Invariance and Stability to Deformations of Deep Convolutional Representations

Julien Mairal

Inria Grenoble

Theory of Deep Learning Workshop, ICML, 2018

This is mostly the work of Alberto Bietti

- A. Bietti and J. Mairal. **Group Invariance, Stability to Deformations, and Complexity of Deep Convolutional Representations.** arXiv:1706.03078. 2018.
- A. Bietti and J. Mairal. Invariance and Stability of Deep Convolutional Representations. NIPS. 2017.

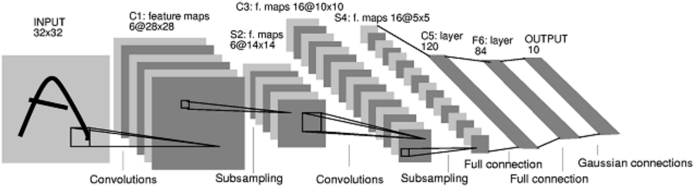
Objectives

Deep convolutional signal representations

- Are they **stable to deformations**?
- How can we achieve **invariance to transformation groups**?
- Do they **preserve signal information**?

Learning aspects

- Building a **functional space** for CNNs (or similar objects).
- Deriving a measure of **model complexity**.



A kernel perspective

Recipe

- Map data x to **high-dimensional space**, $\Phi(x)$ in $\mathcal{H}$ (RKHS), with Hilbertian geometry (projections, barycenters, angles, . . . , exist!).
- Non-linear function f in $\mathcal{H}$ becomes linear: $f(x) = \langle f, \Phi(x) \rangle_{\mathcal{H}}$.
- Learning with a positive definite kernel $K(x, x') = \langle \Phi(x), \Phi(x') \rangle_{\mathcal{H}}$.

[Schölkopf and Smola, 2002, Shawe-Taylor and Cristianini, 2004]...

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What is the relation with deep neural networks?

- It is possible to design a RKHS $\mathcal{H}$ where a large class of deep neural networks live [Mairal, 2016].

$$f(x) = \sigma_k(W_k \sigma_{k-1}(W_{k-1} \ldots \sigma_2(W_2 \sigma_1(W_1 x)) \ldots)) = \langle f, \Phi(x) \rangle_{\mathcal{H}}.$$

- This is the construction of "**convolutional kernel networks**".

[Schölkopf and Smola, 2002, Shawe-Taylor and Cristianini, 2004]...

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Why do we care?

- $\Phi(x)$ is related to the **network architecture** and is **independent of training data**. Is it stable? Does it lose signal information?
- f is a **predictive model**. Can we control its stability?

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

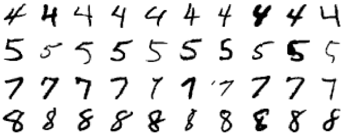
- $\|f\|_{\mathcal{H}}$ controls both **stability and generalization**!

[Schölkopf and Smola, 2002, Shawe-Taylor and Cristianini, 2004]...

A signal processing perspective

plus a bit of harmonic analysis

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



[Mallat, 2012, Bruna and Mallat, 2013, Sifre and Mallat, 2013]...

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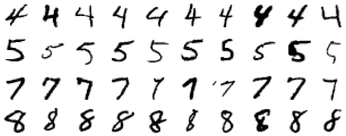

Relation with deep convolutional representations

Stability to deformations studied for wavelet-based scattering transform.

[Mallat, 2012, Bruna and Mallat, 2013, Sifre 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.
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- $C_2 \rightarrow 0$: translation invariance.

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Summary of our results

Multi-layer construction of the RKHS $\mathcal{H}$

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- **Signal preservation** of the multi-layer kernel mapping Φ.
- Conditions of **non-trivial stability** for Φ.
- Constructions to achieve **group invariance**.

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On learning

- Bounds on the RKHS norm $\|.\|_{\mathcal{H}}$ to control **stability and generalization** of a predictive model f.

