

Invariance and Stability to Deformations of Deep Convolutional Representations

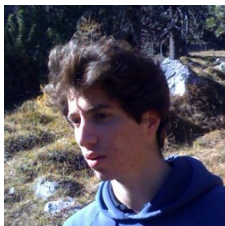
Julien Mairal

Inria Grenoble

ML and AI workshop, Telecom ParisTech, 2018



This is mostly the work of Alberto Bietti

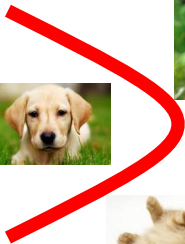


- A. Bietti and J. Mairal. **Group Invariance, Stability to Deformations, and Complexity of Deep Convolutional Representations.** arXiv:1706.03078. 2018.
- A. Bietti and J. Mairal. Invariance and Stability of Deep Convolutional Representations. NIPS. 2017.

Learning a predictive model

The goal is to learn a **prediction function** $f : \mathbb{R}^p \rightarrow \mathbb{R}$ given labeled training data $(x_i, y_i)_{i=1, \dots, n}$ with x_i in \mathbb{R}^p , and y_i in \mathbb{R} :

$$\min_{f \in \mathcal{F}} \underbrace{\frac{1}{n} \sum_{i=1}^n L(y_i, f(x_i))}_{\text{empirical risk, data fit}} + \underbrace{\lambda \Omega(f)}_{\text{regularization}} .$$



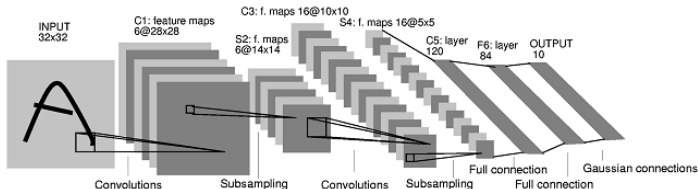
Objectives

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**.

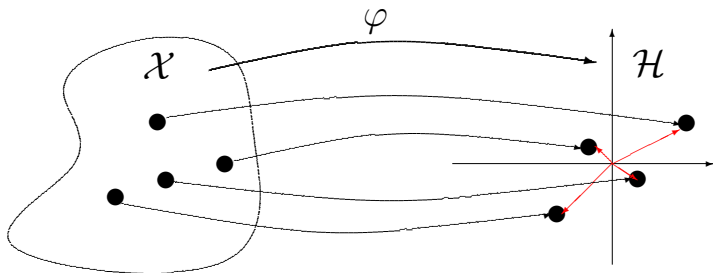


A kernel perspective

$$\min_{f \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^n L(y_i, f(x_i)) + \lambda \|f\|_{\mathcal{H}}^2.$$

- map data to a Hilbert space (RKHS) and work with **linear forms**:

$$\Phi : \mathcal{X} \rightarrow \mathcal{H} \quad \text{and} \quad f(x) = \langle \Phi(x), f \rangle_{\mathcal{H}}.$$



A kernel perspective

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Main purpose: embed data in a vectorial space where

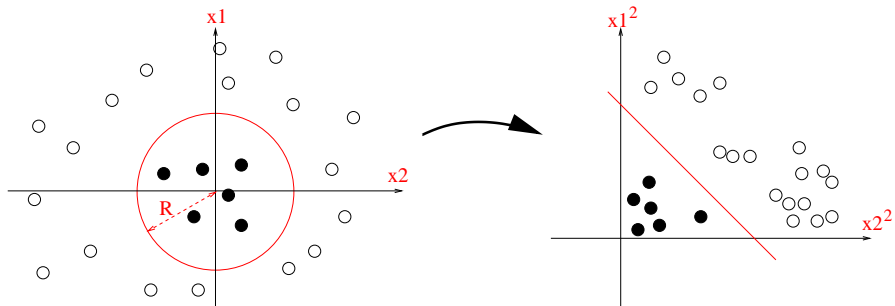
- many **geometrical operations** exist (angle computation, projection on linear subspaces, definition of barycenters....).
- one may learn potentially **rich infinite-dimensional models**.
- **regularization** is natural:

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

A kernel perspective

Second purpose: unhappy with the current Euclidean structure?

