

Group Invariance, Stability to Deformations, and Complexity of Deep Convolutional Representations

Alberto Bietti Julien Mairal

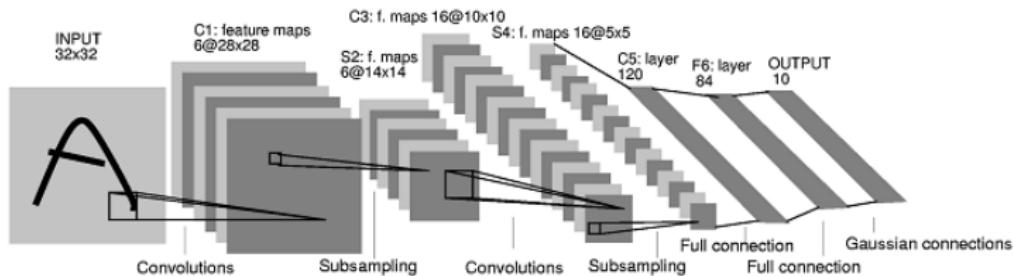
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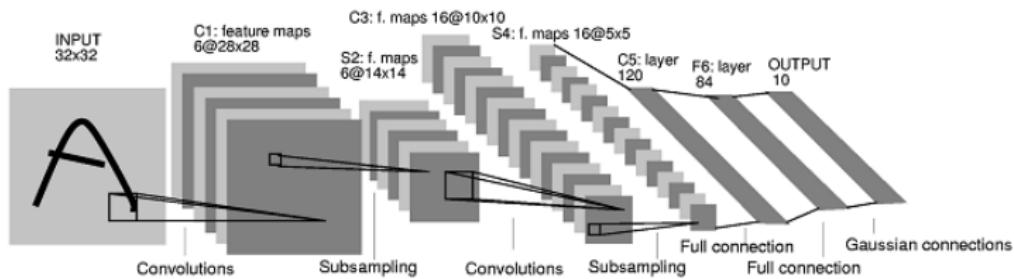
Success of deep convolutional networks



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

- Neural networks: $f(x) = W_{n+1}\sigma(W_n\sigma(W_{n-1}\dots\sigma(W_2\sigma(W_1x))\dots))$
- **Convolutional** structure in the linear operations W_k

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?**
- How can we measure **model complexity?**

A kernel perspective

Kernels?

- Map data x to high-dimensional space, $\Phi(x) \in \mathcal{H}$ (\mathcal{H} : “RKHS”)
- Non-linear function $f \in \mathcal{H}$ becomes linear: $f(x) = \langle f, \Phi(x) \rangle$
- 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 $K(x, x') = \langle \Phi(x), \Phi(x') \rangle$
- CKN kernels (Mairal, 2016) satisfy:

$$f(x) = W_{n+1}\sigma(W_n\sigma(W_{n-1}\dots\sigma(W_2\sigma(W_1x))\dots)) = \langle f, \Phi(x) \rangle$$

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 generalization!**
 - discriminating small deformations requires large $\|f\|$
 - learning stable functions is “easier”

Outline

① Construction of the Convolutional Representation

② Invariance and Stability

③ Model Complexity and Generalization

A generic deep convolutional representation

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

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

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- ▶ M_k : **non-linear mapping** operator, maps each patch to a new point with a **pointwise** non-linear function $\varphi_k(\cdot)$

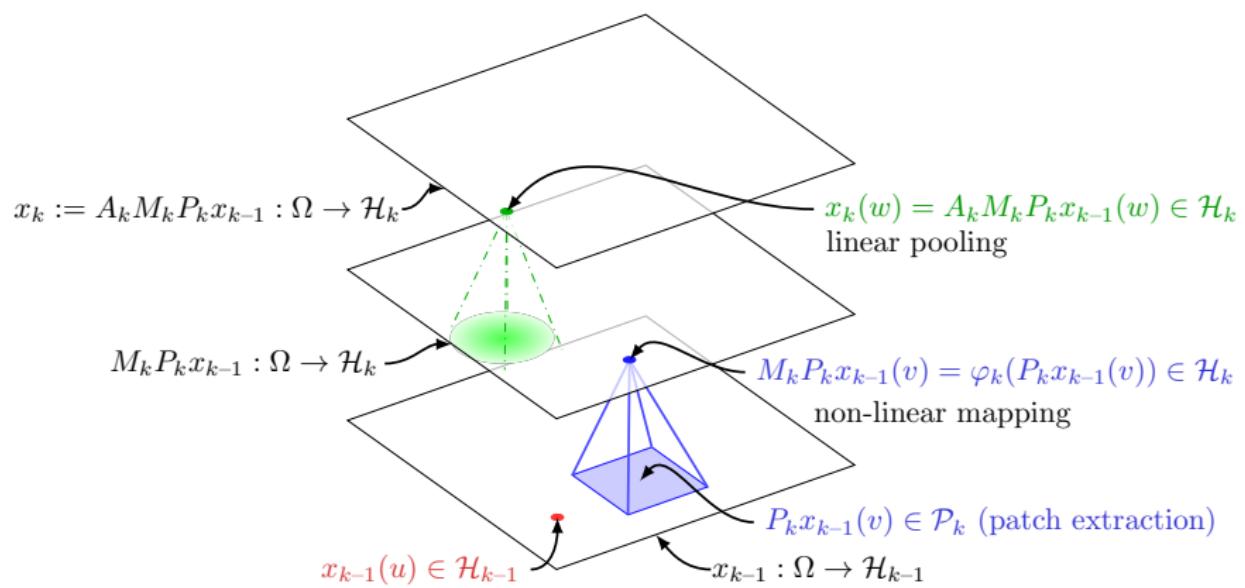
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$$x_k = A_k M_k P_k x_{k-1}$$

