Invariance and Stability to Deformations of Deep Convolutional Representations

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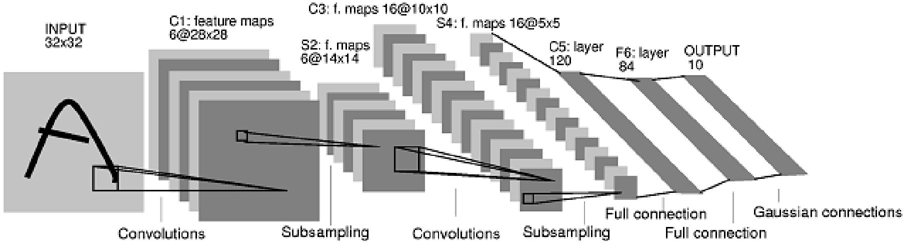
Success of deep convolutional networks



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

Understanding deep convolutional representations

- Are they **stable to deformations**?
- How can we achieve **invariance to transformation groups**?
- Do they **preserve signal information**?
- What are good measures of **model complexity**?

A kernel perspective

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

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- Learning with a positive definite kernel $K(x, x') = \langle \Phi(x), \Phi(x') \rangle$
- Here, we construct **convolutional kernels**, following Mairal (2016)
  - Good empirical performance on image tasks using kernel approximations (Mairal et al., 2014; Mairal, 2016)
  - RKHS contains CNNs, leads to good regularizers (Bietti and Mairal, 2019a; Bietti et al., 2019)
  - (Also related to *neural tangent kernels* for CNNs (Bietti and Mairal, 2019b))

A kernel perspective

Why? Separate learning from representation: $f(x) = \langle f, \Phi(x) \rangle$

- $\Phi(x)$: CNN **architecture** (stability, invariance, signal preservation)
- f: CNN **model**, learning, generalization through RKHS norm $\|f\|$

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

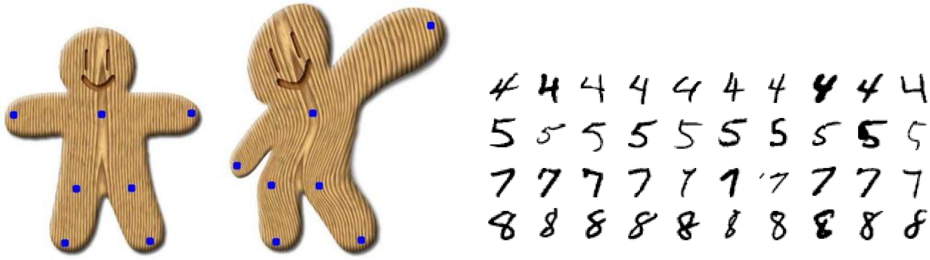
- $\|f\|$ **controls both stability and model complexity**!

  $\rightarrow$ discriminating small perturbations requires large $\|f\|$

  $\rightarrow$ learning stable functions may be "easier"

A signal processing perspective

- Consider images defined on a **continuous** domain $\Omega = \mathbb{R}^2$.
- $\tau : \Omega \to \Omega$: C^1-diffeomorphism.
- $L_\tau x(u) = x(u - \tau(u))$: action operator.
- Much richer group of transformations than translations.



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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.

Outline

A generic deep convolutional representation

- $x_0 : \Omega \to \mathcal{H}_0$: 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