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

Outline

1. Construction of the multi-layer convolutional representation
2. Invariance and stability
3. Learning aspects: model complexity

A generic deep convolutional representation

Initial map x_0 in $L^2(\Omega, \mathcal{H}_0)$

$x_0 : \Omega \to \mathcal{H}_0$: **continuous** input signal

- $u \in \Omega = \mathbb{R}^d$: location $(d = 2$ for images).
- $x_0(u) \in \mathcal{H}_0$: input value at location u $(\mathcal{H}_0 = \mathbb{R}^3$ for RGB images).

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Building map x_k in $L^2(\Omega, \mathcal{H}_k)$ from x_{k-1} in $L^2(\Omega, \mathcal{H}_{k-1})$

$x_k : \Omega \to \mathcal{H}_k$: **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 ($P_k x_{k-1}(u)$ is a patch centered at u).

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

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

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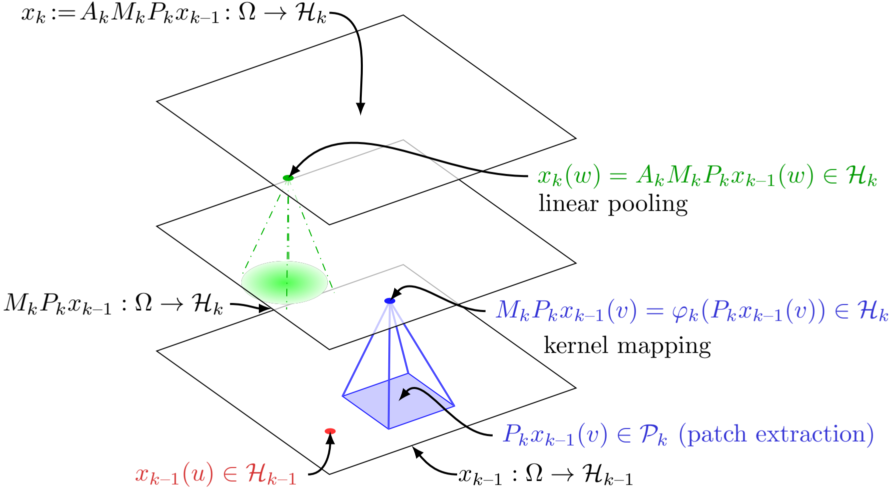
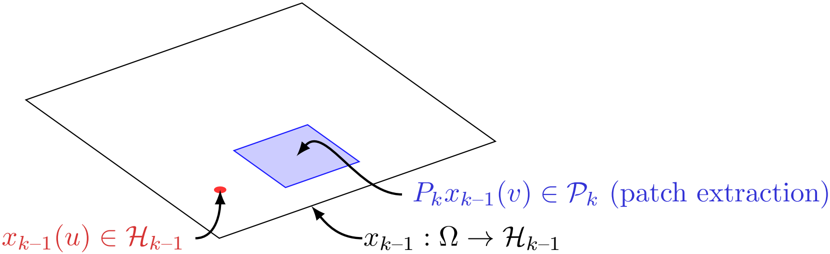


Patch extraction operator P_k

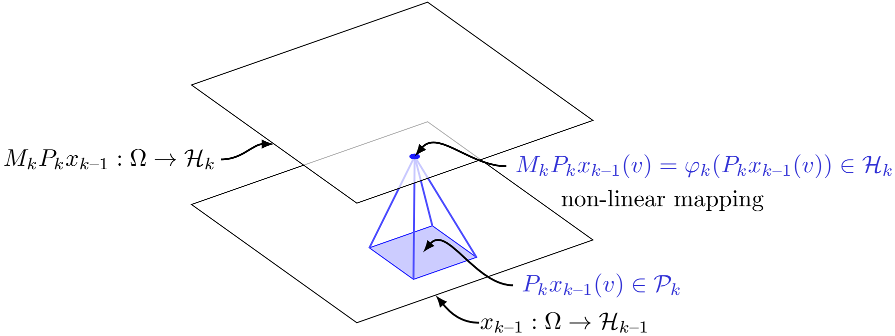
$$P_k x_{k-1}(u) := (v \in S_k \mapsto x_{k-1}(u+v)) \in \mathcal{P}_k = \mathcal{H}_{k-1}^{S_k}.$$