- lift data to a higher-dimensional space with **nicer properties** (e.g., linear separability, clustering structure).
- then, the **linear** form $f(x) = \langle \Phi(x), f \rangle_{\mathcal{H}}$ in \mathcal{H} may correspond to a **non-linear** model in \mathcal{X} .



A kernel perspective

Recipe

- Map data x to **high-dimensional space**, $\Phi(x)$ in \mathcal{H} (RKHS), with Hilbertian geometry (projections, barycenters, angles, \dots , exist!).
- predictive models f in \mathcal{H} are **linear forms** in \mathcal{H} : $f(x) = \langle f, \Phi(x) \rangle_{\mathcal{H}}$.
- 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].

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

- 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?

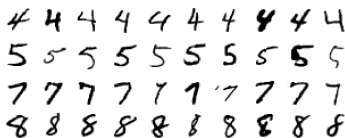
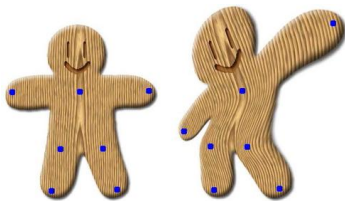
$$|f(x) - f(x')| \leq \|f\|_{\mathcal{H}} \|\Phi(x) - \Phi(x')\|_{\mathcal{H}}.$$

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

A signal processing perspective

plus a bit of harmonic analysis

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

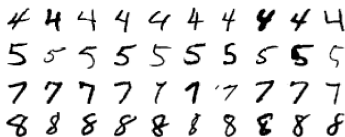
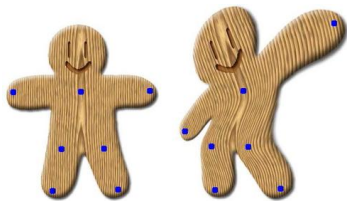


[Mallat, 2012, Allasonnière, Amit, and Trouvé, 2007, Trouvé and Younes, 2005]...

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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

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Summary of our results

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

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Signal representation

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

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On learning

- Bounds on the RKHS norm $\|\cdot\|_{\mathcal{H}}$ 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 $L^2(\Omega, \mathcal{H}_0)$

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

- $u \in \Omega = \mathbb{R}^d$: location ($d = 2$ for images).
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Building map x_k in $L^2(\Omega, \mathcal{H}_k)$ from x_{k-1} in $L^2(\Omega, \mathcal{H}_{k-1})$

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

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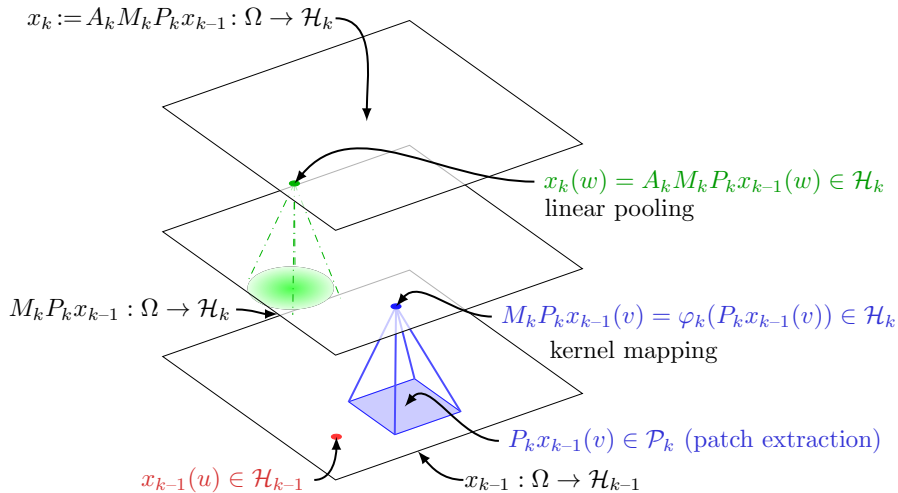
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$$x_k = A_k M_k P_k x_{k-1}.$$

