, maps each patch to a new point with a **pointwise** non-linear function $\varphi_k(\cdot)$ (kernel mapping)

Construction of convolutional kernels

Construct a sequence of feature maps x_1, \dots, x_n

- $x_0 : \Omega \rightarrow \mathcal{H}_0$: 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)
- $x_k : \Omega \rightarrow \mathcal{H}_k$: **feature map** at layer k

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

- ▶ P_k : **patch extraction** operator, extract small patch of feature map x_{k-1} around each point u
- ▶ M_k : **non-linear mapping** operator, maps each patch to a new point with a **pointwise** non-linear function $\varphi_k(\cdot)$ (kernel mapping)
- ▶ A_k : (linear, Gaussian) **pooling** operator at scale σ_k

Construction of convolutional kernels

Construct a sequence of feature maps x_1, \dots, x_n

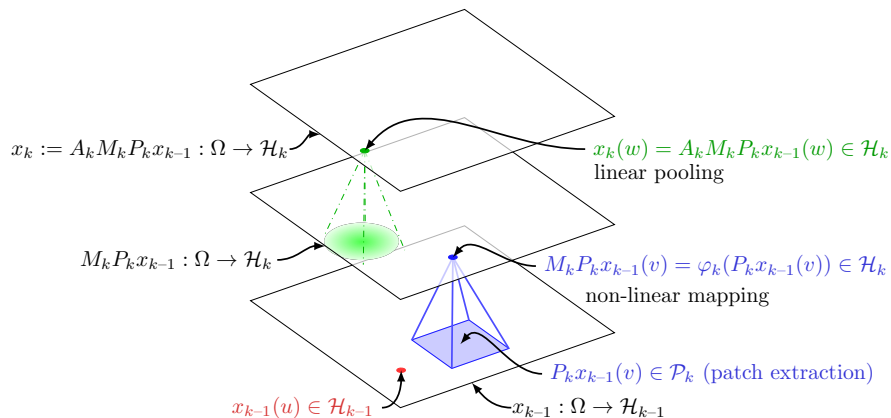
- $x_0 : \Omega \rightarrow \mathcal{H}_0$: initial (**continuous**) signal
 - ▶ $u \in \Omega = \mathbb{R}^d$: location ($d = 2$ for images)
 - ▶ $x_0(u) \in \mathcal{H}_0$: value ($\mathcal{H}_0 = \mathbb{R}^3$ for RGB images)
- $x_k : \Omega \rightarrow \mathcal{H}_k$: **feature map** at layer k

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

- ▶ P_k : **patch extraction** operator, extract small patch of feature map x_{k-1} around each point u
- ▶ M_k : **non-linear mapping** operator, maps each patch to a new point with a **pointwise** non-linear function $\varphi_k(\cdot)$ (kernel mapping)
- ▶ A_k : (linear, Gaussian) **pooling** operator at scale σ_k

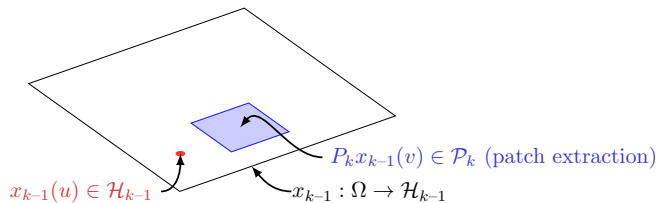
Goal: control stability of these operators through their norms

CKN construction



Patch extraction operator P_k

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



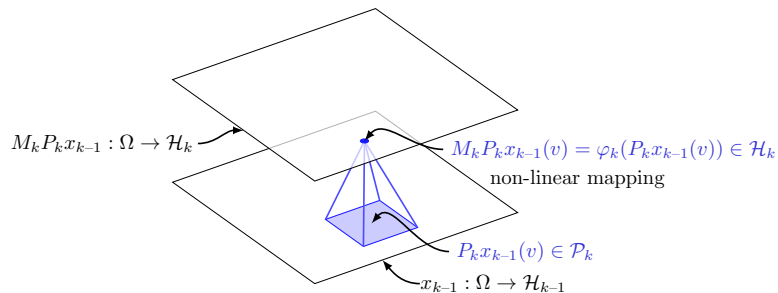
Patch extraction operator P_k

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

- 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

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



Non-linear mapping operator M_k

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

- $\varphi_k : \mathcal{P}_k \rightarrow \mathcal{H}_k$ pointwise non-linearity on patches (kernel map)
- We assume **non-expansivity**: for $z, z' \in \mathcal{P}_k$

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

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

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

φ_k from kernels

Kernel mapping of **homogeneous dot-product kernels**:

$$K_k(z, z') = \|z\| \|z'\| \kappa_k\left(\frac{\langle z, z' \rangle}{\|z\| \|z'\|}\right) = \langle \varphi_k(z), \varphi_k(z') \rangle.$$

$$\kappa_k(u) = \sum_{j=0}^{\infty} b_j u^j \text{ with } b_j \geq 0, \kappa_k(1) = 1$$

- Commonly used for hierarchical kernels
- $\|\varphi_k(z)\| = K_k(z, z)^{1/2} = \|z\|$
- $\|\varphi_k(z) - \varphi_k(z')\| \leq \|z - z'\|$ if $\kappa'_k(1) \leq 1$
- \implies **non-expansive**