$$P_k x_{k-1}$$

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

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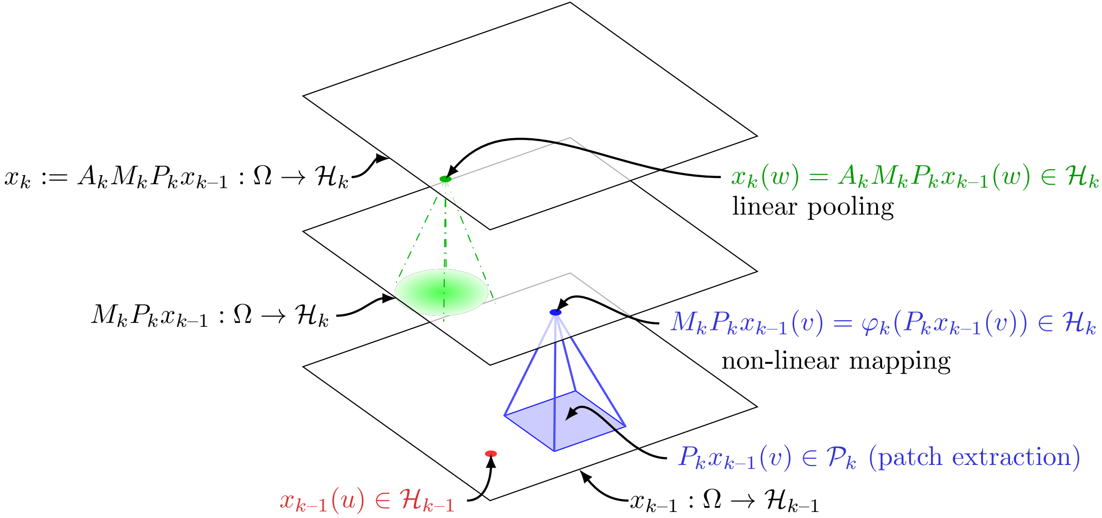
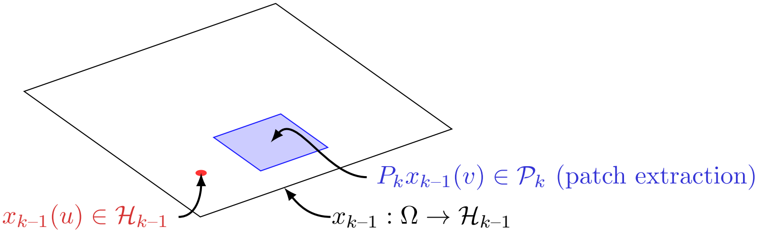
  - A_k: (linear, Gaussian) **pooling** operator at scale σ_k

A generic deep convolutional representation



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

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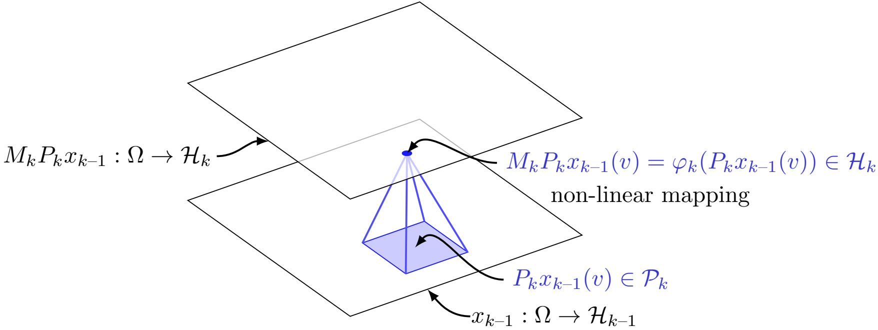

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- $\varphi_k : \mathcal{P}_k \to \mathcal{H}_k$ pointwise non-linearity on patches (kernel map)
- We assume **non-expansivity**: for $z, z' \in \mathcal{P}_k$

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

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

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- (at the cost of paying $\prod_k \rho_k$ later)

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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- $\implies$ **non-expansive**
- Examples:
  - $\kappa_{\text{exp}}(\langle z, z'\rangle) = e^{\langle z, z'\rangle - 1}$ (Gaussian kernel on the sphere)
  - $\kappa_{\text{inv-poly}}(\langle z, z'\rangle) = \frac{1}{2 - \langle z, z'\rangle}$
  - arc-cosine kernel of degree 1 (random features with ReLU activation)