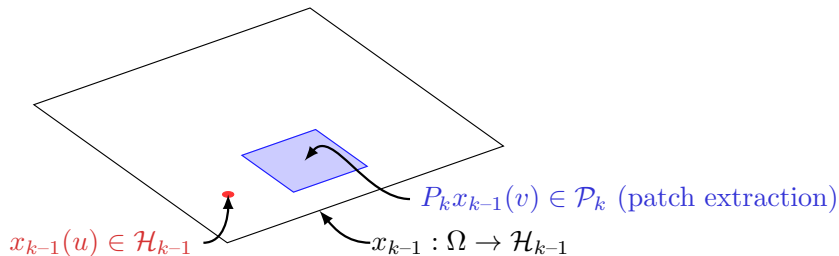
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- A_k : (linear) **pooling** operator at scale σ_k .

A generic deep convolutional representation



Patch extraction operator P_k

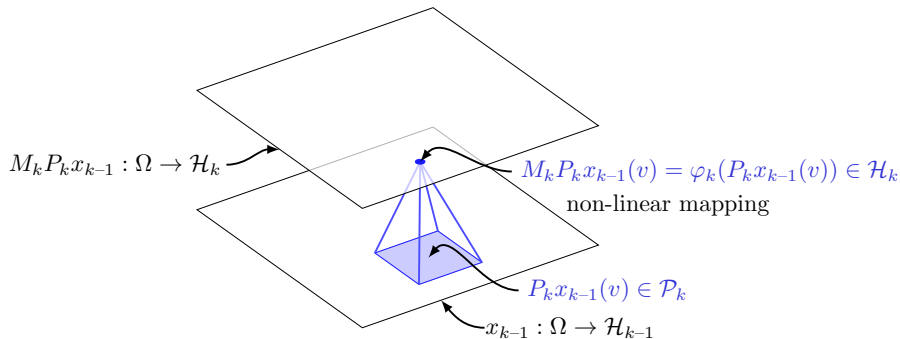
$$P_k x_{k-1}(u) := (v \in S_k \mapsto x_{k-1}(u + v)) \in \mathcal{P}_k = \mathcal{H}_{k-1}^{S_k}.$$



- 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

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- $\varphi_k : \mathcal{P}_k \rightarrow \mathcal{H}_k$ pointwise non-linearity on patches.
- We assume **non-expansivity**

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

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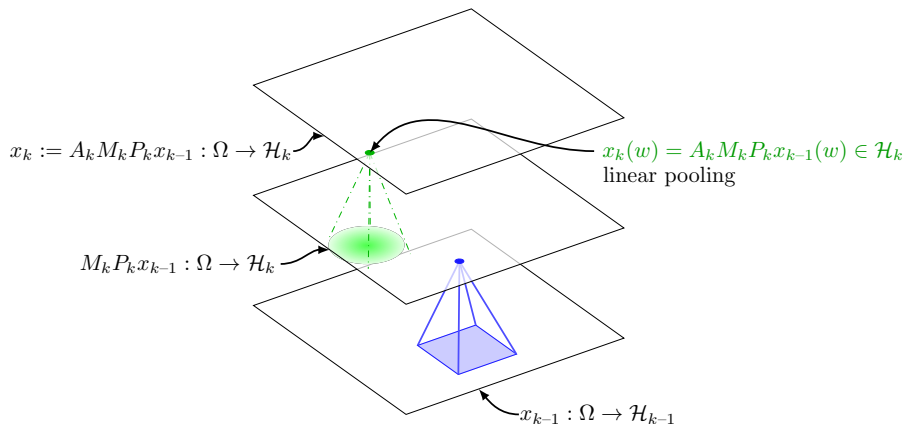
Examples