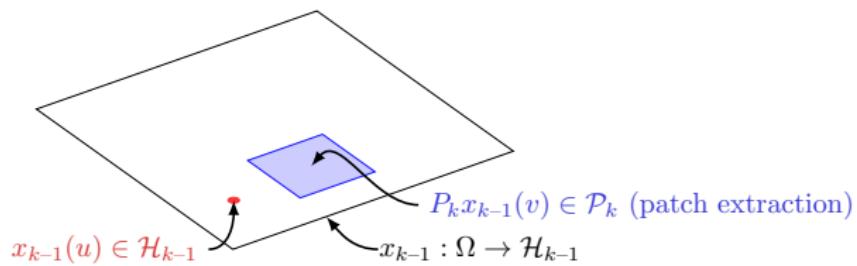
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- ▶ A_k : (linear, Gaussian) **pooling** operator at scale σ_k

A generic deep convolutional representation



Patch extraction operator P_k

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



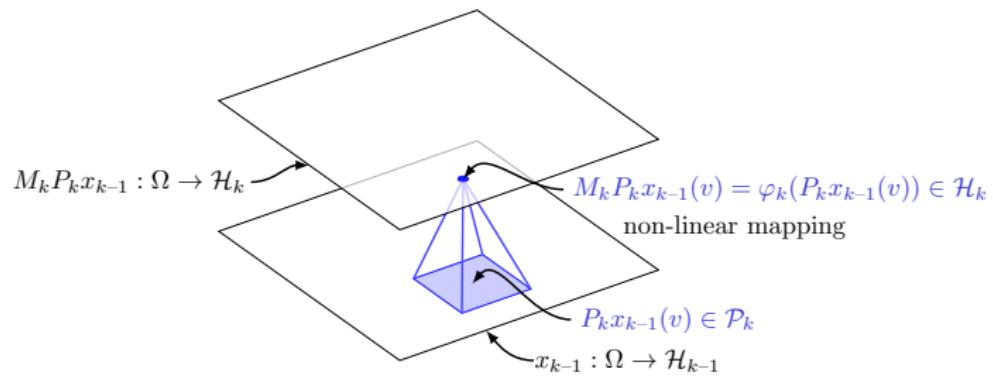
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- S_k : patch shape, e.g. box
- P_k is **linear**, and **preserves the norm**: $\|P_k x_{k-1}\| = \|x_{k-1}\|$

Non-linear mapping operator M_k

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- $\varphi_k : \mathcal{P}_k \rightarrow \mathcal{H}_k$ 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 $x, x' \in L^2(\Omega, \mathcal{P}_k)$

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- We assume: for $z, z' \in \mathcal{P}_k$

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- (can think instead: $\varphi_k(z) = \text{ReLU}(W_k z)$, ρ_k -**Lipschitz** with $\rho_k = \|W_k\|$)

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)
 - $\kappa_{\text{inv-poly}}(\langle z, z' \rangle) = \frac{1}{2 - \langle z, z' \rangle}$

φ_k from kernels: CKNs approximation

Convolutional Kernel Networks approximation (Mairal, 2016):