φ_k from kernels

Kernel mapping of **homogeneous dot-product kernels**:

$$K_k(z, z') = \|z\| \|z'\| \kappa_k\left(\frac{\langle z, z' \rangle}{\|z\| \|z'\|}\right) = \langle \varphi_k(z), \varphi_k(z') \rangle.$$

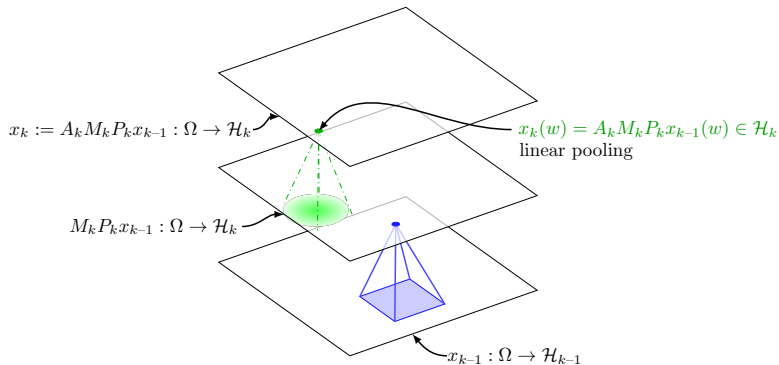
$$\kappa_k(u) = \sum_{j=0}^{\infty} b_j u^j \text{ with } b_j \geq 0, \kappa_k(1) = 1$$

Examples

- $\kappa_{\text{exp}}(\langle z, z' \rangle) = e^{\langle z, z' \rangle - 1}$ (Gaussian kernel on the sphere)
- $\kappa_{\text{inv-poly}}(\langle z, z' \rangle) = \frac{1}{2 - \langle z, z' \rangle}$
- $\kappa_{\sigma}(\langle z, z' \rangle) = \mathbb{E}_w[\sigma(w^\top z)\sigma(w^\top z')]$ (Random features)
 - ▶ arc-cosine kernels for the ReLU $\sigma(u) = \max(0, u)$

Pooling operator A_k

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



Pooling operator A_k

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

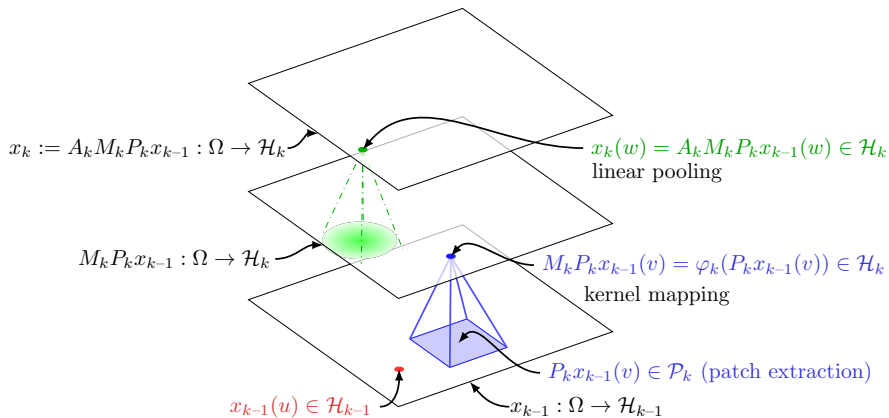
- h_{σ_k} : pooling filter at scale σ_k
- $h_{\sigma_k}(u) := \sigma_k^{-d} h(u/\sigma_k)$ with $h(u)$ **Gaussian**
- **linear, non-expansive operator**: $\|A_k\| \leq 1$

Pooling operator A_k

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

- 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**: $\|A_k\| \leq 1$
- In practice: **discretization**, sampling at resolution σ_k after pooling
- “Preserves information” when **subsampling** \leq **patch size**

Recap: P_k, M_k, A_k



Multilayer construction

Assumption on x_0

- x_0 is typically a **discrete** signal acquired 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 construction

Assumption on x_0

- x_0 is typically a **discrete** signal acquired 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

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

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

Multilayer construction

Assumption on x_0

- x_0 is typically a **discrete** signal acquired 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

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

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

Final kernel

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

Stability to deformations

Theorem (Stability of CKN (Bietti and Mairal, 2019a))

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
 \implies **need several layers with small patches** $n = O(\log(\sigma_n/\sigma_0)/\log \beta)$

Stability to deformations for convolutional NTK

Theorem (Stability of NTK (Bietti and Mairal, 2019b))

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

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

Comparison with random feature CKN on deformed MNIST digits:



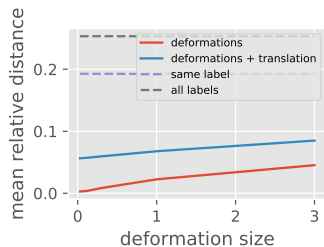
Stability to deformations for convolutional NTK

Theorem (Stability of NTK (Bietti and Mairal, 2019b))

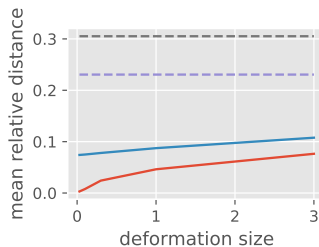
Let $\Phi_n(x) = \Phi^{NTK}(A_0 x)$, and assume $\|\nabla \tau\|_\infty \leq 1/2$

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

Comparison with random feature CKN on deformed MNIST digits:



(a) CKN



(b) NTK

Experiments with convolutional kernels on Cifar10

Convolutional kernels with 3x3 patches + kernel ridge regression (danger: lots of compute!)

