Approximation and Generalization with Convolutional Kernels

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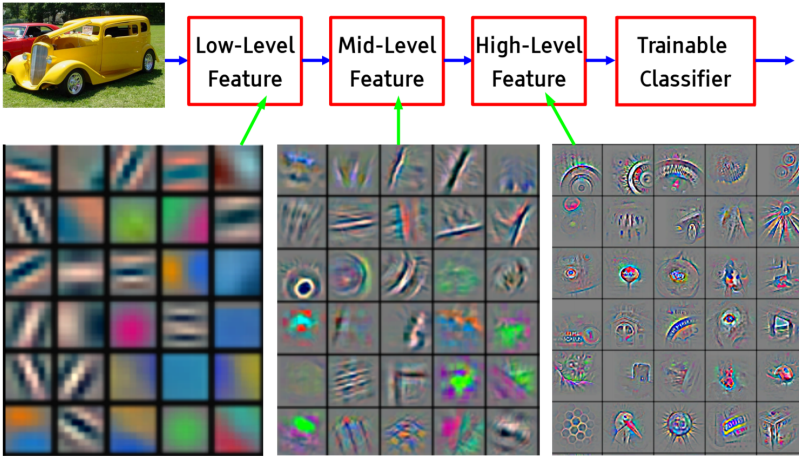
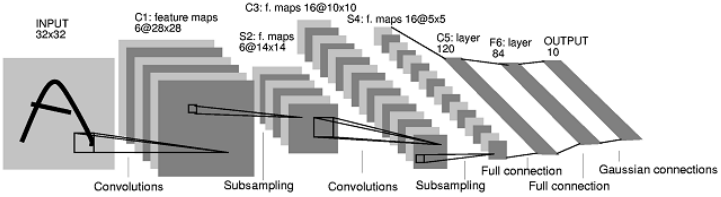
Convolutional networks

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

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** to zero training error with (stochastic) gradient descent!

Which function does optimization find?

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A functional space viewpoint

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

$$\min_f \Omega(f) \quad \text{s.t.} \quad y_i = f(x_i), \quad i = 1, \dots, n$$

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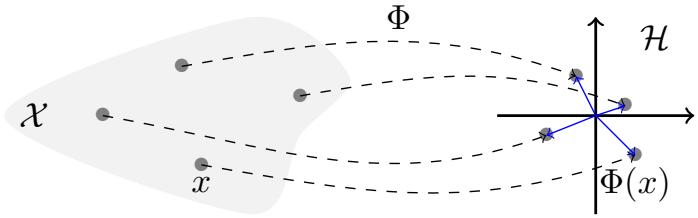
What is an appropriate functional space / norm?

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 $K = [K(x_i, x_j)]_{ij} \in \mathbb{R}^{N \times N}$

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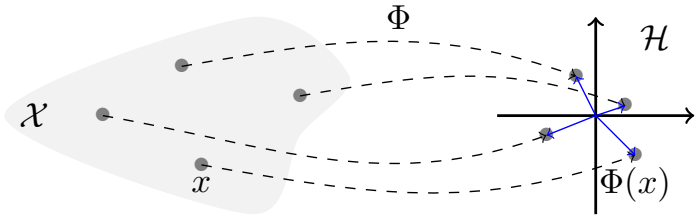


Clean and well-developed theory

- 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**

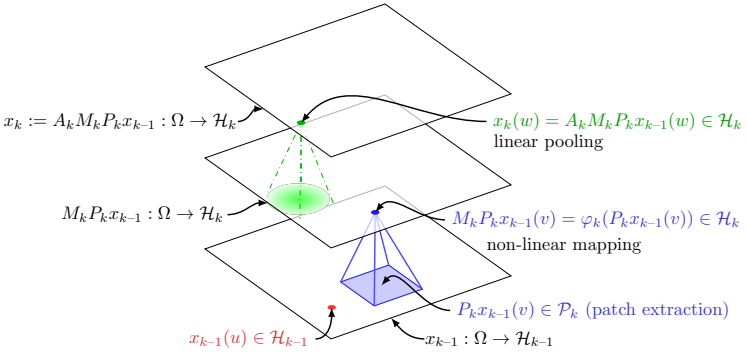
$$K(x, x') = \langle \Phi(x), \Phi(x') \rangle \text{ with } \Phi(x) = \varphi_2(\varphi_1(x))$$

- *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

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

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

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

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

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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

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

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

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RF and NTK extend to deep architectures

Approximation and regularization with kernels

What functions can we represent with a bounded RKHS norm?