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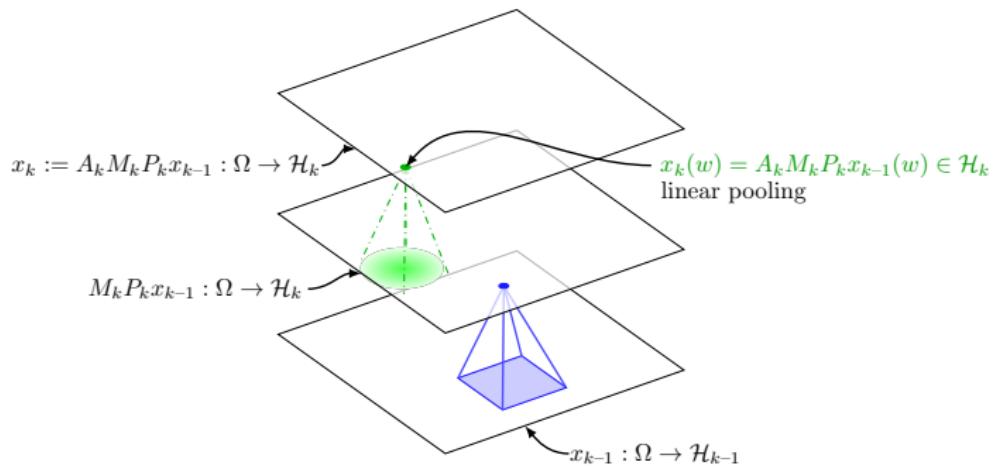
- Approximate $\varphi_k(z)$ by **projection** on $\text{span}(\varphi_k(z_1), \dots, \varphi_k(z_p))$ (Nystrom)
- Leads to **tractable**, p -dimensional representation $\psi_k(z)$
- Norm is preserved, and projection is non-expansive:

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

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

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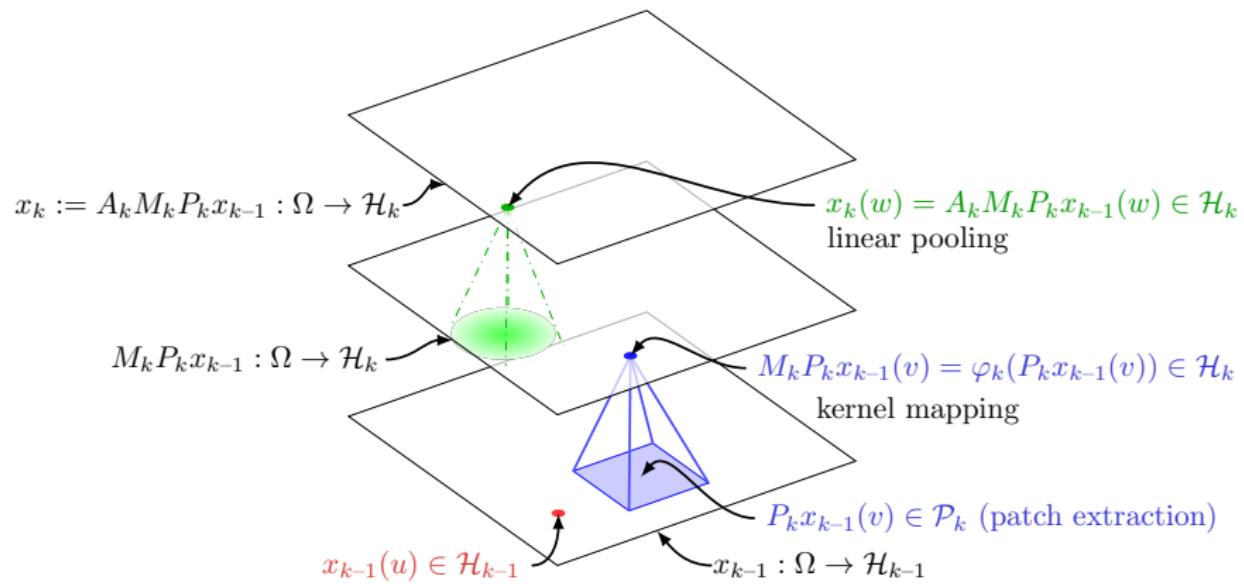
- h_{σ_k} : pooling filter at scale σ_k
- $h_{\sigma_k}(u) := \sigma_k^{-d} h(u/\sigma_k)$ with $h(u)$ **Gaussian**
- **linear, non-expansive operator**: $\|A_k\| \leq 1$

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- **linear, non-expansive operator**: $\|A_k\| \leq 1$
- In practice: **discretization**, sampling at resolution σ_k after pooling
- **Recovery** with kernels possible when **subsampling** \leq **patch size**

Recap: P_k , M_k , A_k



Multilayer construction

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

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

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 - ▶ Natural assumption: $x_0 = A_0 x$, with x the original continuous signal, A_0 local integrator (**anti-aliasing**)