Conv. layers	subsampling	kernel	test acc.
2	2-5	ReLU RF	86.63%
2	2-5	ReLU NTK	87.19%

Experiments with convolutional kernels on Cifar10

Convolutional kernels with 3x3 patches + kernel ridge regression (danger: lots of compute!)

Conv. layers	subsampling	kernel	test acc.
2	2-5	ReLU RF	86.63%
2	2-5	ReLU NTK	87.19%
2	2-5	exp, $\sigma = 0.6$	87.93%
3	2-2-2	exp, $\sigma = 0.6$	88.2%

Experiments with convolutional kernels on Cifar10

Convolutional kernels with 3x3 patches + kernel ridge regression (danger: lots of compute!)

Conv. layers	subsampling	kernel	test acc.
2	2-5	ReLU RF	86.63%
2	2-5	ReLU NTK	87.19%
2	2-5	exp, $\sigma = 0.6$	87.93%
3	2-2-2	exp, $\sigma = 0.6$	88.2%
16 (Li et al., 2019)	last layer only	ReLU RF	87.28%
16 (Li et al., 2019)	last layer only	ReLU NTK	86.77%
10	every 3 layers	exp	88.2%

Li et al. (2019): no pooling before last layer, more complicated pre-processing

Shankar et al. (2020): similar performance to us (88.2%), reaches 90% when adding flips

Outline

- 1 Convolutional kernels and their stability
- 2 Approximation and regularization properties

Approximation with convolutional networks

- **What functions does the RKHS contain? What is their norm?**
- Role of **convolution** vs **fully-connected**?
- Role of **depth**?

Approximation with convolutional networks

- **What functions does the RKHS contain? What is their norm?**
- Role of **convolution** vs **fully-connected**?
- Role of **depth**?
- Limitations of kernels?

Prelude: “teacher” CNNs with smooth activations are in the RKHS

- Consider a CNN with filters $W_k^{ij}(u), u \in S_k$
- **Smooth** activations σ with smoothness controlled by some $C_{\kappa,\sigma}(\cdot)$
- The CNN can be **constructed hierarchically** in \mathcal{H}_{CKN}
- Complexity is controlled by the RKHS norm:

$$\|f_\sigma\|_{\mathcal{H}}^2 \leq \|W_{n+1}\|_2^2 C_{\kappa,\sigma}^2(\|W_n\|_2^2 C_{\kappa,\sigma}^2(\|W_{n-1}\|_2^2 C_{\kappa,\sigma}^2(\dots)))$$

(Bietti and Mairal, 2019a)

Prelude: “teacher” CNNs with smooth activations are in the RKHS

- Consider a CNN with filters $W_k^{ij}(u)$, $u \in S_k$
- **Smooth** activations σ with smoothness controlled by some $C_{\kappa,\sigma}(\cdot)$
- The CNN can be **constructed hierarchically** in \mathcal{H}_{CKN}
- Complexity is controlled by the RKHS norm (linear layers):

$$\|f_\sigma\|_{\mathcal{H}}^2 \leq \|W_{n+1}\|_2^2 \cdot \|W_n\|_2^2 \cdot \|W_{n-1}\|_2^2 \cdots \|W_1\|_2^2$$

- Linear layers: product of spectral norms

(Bietti and Mairal, 2019a)

Prelude: “teacher” CNNs with smooth activations are in the RKHS

- Consider a CNN with filters $W_k^{ij}(u)$, $u \in S_k$
- **Smooth** activations σ with smoothness controlled by some $C_{\kappa,\sigma}(\cdot)$
- The CNN can be **constructed hierarchically** in \mathcal{H}_{CKN}
- Complexity is controlled by the RKHS norm (linear layers):

$$\|f_\sigma\|_{\mathcal{H}}^2 \leq \|W_{n+1}\|_2^2 \cdot \|W_n\|_2^2 \cdot \|W_{n-1}\|_2^2 \cdots \|W_1\|_2^2$$

- Linear layers: product of spectral norms
- **Can we give a more precise characterization of the RKHS?**

(Bietti and Mairal, 2019a)

The fully-connected case

Fully-connected models \implies dot-product kernels

$$K(x, y) = \kappa(x^\top y) \text{ for } x, y \in \mathbb{S}^{d-1}$$

- Infinitely wide random networks (Neal, 1996; Cho and Saul, 2009; Lee et al., 2018)
- NTK for infinitely wide networks (Jacot et al., 2018)