- S_k: patch shape, e.g. box.
- P_k is **linear**, and **preserves the norm**: $\|P_k x_{k-1}\| = \|x_{k-1}\|$.
- Norm of a map: $\|x\|^2 = \int_\Omega \|x(u)\|^2 du < \infty$ for x in $L^2(\Omega, \mathcal{H})$.

Non-linear pointwise 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.
- 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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- or intead: for $z, z' \in \mathcal{P}_k$

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- but at some point, we pay a "price" in $\Pi_{i=1}^k \rho_i$.

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 $b_j \geq 0$, $\kappa_k(1) = 1$.
- $\|\varphi_k(z)\| = K_k(z, z)^{1/2} = \|z\|$ (**norm preservation**).
- $\|\varphi_k(z) - \varphi_k(z')\| \leq \|z - z'\|$ if $\kappa_k'(1) \leq 1$ (**non-expansiveness**).

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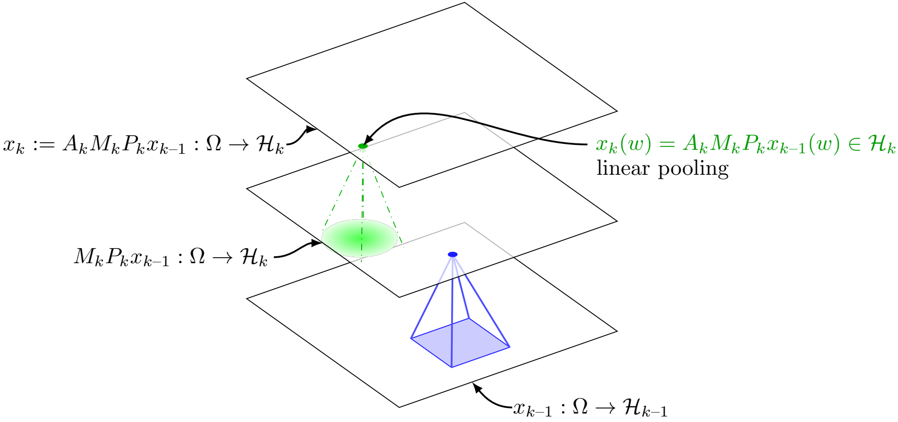
Examples

- $\kappa_{\text{exp}}(\langle z, z'\rangle) = e^{\langle z, z'\rangle - 1} = e^{-\frac{1}{2}\|z - z'\|^2}$ (if $\|z\| = \|z'\| = 1$).
- $\kappa_{\text{inv-poly}}(\langle z, z'\rangle) = \frac{1}{2 - \langle z, z'\rangle}$.

[Schoenberg, 1942, Scholkopf, 1997, Smola et al., 2001, Cho and Saul, 2010, Zhang et al., 2016, 2017, Daniely et al., 2016, Bach, 2017, Mairal, 2016]...