φ_k from kernels: CKNs approximation

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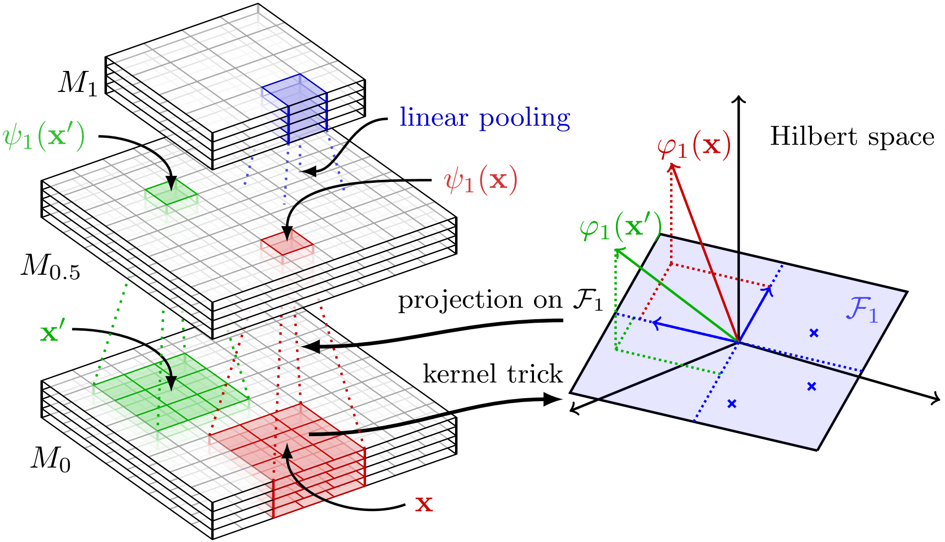
Convolutional Kernel Networks approximation (Mairal, 2016):

- Approximate $\varphi_k(z)$ by **projection** on $span(\varphi_k(z_1), \ldots, \varphi_k(z_p))$ (Nystrom)
- Leads to **tractable**, p-dimensional representation $\psi_k(z)$
- Norm is preserved, and projection is non-expansive:

$$\begin{aligned} \|\psi_k(z) - \psi_k(z')\| &= \|\Pi_k \varphi_k(z) - \Pi_k \varphi_k(z')\| \\ &\leq \|\varphi_k(z) - \varphi_k(z')\| \leq \|z - z'\| \end{aligned}$$

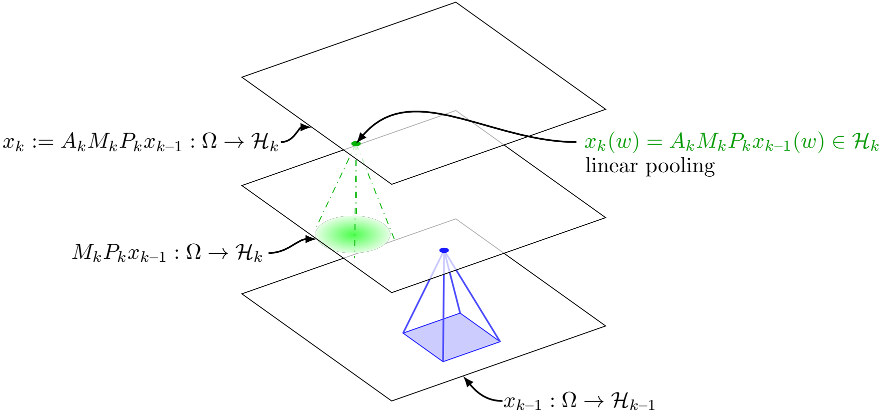
- Anchor points $z_1, \ldots, z_p$ ($\approx$ filters) can be **learned from data** (K-means or backprop)

φ_k from kernels: CKNs approximation



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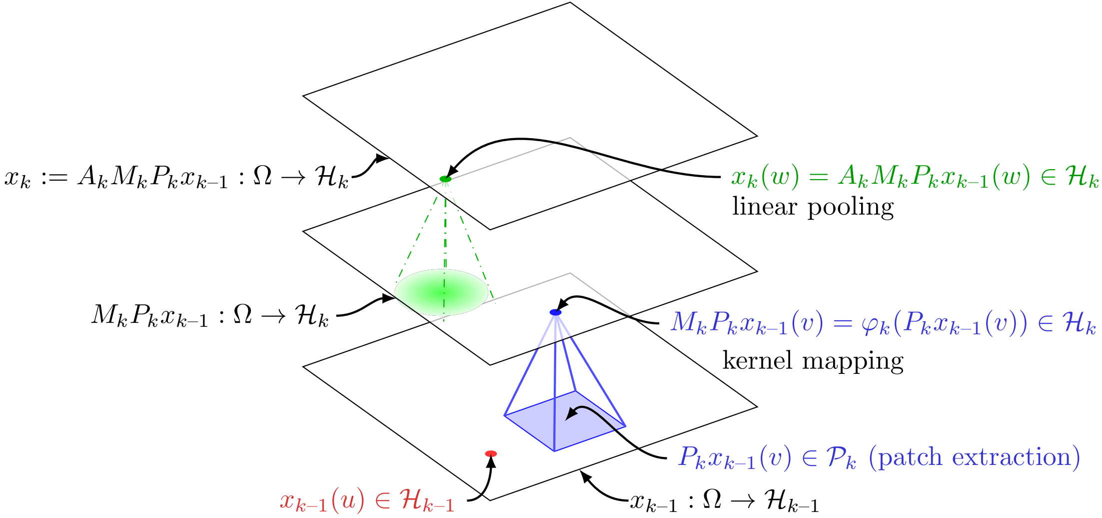
- h_{σ_k}: pooling filter at scale σ_k
- $h_{\sigma_k}(u) := \sigma_k^{-d} h(u/\sigma_k)$ with $h(u)$ **Gaussian**
- **linear, non-expansive operator**: $\|A_k\| \leq 1$