Translation-invariant kernel: $K(x, y) = \kappa(x - y)$

$$\|f\|_{\mathcal{H}}^2 = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \frac{|\hat{f}(\omega)|^2}{\hat{\kappa}(\omega)} d\omega.$$

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Dot-product kernel: $K(x, y) = \kappa(\langle x, y \rangle)$ (*e.g.*, RF/NTK for fully-connected networks)

$$f(x) = \sum_{k \geq 0} \sum_{j=1}^{N(d,k)} f_{k,j} Y_{k,j}(x), \quad x \in \mathbb{S}^{d-1}$$

$$\|f\|_{\mathcal{H}}^2 = \sum_{k \geq 0} \sum_{j=1}^{N(d,k)} \frac{f_{k,j}^2}{\mu_k(\kappa)}.$$

Example: polynomials decays $\mu_k \sim k^{-2\beta}$ (*e.g.*, ReLU RF/NTK) $\Leftrightarrow \|f\|_{\mathcal{H}} \approx \|\nabla^\beta f\|_{L^2(\mathbb{S}^{d-1})}$

Issues with fully-connected kernels

- Architecture/depth plays minor role (Bietti and Bach, 2021)
- Curse of dimensionality (unless target is very smooth)

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Learning on high-dimensional signals/images

- Architecture is important (*e.g.*, for stability, Bietti and Mairal, 2019a)
- **Q: How do convolutional kernels break the curse of dimensionality?**

Simple structured kernels on patches

- Signal x: "pixels" $x[u] \in \mathbb{R}^p$ for $u \in \Omega = \{0, \dots, |\Omega| - 1\}$ (Ω circular)
- Patches $x_u = (x[u + v])_{v \in S} \in \mathbb{R}^{p|S|}$, *e.g.*, $S = \{-1, 0, 1\}$
- Dot-product kernel k on patches with RKHS $\mathcal{H}$

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One-layer convolutional kernel, no pooling

$$K(x, x') = \sum_{u \in \Omega} k(x_u, x'_u)$$

Functions in RKHS: $f(x) = \sum_u g_u(x_u)$. **Penalty**: $\|g\|^2_{L^2(\Omega, \mathcal{H})} = \sum_u \|g_u\|^2_{\mathcal{H}}$

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- Much smaller RKHS than fully-connected architecture!
- For target $f^*(x) = g^*(x_{\bar{u}})$, breaks curse of dimensionality ($p|\Omega| \to p|S|$)
- Still missing: invariance, expressivity on larger visual neighborhoods

One-layer convolutional kernel with pooling

- $h[u]$: pooling filter (*e.g.*, Gaussian)
- A_h: (circular) convolution operator $A_h x[u] = \sum_{v \in \Omega} h[u-v]x[v]$
- $\Phi(x)[u] = \varphi(x_u) \in \mathcal{H}$ (φ: kernel mapping of k)

1-layer convolutional kernel

$$K(x, x') = \sum_{u \in \Omega} \sum_{v, v'} h[u-v]h[u-v']k(x_v, x'_{v'}) = \langle A_h \Phi(x), A_h \Phi(x') \rangle_{L^2(\Omega, \mathcal{H})}$$

Functions in RKHS: Same functions $f(x) = \sum_u g[u](x_u)$, different **penalty**: $\|A_h^\dagger g\|^2_{L^2(\Omega,\mathcal{H})}$.

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$\implies$ Encourages spatial smoothness: for $g_z[u] := g[u](z)$, we have

$$\widehat{A_h^\dagger g_z}[w] = \frac{\hat{g}_z[w]}{\hat{h}[w]}$$

Large pooling $\leftrightarrow$ fast decay of $\hat{h}[w]$ $\leftrightarrow$ stronger penalty on high frequencies of g_z.

Generalization benefits of pooling

Translation-invariant target $f^*(x) = \sum_u g(x_u)$, with $g \in \mathcal{H}$.

Learn using kernel K_h with pooling with filter $h \geq 0$, $\|h\|_1 = 1$, *e.g.*:

- **no pooling**: $h[u] = \delta_{u,0}$
- **global pooling**: $h[u] = 1/|\Omega|$
- $A_h(g, \ldots, g) = (g, \ldots, g) \implies$ **same RKHS norm** for any h!