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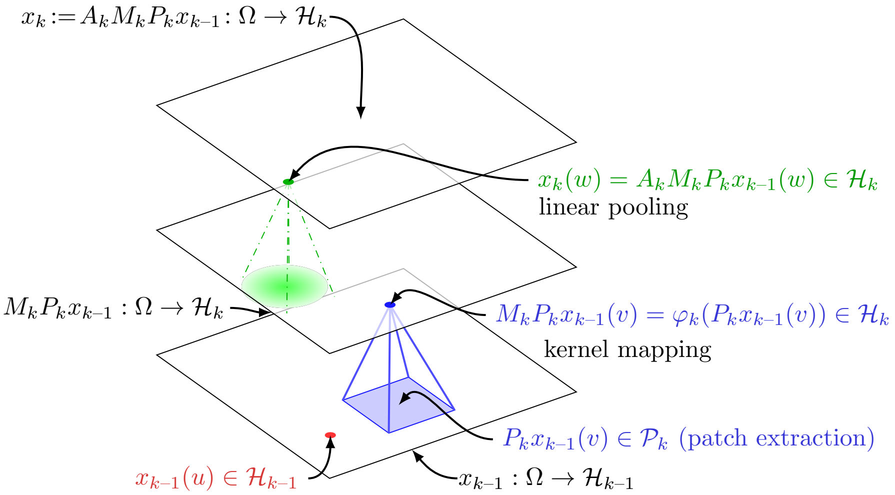
- h_{σ_k}: pooling filter at scale σ_k.
- $h_{\sigma_k}(u) := \sigma_k^{-d} h(u/\sigma_k)$ with $h(u)$ **Gaussian**.
- **linear, non-expansive operator**: $\|A_k\| \leq 1$ (operator norm).

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

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

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

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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: example in 1D

- Discrete signal $\bar{x_k}$ in $\ell^2(\mathbb{Z}, \bar{\mathcal{H}_k})$ vs continuous ones x_k in $L^2(\mathbb{R}, \mathcal{H}_k)$.
- $\bar{x}_k$: subsampling factor s_k after pooling with scale $\sigma_k \approx s_k$:

$$\bar{x}_k[n] = \bar{A}_k \bar{M}_k \bar{P}_k \bar{x}_{k-1}[n s_k].$$

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- How? Recover patches with **linear functions** (contained in $\bar{\mathcal{H}}_k$)

$$\langle f_w, \bar{M}_k \bar{P}_k \bar{x}_{k-1}(u) \rangle = f_w(\bar{P}_k \bar{x}_{k-1}(u)) = \langle w, \bar{P}_k \bar{x}_{k-1}(u) \rangle,$$

and

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Warning: no claim that recovery is practical and/or stable.

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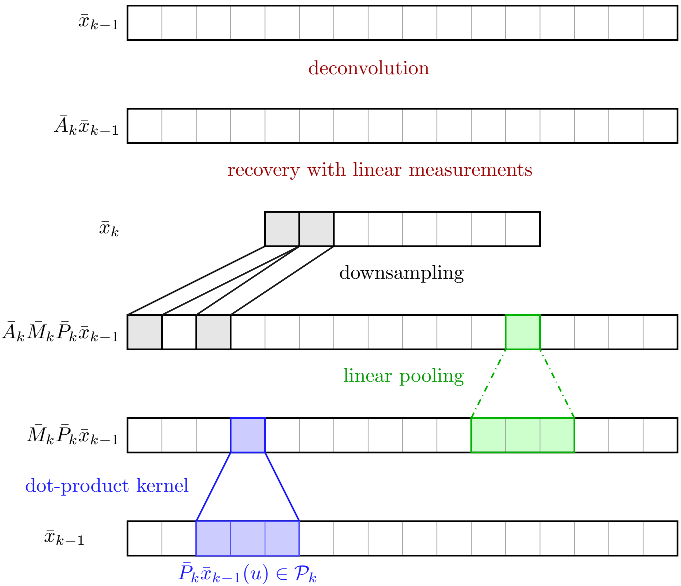

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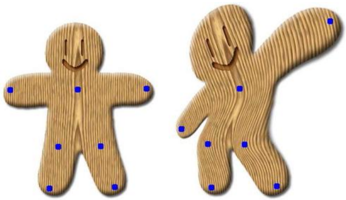

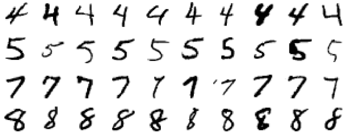

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Warmup: translation invariance

Representation

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How to achieve translation invariance?