The fully-connected case

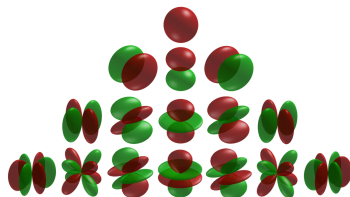
Fully-connected models \implies dot-product kernels

$$K(x, y) = \kappa(x^\top y) \text{ for } x, y \in \mathbb{S}^{d-1}$$

- Infinitely wide random networks (Neal, 1996; Cho and Saul, 2009; Lee et al., 2018)
- NTK for infinitely wide networks (Jacot et al., 2018)

Precise description of the RKHS (Mercer decomposition)

- Rotation-invariant kernel on the sphere
- \implies RKHS description in the $L^2(\mathbb{S}^{d-1})$ basis of **spherical harmonics** $Y_{k,j}$



The fully-connected case

Fully-connected models \implies dot-product kernels

$$K(x, y) = \kappa(x^\top y) \text{ for } x, y \in \mathbb{S}^{d-1}$$

- Infinitely wide random networks (Neal, 1996; Cho and Saul, 2009; Lee et al., 2018)
- NTK for infinitely wide networks (Jacot et al., 2018)

Precise description of the RKHS (Mercer decomposition)

- Rotation-invariant kernel on the sphere
- \implies RKHS description in the $L^2(\mathbb{S}^{d-1})$ basis of **spherical harmonics** $Y_{k,j}$

$$\kappa(x^\top y) = \sum_{k=0}^{\infty} \mu_k \sum_{j=1}^{N(d,k)} Y_{k,j}(x) Y_{k,j}(y), \quad \text{for } x, y \in \mathbb{S}^{d-1}$$

The fully-connected case

Fully-connected models \implies dot-product kernels

$$K(x, y) = \kappa(x^\top y) \text{ for } x, y \in \mathbb{S}^{d-1}$$

- Infinitely wide random networks (Neal, 1996; Cho and Saul, 2009; Lee et al., 2018)
- NTK for infinitely wide networks (Jacot et al., 2018)

Precise description of the RKHS (Mercer decomposition)

- Rotation-invariant kernel on the sphere
- \implies RKHS description in the $L^2(\mathbb{S}^{d-1})$ basis of **spherical harmonics** $Y_{k,j}$

$$\mathcal{H} = \left\{ f = \sum_{k=0}^{\infty} \sum_{j=1}^{N(d,k)} a_{k,j} Y_{k,j}(\cdot) \text{ s.t. } \|f\|_{\mathcal{H}}^2 := \sum_{k,j} \frac{a_{k,j}^2}{\mu_k} < \infty \right\}$$

Approximation for two-layer ReLU networks

Approximation of functions on the sphere (Bach, 2017)

- Decay of $\mu_k \leftrightarrow$ regularity of functions in the RKHS
- Polynomial decays $\mu_k \approx k^{-2\beta}$: similar to Sobolev space of order β , norm:

$$\|f\|_{\mathcal{H}} \approx \|\Delta_{\mathbb{S}^{d-1}}^{\beta/2} f\|_{L^2(\mathbb{S}^{d-1})}$$

- Leads to sufficient conditions for RKHS membership
- Rates of approximation for Lipschitz functions

Approximation for two-layer ReLU networks

Approximation of functions on the sphere (Bach, 2017)

- Decay of $\mu_k \leftrightarrow$ regularity of functions in the RKHS
- Polynomial decays $\mu_k \approx k^{-2\beta}$: similar to Sobolev space of order β , norm:

$$\|f\|_{\mathcal{H}} \approx \|\Delta_{\mathbb{S}^{d-1}}^{\beta/2} f\|_{L^2(\mathbb{S}^{d-1})}$$

- Leads to sufficient conditions for RKHS membership
- Rates of approximation for Lipschitz functions

NTK vs random features (Bietti and Mairal, 2019b)

- f has $\beta = p/2$ η -bounded derivatives $\implies f \in \mathcal{H}_{NTK}$, $\|f\|_{\mathcal{H}_{NTK}} \leq O(\eta)$
- $\beta = p/2 + 1$ needed for RF (Bach, 2017)
- $\implies \mathcal{H}_{NTK}$ is (slightly) “**larger**” than \mathcal{H}_{RF}
- Similar improvement for approximation of Lipschitz functions

Deep fully-connected ReLU networks: limitations

$$\kappa_L(x^\top y) = \underbrace{\kappa \circ \cdots \circ \kappa}_{L \text{ times}}(x^\top y)$$

Deep = Shallow (Bietti and Bach, 2021)

- RF or NTK kernels for deep and shallow networks have the same decay! (thus same \mathcal{H})
- Proof using differentiability of κ : we have $\mu_k \sim k^{d-2\nu+1}$ when

$$\begin{aligned}\kappa(1-t) &= \text{poly}(t) + c_1 t^\nu + o(t^\nu) \\ \kappa(-1+t) &= \text{poly}(t) + c_{-1} t^\nu + o(t^\nu).\end{aligned}$$

- Such expansions are preserved when taking composition with ReLU/arc-cosine kernel

Deep fully-connected ReLU networks: limitations

$$\kappa_L(x^\top y) = \underbrace{\kappa \circ \dots \circ \kappa}_{L \text{ times}}(x^\top y)$$

Deep = Shallow (Bietti and Bach, 2021)