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Basic generalization bound with 1-Lipschitz loss on $\mathcal{F} = \{\|f\|_{K_h} \leq B\}$

$$\mathbb{E}\, L(f_n) - \min_{f \in \mathcal{F}} L(f) \lesssim \frac{B\sqrt{\mathbb{E}_x[K_h(x,x)]}}{\sqrt{n}}$$

Under simple data models, $\mathbb{E}_x[k(x_u, x_u)] = 1$, $\mathbb{E}_x[k(x_u, x_v)] \leq \epsilon \ll 1$ for $u \neq v$

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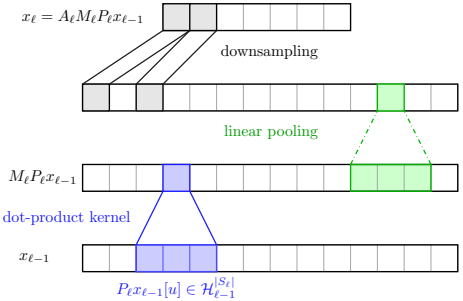
- General h: $\mathbb{E}[K_h(x,x)] \leq |\Omega|\|h\|_2^2 + \epsilon|\Omega|(1 - \|h\|_2^2)$

More layers

- Same construction, replace $x \in L^2(\Omega, \mathbb{R}^p)$ by $A\Phi(x) \in L^2(\Omega, \mathcal{H})$
- Dot-product kernel can still be defined with inputs in a Hilbert space

$$K(x, x') = \langle \Psi(x), \Psi(x') \rangle, \qquad \text{with } \Psi(x) = A_L M_L P_L \cdots A_1 M_1 P_1 x$$



P_ℓ with patch shape S_ℓ, A_ℓ with Gaussian pooling h_ℓ at scale σ_ℓ

Some experiments on Cifar10

2-layers, 3x3 patches, pooling/downsampling sizes (2,5). Patch kernels κ_1, κ_2.

κ_1	κ_2	Test acc. (10k examples)	Test acc. (50k examples)
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%)

In parentheses: Nyström approximation of the kernel (Mairal, 2016) with [256,4096] filters, instead of the full kernel.

Two-layer convolutional kernel

- Quadratic patch kernel $k_2(z, z') = (z^\top z')^2 = \langle z \otimes z, z' \otimes z' \rangle_{(\mathcal{H} \otimes \mathcal{H})^{|S_2| \times |S_2|}}$
- $\mathcal{H} \otimes \mathcal{H}$: contains functions $g(x_u, x_v)$ of 2 patches (Wahba, 1990)

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RKHS of 2-layer convolutional kernel (patch size $|S_2| = 1$): Contains functions

$$f(x) = \sum_{u,v\in\Omega} G[u, v](x_u, x_v),$$

with $G[u, v] = 0$ if $|u - v| > \text{diam}(\text{supp}(h_1))$. **Penalty**:

$$\|A_2^\dagger \,\text{diag}((A_1 \otimes A_1)^\dagger G)\|^2_{L^2(\Omega_2, \mathcal{H}\otimes\mathcal{H})}$$

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- $(A_1 \otimes A_1)^\dagger$: encourages 2D smoothness of "image" $G[u, v]$, bandwidth σ_1
- $A_2^\dagger$: encourage 1D smoothness along diagonal of G, bandwidth σ_2
- $\sigma_1 > \sigma_2 \implies G[u, v]$ can depend more strongly on $u - v$ than u or v

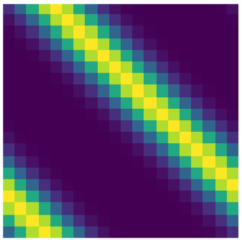
Two-layer convolutional kernel

RKHS of 2-layer convolutional kernel (any patch size $|S_2|$): Contains functions

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

with $G_{pq}[u,v] = 0$ if $|u - v - (p - q)| > \mathrm{diam}(\mathrm{supp}(h_1))$. **Penalty**:

$$\sum_{p,q \in S_2} \|A_2^\dagger \, \mathrm{diag}((L_p A_1 \otimes L_q A_1)^\dagger G_{pq})\|^2_{L^2(\Omega_2, \mathcal{H} \otimes \mathcal{H})}$$



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"Variance" term: $\sqrt{\mathbb{E}_x[K(x,x)]} \leq |\Omega||S_2|^2 \sum_v \langle h_2, L_v h_w \rangle \langle h_1, L_v h_1 \rangle^2 + O(\epsilon)$

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"Variance" term: $\sqrt{\mathbb{E}_x[K(x,x)]} \leq |\Omega||S_2|^2 \sum_v \langle h_2, L_v h_w \rangle \langle h_1, L_v h_1 \rangle^2 + O(\epsilon)$

Extensions:

- κ_2 higher-degree polynomial $\implies$ higher-order interactions
- more layers: also higher-order interactions, but more structured penalty

More experiments: 3 layers

3-layers, 3x3 patches, pooling/downsampling sizes (2,2,2), patch kernels κ_1, κ_2 and κ_3.