Recap: P_k, M_k, A_k



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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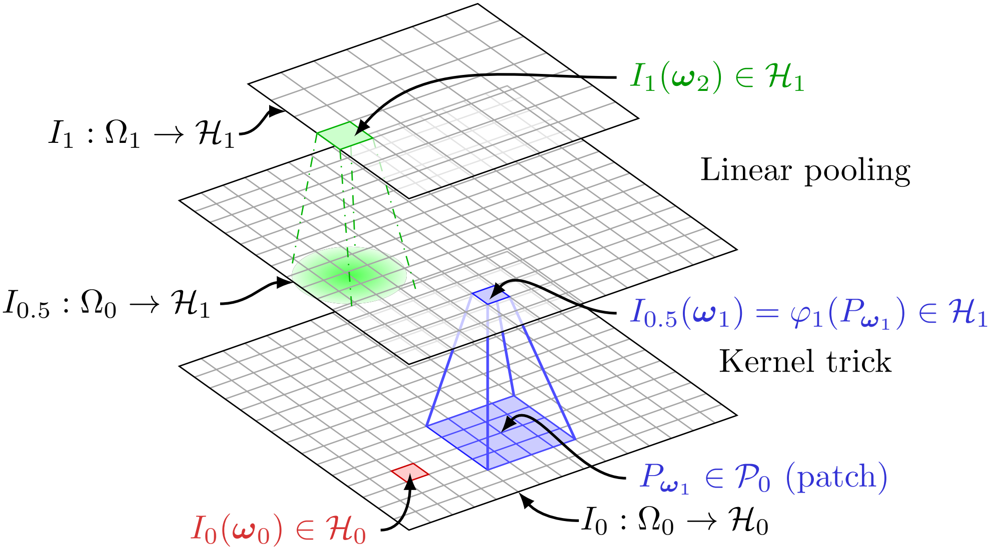
Prediction layer

- e.g., linear $f(x) = \langle w, \Phi_n(x) \rangle$.
- "linear kernel" $\mathcal{K}(x, x') = \langle \Phi_n(x), \Phi_n(x') \rangle = \int_\Omega \langle x_n(u), x'_n(u) \rangle du$.

Discretization and signal preservation



Discretization and signal preservation

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

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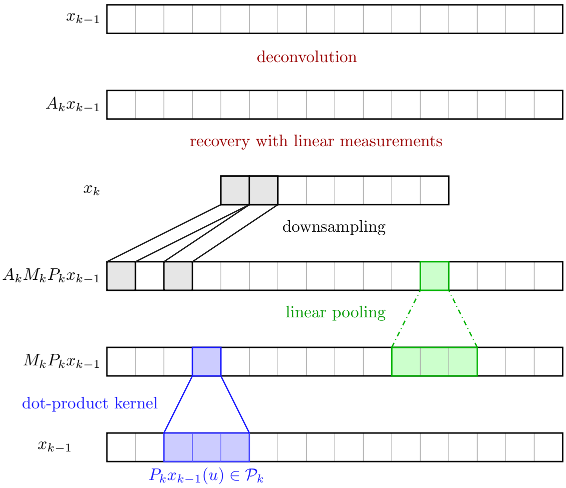
- **How**? Kernels! Recover patches with **linear functions** (contained in RKHS)

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

Signal recovery: example in 1D



Outline

Stability to deformations: definitions

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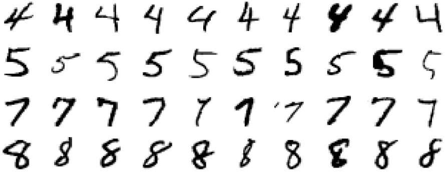