- Translation: $L_c x(u) = x(u - c)$.

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- Translation: $L_c x(u) = x(u - c)$.
- *Equivariance* - all operators commute with L_c: $\square L_c = L_c \square$.

$$\begin{aligned}
\|\Phi_n(L_c x) - \Phi_n(x)\| &= \|L_c \Phi_n(x) - \Phi_n(x)\| \\
&\leq \|L_c A_n - A_n\| \cdot \|M_n P_n \Phi_{n-1}(x)\| \\
&\leq \|L_c A_n - A_n\| \|x\|.
\end{aligned}$$

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- Mallat [2012]: $\|L_\tau A_n - A_n\| \leq \frac{C_2}{\sigma_n} \|\tau\|_\infty$ (operator norm).

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- Translation: $L_c x(u) = x(u-c)$.
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$$\begin{aligned} \|\Phi_n(L_c x) - \Phi_n(x)\| &= \|L_c \Phi_n(x) - \Phi_n(x)\| \\ &\leq \|L_c A_n - A_n\| \cdot \|M_n P_n \Phi_{n-1}(x)\| \\ &\leq \|L_c A_n - A_n\| \|x\|. \end{aligned}$$

- Mallat [2012]: $\|L_c A_n - A_n\| \leq \frac{C_2}{\sigma_n} c$ (operator norm).
- **Scale σ_n of the last layer controls translation invariance.**

Stability to deformations

Representation

$$\Phi_n(x) \triangleq A_n M_n P_n A_{n-1} M_{n-1} P_{n-1} \cdots A_1 M_1 P_1 A_0 x.$$

How to achieve stability to deformations?

- Patch extraction P_k and pooling A_k **do not commute** with L_τ!

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- $\|A_k L_\tau - L_\tau A_k\| \leq C_1 \|\nabla \tau\|_\infty$ [from Mallat, 2012].

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

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

Stability to deformations: final result

Theorem

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

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

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

related work on stability [Wiatowski and Bölcskei, 2017]

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Stability to deformations: final result

Theorem

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

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

- translation invariance: large σ_n.
- stability: small patch sizes.
- signal preservation: subsampling factor $\approx$ patch size.
- $\Longrightarrow$ **needs several layers.**
- requires additional discussion to make stability non-trivial.
- (also valid for generic CNNs with ReLUs: multiply by $\prod_k \rho_k = \prod_k \|W_k\|$, but no signal preservation).

related work on stability [Wiatowski and Bölcskei, 2017]

Beyond the translation group

Can we achieve invariance to other groups?

- Group action: $L_g x(u) = x(g^{-1}u)$ (e.g., rotations, reflections).
- Feature maps $x(u)$ defined on $u \in G$ (G: locally compact group).

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Recipe: Equivariant inner layers + global pooling in last layer

- **Patch extraction**:

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

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

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

related work [Sifre and Mallat, 2013, Cohen and Welling, 2016, Raj et al., 2016]...

Group invariance and stability

Previous construction is similar to Cohen and Welling [2016] for CNNs.

A case of interest: the roto-translation group

- $G = \mathbb{R}^2 \rtimes SO(2)$ (mix of translations and rotations).
- **Stability** with respect to the translation group.
- **Global invariance** to rotations (only global pooling at final layer).
  - Inner layers: only pool 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

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

What does the RKHS contain?

Homogeneous version of [Zhang et al., 2016, 2017]

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- RKHS contains **homogeneous functions**:

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

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What does the RKHS contain?