κ_1	κ_2	κ_3	Test ac. (10k)	Test ac. (50k)
Exp	Exp	Exp	80.7%	**88.2%**
Exp	Poly2	Poly2	80.5%	87.9%
Exp	Poly4	Lin	80.2%	-
Exp	Lin	Poly4	79.2%	-
Exp	Lin	Lin	74.1%	-

Shankar et al. (2020) also obtains 88.2% but using 10 layers

More experiments: larger patches

2-layers, 3x3 patches at first layer, pooling/downsampling sizes (2,5)
patch kernels κ_1/κ_2 and different patch sizes at the second layer.

κ_1	κ_2	$\lvert S_2\rvert$	Test ac. (10k)	Test ac. (50k)
Exp	Exp	5x5	81.1%	**88.3%**
Exp	Poly4	5x5	81.3%	**88.3%**
Exp	Poly3	5x5	81.1%	-
Exp	Poly2	7x7	80.1%	-
Exp	Poly2	5x5	80.1%	-
Exp	Poly2	3x3	79.4%	-
Exp	Poly2	1x1	76.3%	-
ReLU	ReLU	3x3	78.51%	86.6%
NTK	(NTK)	3x3	79.24%	87.2%

Conclusion and perspectives

Learning with convolutional kernels

- Additive interaction models on patches
- Pooling is important for encouraging spatial regularities, and better sample complexity
- 2/3 layers seems enough on Cifar10

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What is missing compared to full DL?

- **Feature selection**: avoid dependence on dimensionality (of the patch) by finding good weights at the first layer
  - Bach (2017)
  - Finding good filters (e.g. Gabors) could also avoid the need for explicit pooling
- **Hierarchy**: efficiently find hierarchical **compositions** of functions
  - Allen-Zhu and Li (2020): SGD can do it under strong assumptions

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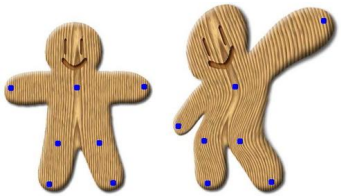
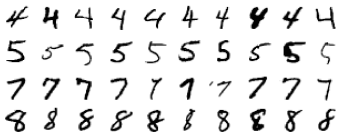
Stability to deformations

Deformations

- $\tau : \Omega \to \Omega$: 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)

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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
- $C_2 \to 0$: 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)

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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 $x_1, \dots, x_n$

- $x_0 : \Omega \to \mathcal{H}_0$: 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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$$P_k x_{k-1}$$

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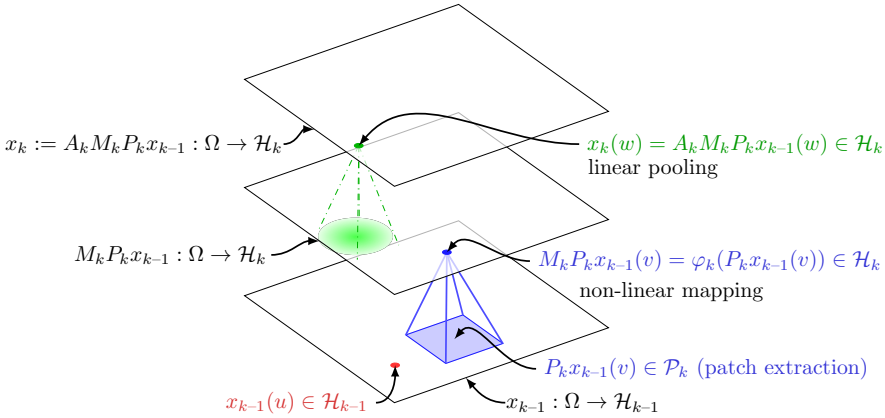
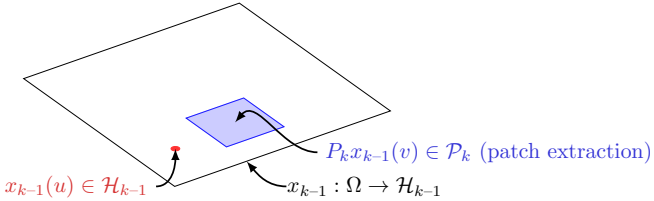
Goal: control stability of these operators through their norms