- RF or NTK kernels for deep and shallow networks have the same decay! (thus same \mathcal{H})
- Proof using differentiability of κ : we have $\mu_k \sim k^{d-2\nu+1}$ when

$$\begin{aligned}\kappa(1-t) &= \text{poly}(t) + c_1 t^\nu + o(t^\nu) \\ \kappa(-1+t) &= \text{poly}(t) + c_{-1} t^\nu + o(t^\nu).\end{aligned}$$

- Such expansions are preserved when taking composition with ReLU/arc-cosine kernel

Consequences

- \implies kernel regime cannot explain power of depth in fully-connected nets
- \implies power of deep kernels comes from **architecture**

Deep = shallow: numerical experiments

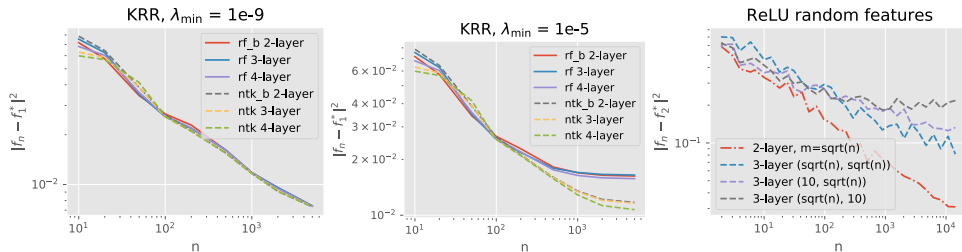


Figure 1: (left, middle) expected squared error vs sample size n for kernel ridge regression estimators with different kernels on f_1^* and with two different budgets on optimization difficulty λ_{\min} (the minimum regularization parameter allowed). (right) ridge regression with one or two layers of random ReLU features on f_2^* , with different scalings of the number of “neurons” at each layer in terms of n .

Deep = shallow: numerical experiments

MNIST

L	RF	NTK
2	98.60 ± 0.03	98.49 ± 0.02
3	98.67 ± 0.03	98.53 ± 0.02
4	98.66 ± 0.02	98.49 ± 0.01
5	98.65 ± 0.04	98.46 ± 0.02

F-MNIST

L	RF	NTK
2	90.75 ± 0.11	90.65 ± 0.07
3	90.87 ± 0.16	90.62 ± 0.08
4	90.89 ± 0.13	90.55 ± 0.07
5	90.88 ± 0.08	90.50 ± 0.05

(on 50k samples)

Approximating functions on signals: motivation

Curse of dimensionality

- Natural signals are very high-dimensional ($d \approx |\Omega|$, where Ω is the domain)
- Approximating general f^* requires exponentially large norm or very high smoothness

Approximating functions on signals: motivation

Curse of dimensionality

- Natural signals are very high-dimensional ($d \approx |\Omega|$, where Ω is the domain)
- Approximating general f^* requires exponentially large norm or very high smoothness

Adding structure: localized functions e.g., $f^*(x) = g^*(P_X[u_0])$

- With fully-connected kernel, still need norm exp. large in d
- For basic convolutional kernel, norm only scales with the dimension of the patch $P_X[u_0]$:

$$K(x, x') = \langle MP_X, MP_{X'} \rangle = \sum_{u \in \Omega} k(P_X[u], P_{X'}[u])$$

- See also Ciliberto et al. (2019) for similar part-based kernels for structured prediction

Warmup: one layer with pooling

$$K(x, x') = \langle AMP_x, AMP_{x'} \rangle_{L^2(\Omega, \mathcal{H})}$$

(\mathcal{H} : RKHS of patch kernels)

- RKHS consists of functions of the form (patches denoted $x_u = Px[u] \in \mathbb{R}^p$)

$$f(x) = \sum_{u \in \Omega} G[u](x_u), \quad G[u] \in \mathcal{H}$$

Warmup: one layer with pooling

$$K(x, x') = \langle AMP_x, AMP_{x'} \rangle_{L^2(\Omega, \mathcal{H})}$$

(\mathcal{H} : RKHS of patch kernels)

- RKHS consists of functions of the form (patches denoted $x_u = Px[u] \in \mathbb{R}^p$)

$$f(x) = \sum_{u \in \Omega} G[u](x_u), \quad G[u] \in \mathcal{H}$$

- Squared RKHS norm given by the minimum over such decompositions of

$$\|A^{-\top} G\|_{L^2(\Omega, \mathcal{H})}^2 = \|(A^{-\top} \otimes \Gamma)G\|_{L^2(\Omega) \otimes L^2(\mathbb{S}^{p-1})}^2$$

- ▶ G viewed in $L^2(\Omega) \otimes L^2(\mathbb{S}^{p-1})$ as $(u, z) \mapsto G[u](z)$
- ▶ $\Gamma = T^{-1/2}$ regularization operator of \mathcal{H} , e.g., $\Gamma = \Delta_{\mathbb{S}^{p-1}}^{\beta/2}$
- $\implies A$ (pooling) encourages smoothness of $u \mapsto G[u](z)$
- $\implies \Gamma$ (kernel) encourages smoothness of $z \mapsto G[u](z)$

Beyond one layer: empirical study

Cifar10 with full kernel (or Nyström in parentheses)