- RKHS contains **homogeneous functions**:

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

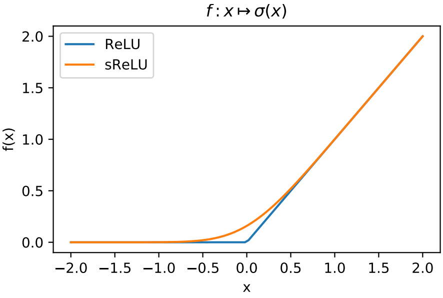
- **Smooth activations**: $\sigma(u) = \sum_{j=0}^{\infty} a_j u^j$ with $a_j \geq 0$.
- Norm: $\|f\|^2_{\mathcal{H}_k} \leq C^2_\sigma(\|g\|^2) = \sum_{j=0}^{\infty} \frac{a_j^2}{b_j}\|g\|^2 < \infty$.

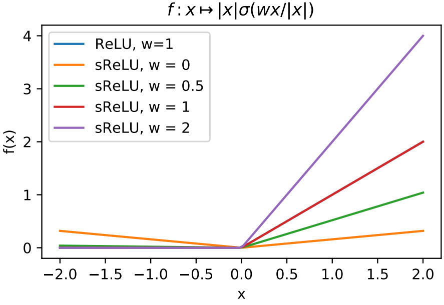
Homogeneous version of [Zhang et al., 2016, 2017]

RKHS of patch kernels K_k

Examples:

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





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

Some CNNs live in the RKHS: "linearization" principle

$$f(x) = \sigma_k(W_k \sigma_{k-1}(W_{k-1} \ldots \sigma_2(W_2 \sigma_1(W_1 x)) \ldots)) = \langle f, \Phi(x) \rangle_{\mathcal{H}}.$$

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

Some CNNs live in the RKHS: "linearization" principle

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- Consider a CNN with filters $W_k^{ij}(u), u \in S_k$.
  - k: layer;
  - i: index of filter;
  - j: index of input channel.
- "Smooth homogeneous" activations σ.
- The CNN can be constructed hierarchically in $\mathcal{H}_\mathcal{K}$.
- Norm (linear layers):

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

- Linear layers: product of spectral norms.

Link with generalization

Direct application of classical generalization bounds

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

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

Link with generalization

Direct application of classical generalization bounds

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

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

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

[see, e.g., Boucheron et al., 2005, Shalev-Shwartz and Ben-David, 2014]...

Deep convolutional representations: conclusions

Study of generic properties of signal representation

- **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

- Same quantity $\|f\|$ controls stability and generalization.
- "higher capacity" is needed to discriminate small deformations.

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Applies to learned models

- Same quantity $\|f\|$ controls stability and generalization.
- "higher capacity" is needed to discriminate small deformations.

Questions:

- Better regularization?
- How does SGD control capacity in CNNs?
- What about networks with no pooling layers? ResNet?

Allez les bleus !

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φ_k from kernel approximations: CKNs [Mairal, 2016]

- Approximate $\varphi_k(z)$ by **projection** (Nyström approximation) on

$$\mathcal{F} = \mathsf{Span}(\varphi_k(z_1), \ldots, \varphi_k(z_p)).$$

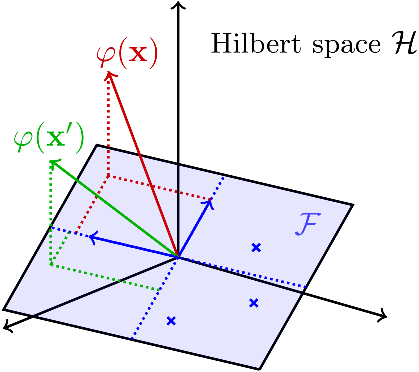

Figure: Nyström approximation.

[Williams and Seeger, 2001, Smola and Schölkopf, 2000, Zhang et al., 2008]...

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- 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).

[Williams and Seeger, 2001, Smola and Schölkopf, 2000, Zhang et al., 2008]...

Discussion

- norm of $\|\Phi(x)\|$ is of the same order (or close enough) to $\|x\|$.
- the kernel representation is non-expansive but not contractive

$$\sup_{x,x' \in L^2(\Omega,\mathcal{H}_0)} \frac{\|\Phi(x) - \Phi(x')\|}{\|x - x'\|} = 1.$$