- Studied for wavelet-based scattering transform (Mallat, 2012; Bruna and Mallat, 2013)

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Warmup: translation invariance

- Representation:

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- Adapt to **current layer resolution**, patch size controlled by σ_{k-1}:

$$\|[P_k A_{k-1}, L_\tau]\| \leq C_{1,\beta} \|\nabla \tau\|_\infty \qquad \sup_{u \in S_k} |u| \leq \beta \sigma_{k-1}$$

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- $C_{1,\beta}$ grows as $\beta^{d+1} \implies$ more stable with **small patches** (e.g., 3x3, VGG et al.)

Stability to deformations: final result

Theorem

If $\|\nabla \tau\|_\infty \leq 1/2$,

$$\|\Phi_n(L_\tau x) - \Phi_n(x)\| \leq \left(C_{1,\beta} \left(n + 1 \right) \|\nabla \tau\|_\infty + \frac{C_2}{\sigma_n} \|\tau\|_\infty \right) \|x\|$$

- translation invariance: large σ_n
- stability: small patch sizes
- signal preservation: subsampling factor $\approx$ patch size
- $\Longrightarrow$ **needs several layers**

Stability to deformations: final result

Theorem

If $\|\nabla\tau\|_\infty \leq 1/2$,

$$\|\Phi_n(L_\tau x) - \Phi_n(x)\| \leq \prod_k \rho_k \left(C_{1,\beta}\,(n+1)\,\|\nabla\tau\|_\infty + \frac{C_2}{\sigma_n}\|\tau\|_\infty \right) \|x\|$$

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- (also valid for generic CNNs with ReLUs: multiply by $\prod_k \rho_k = \prod_k \|W_k\|$, but no direct signal preservation).

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

Outline

RKHS of patch kernels K_k

$$K_k(z, z') = \|z\|\|z'\|\kappa\left(\frac{\langle z, z'\rangle}{\|z\|\|z'\|}\right), \qquad \kappa(u) = \sum_{j=0}^{\infty} b_j u^j$$

- RKHS contains **homogeneous functions**:

$$f : z \mapsto \|z\|\sigma(\langle g, z\rangle/\|z\|)$$

Homogeneous version of (Zhang et al., 2016, 2017)

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$$f : z \mapsto \|z\| \sigma(\langle g, z \rangle / \|z\|)$$

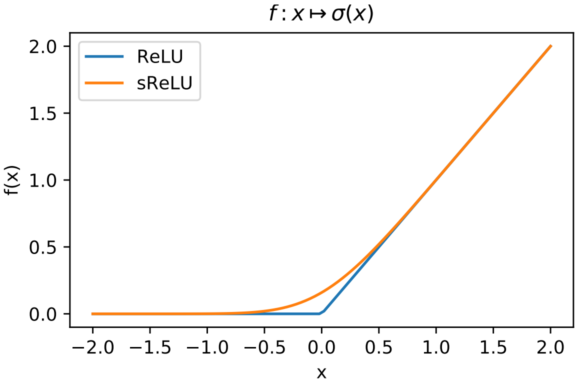
- **Smooth activations**: $\sigma(u) = \sum_{j=0}^{\infty} a_j u^j$
- Norm: $\|f\|_{\mathcal{H}_k}^2 \leq C_\sigma^2(\|g\|^2) = \sum_{j=0}^{\infty} \frac{a_j^2}{b_j} \|g\|^2 < \infty$

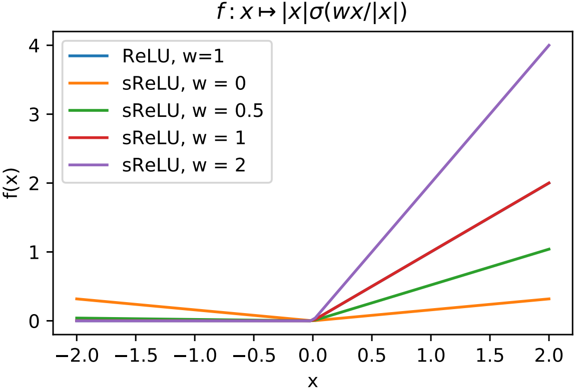
Homogeneous version of (Zhang et al., 2016, 2017)