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

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

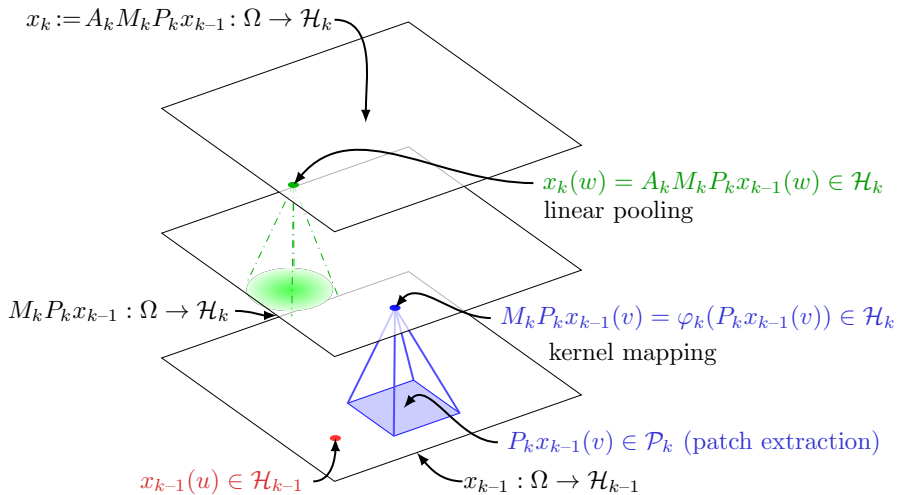


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- h_{σ_k} : pooling filter at scale σ_k .
- $h_{\sigma_k}(u) := \sigma_k^{-d} h(u/\sigma_k)$ with $h(u)$ **Gaussian**.
- **linear, non-expansive operator**: $\|A_k\| \leq 1$ (operator norm).

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

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Prediction layer

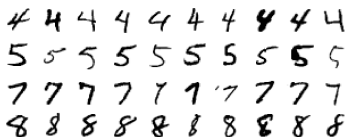
- e.g., linear $f(x) = \langle w, \Phi_n(x) \rangle$.
- “linear kernel” $\mathcal{K}(x, x') = \langle \Phi_n(x), \Phi_n(x') \rangle = \int_{\Omega} \langle x_n(u), x'_n(u) \rangle du$.

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- 2 Invariance and stability
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Invariance, definitions

- $\tau : \Omega \rightarrow \Omega$: C^1 -diffeomorphism with $\Omega = \mathbb{R}^d$.
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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]: $\|L_c A_n - A_n\| \leq \frac{C_2}{\sigma_n} c$ (operator norm).
- **Scale σ_n of the last layer controls translation invariance.**

Stability to deformations

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How to achieve stability to deformations?

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- $\|[A_k, L_\tau]\| \leq C_1 \|\nabla \tau\|_\infty$ [from Mallat, 2012].
- But: $[P_k, L_\tau]$ is **unstable** at high frequencies!

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- $\|[A_k, L_\tau]\| \leq C_1 \|\nabla\tau\|_\infty$ [from Mallat, 2012].
- But: $[P_k, L_\tau]$ is **unstable** at high frequencies!
- Adapt to **current layer resolution**, patch size controlled by σ_{k-1} :

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

Stability to deformations

Representation

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

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

Stability to deformations: final result

Theorem

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

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

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

related work on stability [Wiatowski and Bölcskei, 2017]

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related work on stability [Wiatowski and Bölcskei, 2017]

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.
- \implies **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

- $G = \mathbb{R}^2 \times SO(2)$ (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

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 $\sigma_k \approx s_k$:

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

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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

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

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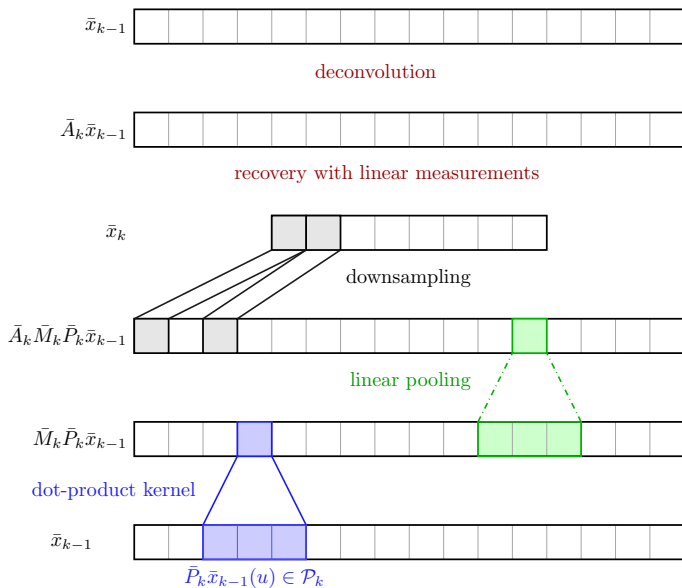
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Warning: no claim that recovery is practical and/or stable.