CKN construction



Patch extraction operator P_k

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



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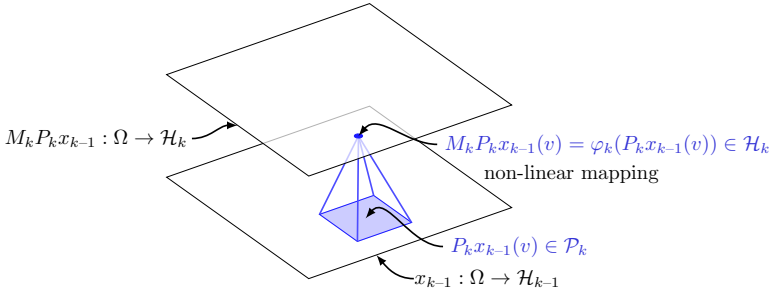
- S_k: patch shape, e.g. box
- P_k is **linear**, and **preserves the L^2 norm**: $\|P_k x_{k-1}\| = \|x_{k-1}\|$

Non-linear mapping operator M_k

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



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- $\varphi_k : \mathcal{P}_k \to \mathcal{H}_k$ 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**:

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

$\kappa_k(u) = \sum_{j=0}^{\infty} b_j u^j$ 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**

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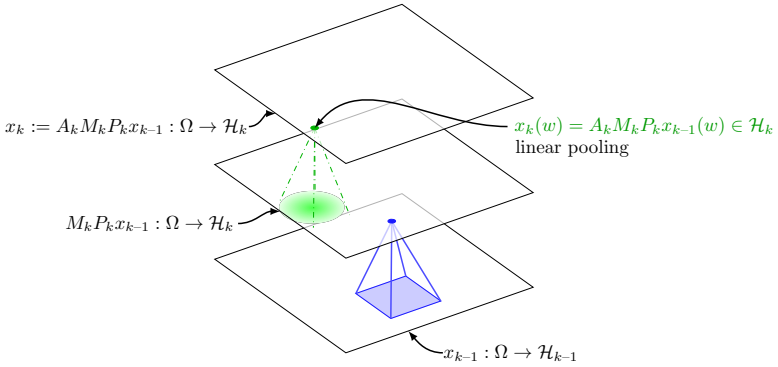
Examples

- $\kappa_{\exp}(\langle z, z'\rangle) = e^{\langle z, z'\rangle - 1}$ (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

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



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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**: $\|A_k\| \leq 1$

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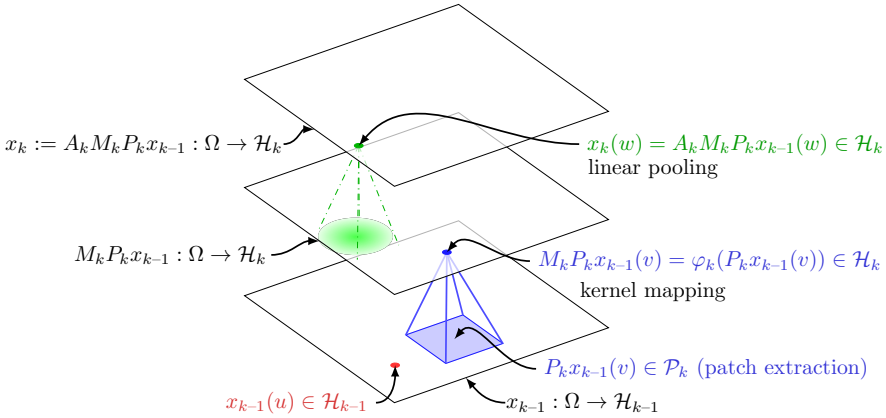
- **linear, non-expansive operator**: $\|A_k\| \leq 1$
- In practice: **discretization**, sampling at resolution σ_k after pooling
- "Preserves information" when **subsampling** $\leq$ **patch size**

Recap: P_k, M_k, A_k



Multilayer construction

Assumption on x_0

- x_0 is typically a **discrete** signal 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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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).

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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

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

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* $\|\nabla\tau\|_\infty \leq 1/2$

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

Comparison with random feature CKN on deformed MNIST digits:

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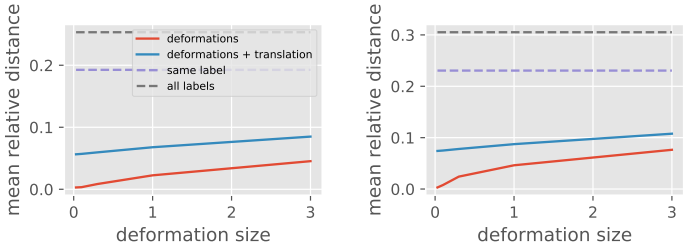

(a) CKN (b) NTK