RKHS of patch kernels K_k

Examples:

- $\sigma(u) = u$ (linear): $C^2_\sigma(\lambda^2) = O(\lambda^2)$
- $\sigma(u) = u^p$ (polynomial): $C^2_\sigma(\lambda^2) = O(\lambda^{2p})$
- $\sigma \approx$ sin, sigmoid, smooth ReLU: $C^2_\sigma(\lambda^2) = O(e^{c\lambda^2})$





Constructing a CNN in the RKHS $\mathcal{H}_\mathcal{K}$

- Consider a CNN with filters $W_k^{ij}(u), u \in S_k$
- "Smooth homogeneous" activations σ
- The CNN can be constructed hierarchically in $\mathcal{H}_\mathcal{K}$
- Norm upper bound:

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

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

- Linear layers: product of spectral norms

Link with generalization

- Simple bound on Rademacher complexity for linear/kernel methods:

$$\mathcal{F}_B = \{f \in \mathcal{H}_\mathcal{K}, \|f\|_\mathcal{H} \leq B\} \implies \mathrm{Rad}_N(\mathcal{F}_B) \leq O\left(\frac{BR}{\sqrt{N}}\right)$$

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- Leads to margin bound $O(\|\hat{f}_N\|_\mathcal{H} R/\gamma\sqrt{N})$ for a learned CNN $\hat{f}_N$ with margin (confidence) $\gamma > 0$
- Related to generalization bounds for neural networks based on **product of spectral norms** (*e.g.*, Bartlett et al., 2017; Neyshabur et al., 2018)

Outline

Regularizing with the RKHS norm in practice

Deep learning struggles with **small datasets** and **adversarial examples**.

(Bietti, Mialon, Chen, and Mairal, 2019)

Regularizing with the RKHS norm in practice

Can we obtain better models through regularization?

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$$\|f\|_{\mathcal{H}} \geq \sup_{x, \|\delta\| \leq 1} \langle f, \Phi(x + \delta) - \Phi(x) \rangle_{\mathcal{H}} \quad \text{(adversarial perturbations)}$$

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- Best performance by combining upper + lower bound approaches

(Bietti, Mialon, Chen, and Mairal, 2019)

Regularizing with the RKHS norm in practice

Can we obtain better models through regularization?

Table 2. Regularization on 300 or 1 000 examples from MNIST, using deformations from Infinite MNIST. $(*)$ indicates that random deformations were included as training examples, while $\|f\|_\tau^2$ and $\|D_\tau f\|^2$ use them as part of the regularization penalty.

Method	300 VGG	1k VGG
Weight decay	89.32	94.08
SN projection	90.69	95.01
grad-ℓ_2	93.63	96.67
$\|f\|_\delta^2$ penalty	94.17	96.99
$\|\nabla f\|^2$ penalty	94.08	96.82
Weight decay $(*)$	92.41	95.64
grad-ℓ_2 $(*)$	95.05	97.48
$\|D_\tau f\|^2$ penalty	94.18	96.98
$\|f\|_\tau^2$ penalty	94.42	97.13
$\|f\|_\tau^2 + \|\nabla f\|^2$	94.75	97.40
$\|f\|_\tau^2 + \|f\|_\delta^2$	95.23	**97.66**
$\|f\|_\tau^2 + \|f\|_\delta^2$ $(*)$	**95.53**	**97.56**
$\|f\|_\tau^2 + \|f\|_\delta^2$ + SN proj	95.20	**97.60**
$\|f\|_\tau^2 + \|f\|_\delta^2$ + SN proj $(*)$	**95.40**	**97.77**

(Bietti, Mialon, Chen, and Mairal, 2019)

Regularizing with the RKHS norm in practice

Can we obtain better models through regularization?

Table 3. Regularization on protein homology detection tasks, with or without data augmentation (DA). Fixed hyperparameters are selected using the first half of the datasets, and we report the average auROC50 score on the second half.