Discretization and signal preservation: example in 1D



Outline

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

RKHS of patch kernels K_k

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

What does the RKHS contain?

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

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What does the RKHS contain?

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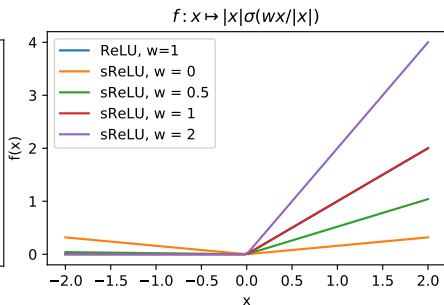
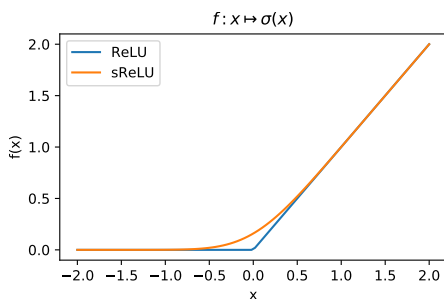
- **Smooth activations**: $\sigma(u) = \sum_{j=0}^{\infty} a_j u^j$ with $a_j \geq 0$.
- **Norm**: $\|f\|_{\mathcal{H}_k}^2 \leq C_\sigma^2 (\|g\|^2) = \sum_{j=0}^{\infty} \frac{a_j^2}{b_j} \|g\|^2 < \infty$.

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

RKHS of patch kernels K_k

Examples:

- $\sigma(u) = u$ (linear): $C_\sigma^2(\lambda^2) = O(\lambda^2)$.
- $\sigma(u) = u^p$ (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 $\mathcal{H}_{\mathcal{X}}$

Some CNNs live in the RKHS: “linearization” principle

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

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

Some CNNs live in the RKHS: “linearization” principle

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

- 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):

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

- Linear layers: product of spectral norms.

Link with generalization

Direct application of classical generalization bounds

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

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

Link with generalization

Direct application of classical generalization bounds

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

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

- 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

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- “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?

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φ_k from kernel approximations: CKNs [Mairal, 2016]

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

$$\mathcal{F} = \text{Span}(\varphi_k(z_1), \dots, \varphi_k(z_p)).$$

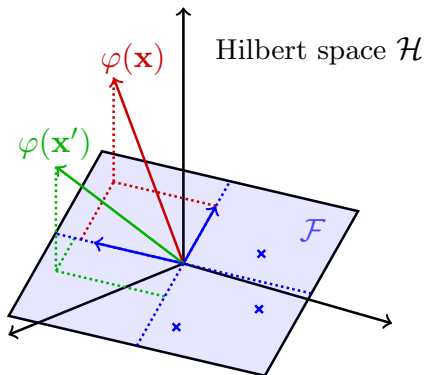


Figure: Nyström approximation.

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

φ_k from kernel approximations: CKNs [Mairal, 2016]

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

$$\mathcal{F} = \text{Span}(\varphi_k(z_1), \dots, \varphi_k(z_p)).$$

- Leads to **tractable**, p -dimensional representation $\psi_k(z)$.
- Norm is preserved, and projection is **non-expansive**:

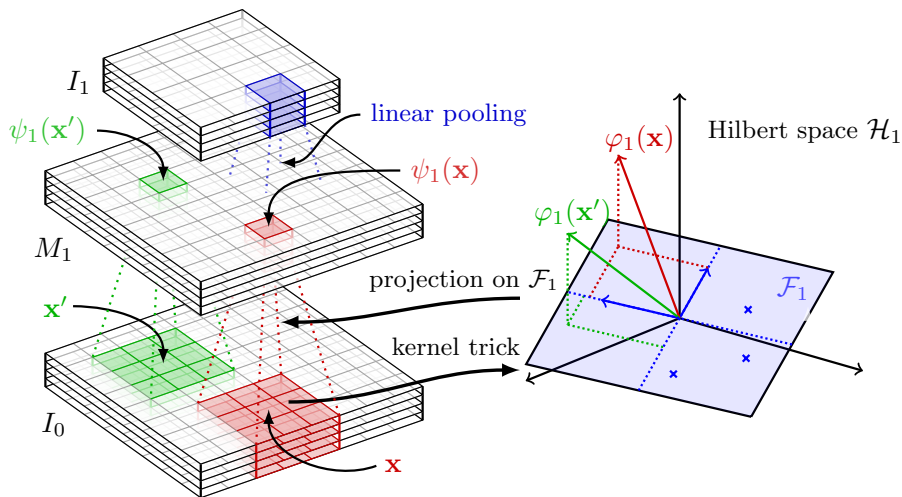
$$\begin{aligned}\|\psi_k(z) - \psi_k(z')\| &= \|\Pi_k \varphi_k(z) - \Pi_k \varphi_k(z')\| \\ &\leq \|\varphi_k(z) - \varphi_k(z')\| \leq \|z - z'\|.\end{aligned}$$

- Anchor points z_1, \dots, 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]...

φ_k from kernel approximations: CKNs [Mairal, 2016]

Convolutional kernel networks in practice.



Discussion

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

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

Future of Convolutional Neural Networks

What are current high-potential problems to solve?

- 1 lack of **robustness** (see next slide).
- 2 learning with **few labeled data**.
- 3 learning with **no supervision** (see Tab. from Bojanowski and Joulin, 2017).

Method	Acc@1
Random (Noroozi & Favaro, 2016)	12.0
SIFT+FV (Sánchez et al., 2013)	55.6
Wang & Gupta (2015)	29.8
Doersch et al. (2015)	30.4
Zhang et al. (2016)	35.2
¹ Noroozi & Favaro (2016)	38.1
BiGAN (Donahue et al., 2016)	32.2
NAT	36.0

Table 3. Comparison of the proposed approach to state-of-the-art unsupervised feature learning on ImageNet. A full multi-layer perceptron is retrained on top of the features. We compare to several self-supervised approaches and an unsupervised approach.

Future of Convolutional Neural Networks

Illustration of instability. Picture from Kurakin et al. [2016].

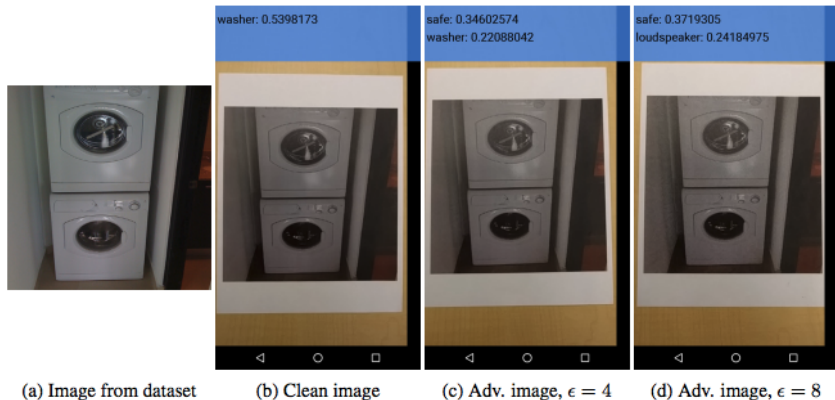


Figure: Adversarial examples are generated by computer; then printed on paper; a new picture taken on a smartphone fools the classifier.

Future of Convolutional Neural Networks

$$\min_{f \in \mathcal{F}} \underbrace{\frac{1}{n} \sum_{i=1}^n L(y_i, f(x_i))}_{\text{empirical risk, data fit}} + \underbrace{\lambda \Omega(f)}_{\text{regularization}} .$$

The issue of regularization

- today, heuristics are used (DropOut, weight decay, early stopping)...
- ...but they are not sufficient.
- how to **control variations of prediction functions**?

$|f(x) - f(x')|$ should be close if x and x' are “similar”.

- what does it mean for x and x' to be “similar”?
- what should be a good **regularization function** Ω ?