κ_1	κ_2	Test acc. (10k)	Test acc. (full)
Exp	Exp	80.5%	87.9% (84.1%)
Exp	Poly3	80.5%	87.7% (84.1%)
Exp	Poly2	79.4%	86.9% (83.4%)
Poly2	Exp	77.4%	- (81.5%)
Poly2	Poly2	75.1%	- (81.2%)
Exp	- (Lin)	74.2%	- (76.3%)

One layer is not enough

Polynomial kernel can be enough for second layer

Interlude: kernel tensor products

κ_2 **polynomial** \implies **products of patch kernels**

$$K((x_1, x_2), (x'_1, x'_2)) = k(x_1, x'_1)k(x_2, x'_2) = \langle \varphi(x_1) \otimes \varphi(x_2), \varphi(x'_1) \otimes \varphi(x'_2) \rangle_{\mathcal{H} \otimes \mathcal{H}}$$

- RKHS $\mathcal{H} \otimes \mathcal{H}$ contains closure of functions $f(x_1, x_2) = \sum_{j=1}^m f_{1,j}(x_1)f_{2,j}(x_2)$

Interlude: kernel tensor products

κ_2 **polynomial** \implies **products of patch kernels**

$$K((x_1, x_2), (x'_1, x'_2)) = k(x_1, x'_1)k(x_2, x'_2) = \langle \varphi(x_1) \otimes \varphi(x_2), \varphi(x'_1) \otimes \varphi(x'_2) \rangle_{\mathcal{H} \otimes \mathcal{H}}$$

- RKHS $\mathcal{H} \otimes \mathcal{H}$ contains closure of functions $f(x_1, x_2) = \sum_{j=1}^m f_{1,j}(x_1)f_{2,j}(x_2)$
- RKHS is often **much smaller** than a dot-product kernel on $x = (x_1, x_2)$
- Helpful for modeling **interactions** between variables/patches (Wahba, 1990; Lin, 2000; Scetbon and Harchaoui, 2020)

Interlude: kernel tensor products

κ_2 **polynomial** \implies **products of patch kernels**

$$K((x_1, x_2), (x'_1, x'_2)) = k(x_1, x'_1)k(x_2, x'_2) = \langle \varphi(x_1) \otimes \varphi(x_2), \varphi(x'_1) \otimes \varphi(x'_2) \rangle_{\mathcal{H} \otimes \mathcal{H}}$$

- RKHS $\mathcal{H} \otimes \mathcal{H}$ contains closure of functions $f(x_1, x_2) = \sum_{j=1}^m f_{1,j}(x_1)f_{2,j}(x_2)$
- RKHS is often **much smaller** than a dot-product kernel on $x = (x_1, x_2)$
- Helpful for modeling **interactions** between variables/patches (Wahba, 1990; Lin, 2000; Scetbon and Harchaoui, 2020)
- Here, the **architecture** determines which interactions matter, and **pooling** will further encourage **spatial regularities** among interaction terms

RKHS of two-layer CKN with quadratic second layer

Kernel $K(x, x') = \langle \Phi(x), \Phi(x') \rangle$, with

$$\Phi(x) = A_2 M_2 P_2 A_1 M_1 P_1 x \in L^2 \left(\Omega, (\mathcal{H} \otimes \mathcal{H})^{|S_2| \times |S_2|} \right)$$

RKHS of two-layer CKN with quadratic second layer

Kernel $K(x, x') = \langle \Phi(x), \Phi(x') \rangle$, with

$$\Phi(x) = A_2 M_2 P_2 A_1 M_1 P_1 x \in L^2 \left(\Omega, (\mathcal{H} \otimes \mathcal{H})^{|S_2| \times |S_2|} \right)$$

RKHS functions of the form

$$f(x) = \sum_{p,q \in S_2} \sum_{u,v \in \Omega} G_{pq}[u, v](x_u, x_v)$$

RKHS of two-layer CKN with quadratic second layer

Kernel $K(x, x') = \langle \Phi(x), \Phi(x') \rangle$, with

$$\Phi(x) = A_2 M_2 P_2 A_1 M_1 P_1 x \in L^2 \left(\Omega, (\mathcal{H} \otimes \mathcal{H})^{|S_2| \times |S_2|} \right)$$

RKHS functions of the form

$$f(x) = \sum_{p,q \in S_2} \sum_{u,v \in \Omega} G_{pq}[u, v](x_u, x_v)$$

Under **localization** constraint: $G_{pq} \in \text{Range}((L_p A_1 \otimes L_q A_1)^\top \text{diag}(\cdot))$



Figure 2. Display of the response of the operator E_{pq} to Dirac inputs $x = \delta_u$ centered at two different locations u . These are bumps centered on points of the $p - q$ diagonal, corresponding to interactions between two patches, at distance around $p - q$.