Method	No DA	DA
No weight decay	0.446	0.500
Weight decay	0.501	0.546
SN proj	0.591	**0.632**
PGD-ℓ_2	0.575	0.595
grad-ℓ_2	0.540	0.552
$\|f\|_\delta^2$	**0.600**	0.608
$\|\nabla f\|^2$	0.585	0.611
PGD-ℓ_2 + SN proj	**0.596**	**0.627**
grad-ℓ_2 + SN proj	0.592	**0.624**
$\|f\|_\delta^2$ + SN proj	**0.630**	**0.644**
$\|\nabla f\|^2$ + SN proj	**0.603**	**0.625**

(Bietti, Mialon, Chen, and Mairal, 2019)

Regularization for robustness

- Robust optimization yields another lower bound (hinge/logistic loss)

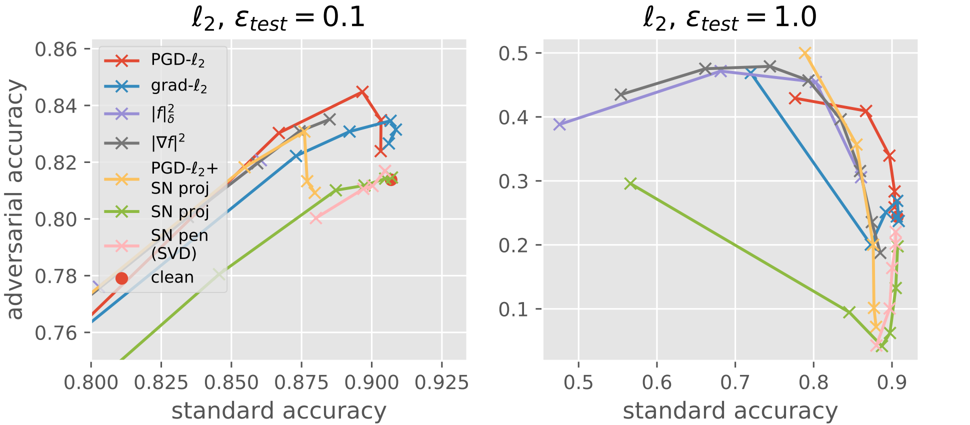
$$\frac{1}{N}\sum_{i=1}^{N}\sup_{\|\delta\|_2\leq\epsilon}\ell(y_i, f(x_i+\delta)) \leq \frac{1}{N}\sum_{i=1}^{N}\ell(y_i, f(x_i)) + \epsilon\|f\|_{\mathcal{H}}$$

- Controlling $\|f\|_{\mathcal{H}}$ allows a more **global** form of robustness
- Leads to margin bounds for *adversarial generalization* with ℓ_2 perturbations
  - Using $\|f\|_{\mathcal{H}} \geq \|f\|_{\text{Lip}}$ near the margin
- But, may cause a loss in accuracy in practice

(Bietti, Mialon, Chen, and Mairal, 2019)

Regularization for robustness

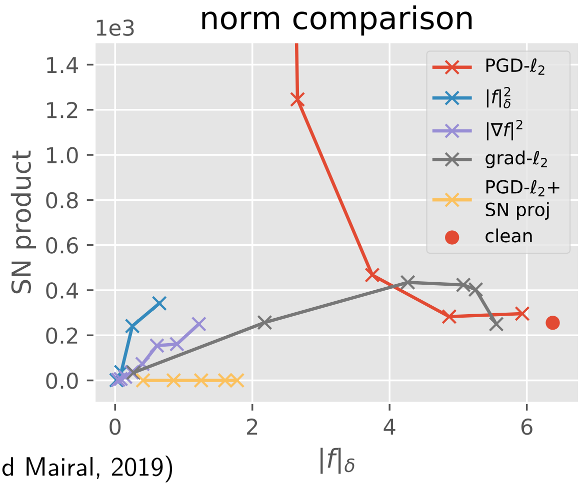
Robust vs standard accuracy trade-offs



(Bietti, Mialon, Chen, and Mairal, 2019)

Regularization for robustness

Upper vs lower bounds



(Bietti, Mialon, Chen, and Mairal, 2019)

Deep convolutional representations: conclusions

Study of generic properties

- Deformation stability with small patches, adapted to resolution
- Signal preservation when subsampling $\leq$ patch size
- Group invariance by changing patch extraction and pooling

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Applies to learned models

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  - "higher capacity" is needed to discriminate small deformations
  - Learning may be "easier" with stable functions
- Better regularization of generic CNNs using RKHS norm

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Links with optimization (Bietti and Mairal, 2019b)

- Similar kernel (NTK) arises from optimization in a certain regime
- Weaker stability guarantees, but better approximation properties

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