RKHS of two-layer CKN with quadratic second layer

Kernel $K(x, x') = \langle \Phi(x), \Phi(x') \rangle$, with

$$\Phi(x) = A_2 M_2 P_2 A_1 M_1 P_1 x \in L^2\left(\Omega, (\mathcal{H} \otimes \mathcal{H})^{|S_2| \times |S_2|}\right)$$

RKHS functions of the form

$$f(x) = \sum_{p,q \in S_2} \sum_{u,v \in \Omega} G_{pq}[u, v](x_u, x_v)$$

Under **localization** constraint: $G_{pq} \in \text{Range}((L_p A_1 \otimes L_q A_1)^\top \text{diag}(\cdot))$

RKHS norm given by the penalty

$$\sum_{p,q \in S_2} \|A_2^{-\top} \text{diag}((L_p A_1 \otimes L_q A_1)^{-\top} G_{pq})\|_{L^2(\Omega, \mathcal{H} \otimes \mathcal{H})}^2.$$

- $(L_p A_1 \otimes L_q A_1)^{-\top} G$ encourages **2D smoothness** of $(u, v) \mapsto G[u, v](z, z')$
- $A_2^{-\top}$ imposes even stronger **1D smoothness** on diagonal $u - v = p - q$

Extensions

- **Higher-order** polynomials \implies higher-order interactions
- **More layers**: also capture higher-order interactions, with different structure

Extensions

- **Higher-order** polynomials \implies higher-order interactions
- **More layers**: also capture higher-order interactions, with different structure
- Empirically, on Cifar10, 2 layers with degree-4 kernels at 2nd layer suffice for best performance

Conclusions

Benefits of convolutional kernels

- Translation invariance + deformation stability with small patches and pooling
- \implies benefits of depth for stability
- Approximation benefits of ≥ 2 layers by efficiently capturing interactions
- Limitations of depth for fully-connected models in kernel regimes

Conclusions

Benefits of convolutional kernels

- Translation invariance + deformation stability with small patches and pooling
- \implies benefits of depth for stability
- Approximation benefits of ≥ 2 layers by efficiently capturing interactions
- Limitations of depth for fully-connected models in kernel regimes

Future directions

- Empirically, any benefits of depth beyond 2 layers?
- Statistical analysis through covariance operator

Conclusions

Benefits of convolutional kernels

- Translation invariance + deformation stability with small patches and pooling
- \implies benefits of depth for stability
- Approximation benefits of ≥ 2 layers by efficiently capturing interactions
- Limitations of depth for fully-connected models in kernel regimes

Future directions

- Empirically, any benefits of depth beyond 2 layers?
- Statistical analysis through covariance operator

Perspectives: beyond kernels

- Kernels provide a nice tractable model, but a limited picture of deep learning
- Feature selection through mean-field/“active” regime, at least at first layer
- Benefits of depth beyond simple interaction models, e.g., through hierarchy

References I

- F. Bach. Breaking the curse of dimensionality with convex neural networks. *Journal of Machine Learning Research (JMLR)*, 18(19):1–53, 2017.
- A. Bietti and F. Bach. Deep equals shallow for relu networks in kernel regimes. In *Proceedings of the International Conference on Learning Representations (ICLR)*, 2021.
- A. Bietti and J. Mairal. Group invariance, stability to deformations, and complexity of deep convolutional representations. *Journal of Machine Learning Research (JMLR)*, 20(25):1–49, 2019a.
- A. Bietti and J. Mairal. On the inductive bias of neural tangent kernels. In *Advances in Neural Information Processing Systems (NeurIPS)*, 2019b.
- J. Bruna and S. Mallat. Invariant scattering convolution networks. *IEEE Transactions on Pattern Analysis and Machine Intelligence (PAMI)*, 35(8):1872–1886, 2013.
- L. Chizat, E. Oyallon, and F. Bach. On lazy training in differentiable programming. In *Advances in Neural Information Processing Systems (NeurIPS)*, 2019.
- Y. Cho and L. K. Saul. Kernel methods for deep learning. In *Advances in Neural Information Processing Systems (NIPS)*, 2009.
- C. Ciliberto, F. Bach, and A. Rudi. Localized structured prediction. In *Advances in Neural Information Processing Systems (NeurIPS)*, 2019.

References II

- T. Cohen and M. Welling. Group equivariant convolutional networks. In *International Conference on Machine Learning (ICML)*, 2016.
- A. Jacot, F. Gabriel, and C. Hongler. Neural tangent kernel: Convergence and generalization in neural networks. In *Advances in Neural Information Processing Systems (NeurIPS)*, 2018.
- R. Kondor and S. Trivedi. On the generalization of equivariance and convolution in neural networks to the action of compact groups. In *Proceedings of the International Conference on Machine Learning (ICML)*, 2018.
- Y. LeCun, B. Boser, J. S. Denker, D. Henderson, R. E. Howard, W. Hubbard, and L. D. Jackel. Backpropagation applied to handwritten zip code recognition. *Neural computation*, 1(4):541–551, 1989.
- Y. LeCun, L. Bottou, Y. Bengio, P. Haffner, et al. Gradient-based learning applied to document recognition. *Proceedings of the IEEE*, 86(11):2278–2324, 1998.
- J. Lee, Y. Bahri, R. Novak, S. S. Schoenholz, J. Pennington, and J. Sohl-Dickstein. Deep neural networks as gaussian processes. In *Proceedings of the International Conference on Learning Representations (ICLR)*, 2018.
- Y. Lin. Tensor product space anova models. *Annals of Statistics*, 28(3):734–755, 2000.
- J. Mairal. End-to-End Kernel Learning with Supervised Convolutional Kernel Networks. In *Advances in Neural Information Processing Systems (NIPS)*, 2016.

References III

- J. Mairal, P. Koniusz, Z. Harchaoui, and C. Schmid. Convolutional kernel networks. In *Advances in Neural Information Processing Systems (NIPS)*, 2014.
- S. Mallat. Group invariant scattering. *Communications on Pure and Applied Mathematics*, 65(10): 1331–1398, 2012.
- R. M. Neal. *Bayesian learning for neural networks*. Springer, 1996.
- A. Rahimi and B. Recht. Random features for large-scale kernel machines. In *Advances in Neural Information Processing Systems (NIPS)*, 2007.
- M. Scetbon and Z. Harchaoui. Harmonic decompositions of convolutional networks. In *Proceedings of the International Conference on Machine Learning (ICML)*, 2020.
- V. Shankar, A. Fang, W. Guo, S. Fridovich-Keil, L. Schmidt, J. Ragan-Kelley, and B. Recht. Neural kernels without tangents. *arXiv preprint arXiv:2003.02237*, 2020.
- K. Simonyan and A. Zisserman. Very deep convolutional networks for large-scale image recognition. In *Proceedings of the International Conference on Learning Representations (ICLR)*, 2014.
- G. Wahba. *Spline models for observational data*, volume 59. Siam, 1990.

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

$$x_k(u) = P_k A_{k-1} \varphi_1(x_{k-1})(u)$$

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

Discretization and signal preservation

- \bar{x}_k : subsampling factor s_k after pooling with scale $\sigma_k \approx s_k$:

$$\bar{x}_k[n] = A_k M_k P_k \bar{x}_{k-1}[ns_k]$$

Discretization and signal preservation

- \bar{x}_k : subsampling factor s_k after pooling with scale $\sigma_k \approx s_k$:

$$\bar{x}_k[n] = A_k M_k P_k \bar{x}_{k-1}[ns_k]$$

- **Claim:** We can recover \bar{x}_{k-1} from \bar{x}_k if **subsampling** $s_k \leq$ **patch size**

Discretization and signal preservation

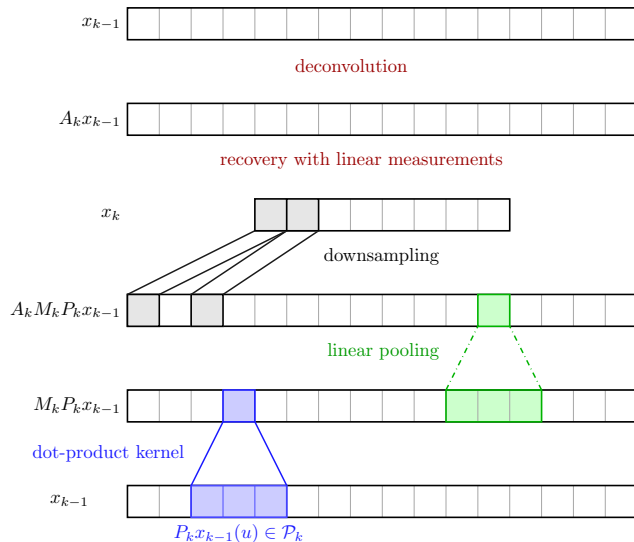
- \bar{x}_k : subsampling factor s_k after pooling with scale $\sigma_k \approx s_k$:

$$\bar{x}_k[n] = A_k M_k P_k \bar{x}_{k-1}[ns_k]$$

- **Claim:** We can recover \bar{x}_{k-1} from \bar{x}_k if **subsampling** $s_k \leq$ **patch size**
- **How?** Kernels! Recover patches with **linear functions** (contained in RKHS)

$$\langle f_w, M_k P_k x(u) \rangle = f_w(P_k x(u)) = \langle w, P_k x(u) \rangle$$

Signal recovery: example in 1D



Beyond the translation group

Global invariance to other groups?

- Rotations, reflections, roto-translations, ...
- Group action $L_g x(u) = x(g^{-1}u)$
- **Equivariance** in inner layers + **(global) pooling** in last layer
- Similar construction to Cohen and Welling (2016); Kondor and Trivedi (2018)

G-equivariant layer construction

- Feature maps $x(u)$ defined on $u \in G$ (G : locally compact group)
 - ▶ Input needs special definition when $G \neq \Omega$

- **Patch extraction:**

$$Px(u) = (x(uv))_{v \in S}$$

- **Non-linear mapping:** equivariant because pointwise!
- **Pooling** (μ : left-invariant Haar measure):

$$Ax(u) = \int_G x(uv)h(v)d\mu(v) = \int_G x(v)h(u^{-1}v)d\mu(v)$$

Group invariance and stability

Roto-translation group $G = \mathbb{R}^2 \rtimes SO(2)$ (translations + rotations)

- **Stability** w.r.t. translation group
- **Global invariance** to rotations (only global pooling at final layer)
 - ▶ Inner layers: patches and pooling only on translation group
 - ▶ Last layer: global pooling on rotations
 - ▶ Cohen and Welling (2016): pooling on rotations in inner layers hurts performance on Rotated MNIST