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- **Prediction layer:** e.g. linear
 - ▶ $f(x_0) = \langle w, x_n \rangle$
 - ▶ “linear kernel” $\mathcal{K}(x_0, x'_0) = \langle x_n, x'_n \rangle = \int_{\Omega} \langle x_n(u), x'_n(u) \rangle du$

Outline

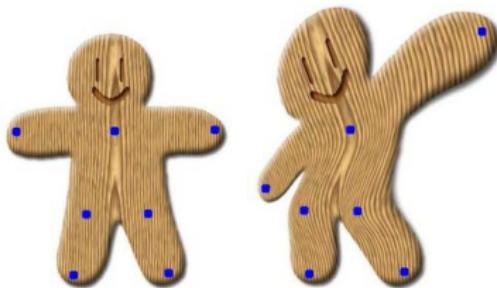
① Construction of the Convolutional Representation

② Invariance and Stability

③ Model Complexity and Generalization

Stability to deformations: definitions

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



4	4	4	4	4	4	4	4	4	4
5	5	5	5	5	5	5	5	5	5
7	7	7	7	7	1	7	7	7	7
8	8	8	8	8	8	8	8	8	8

Stability to deformations: definitions

- 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

Warmup: translation invariance

- Representation:

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

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

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- *Equivariance* - all operators commute with L_c : $\square L_c = L_c \square$

$$\begin{aligned}\|\Phi(L_c x) - \Phi(x)\| &= \|L_c \Phi(x) - \Phi(x)\| \\ &\leq \|L_c A_n - A_n\| \cdot \|x\|\end{aligned}$$

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

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- Mallat (2012): $\|L_c A_n - A_n\| \leq \frac{C_2}{\sigma_n} c$
- **Group invariance** (e.g., rotations) with different construction
 - ▶ Group equivariance in P_k, A_k
 - ▶ Global pooling on the group at last layer

Stability to deformations

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- But: $[P_k, L_\tau]$ is **unstable** at high frequencies!

Stability to deformations

- Representation:

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

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

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

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

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

- Suggests several layers with small patches and subsampling for stability + signal preservation

Stability to deformations: final result

Theorem

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

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

- Suggests several layers with small patches and subsampling for stability + signal preservation
- (for generic CNNs, multiply by $\prod_k \rho_k = \prod_k \|W_k\|$)

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RKHS of patch kernels K_k

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

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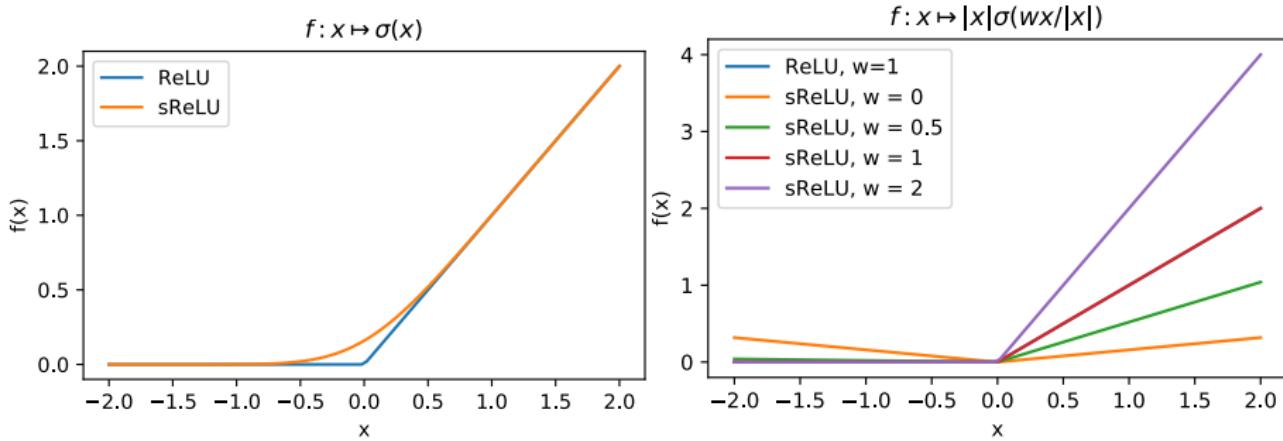
- **Smooth activations**: $\sigma(u) = \sum_{j=0}^{\infty} a_j u^j$
- Norm: $\|f\|_{\mathcal{H}_k}^2 \leq C_\sigma^2(\|g\|^2) = \sum_{j=0}^{\infty} \frac{a_j^2}{b_j} \|g\|^2 < \infty$

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



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

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

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

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- “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

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

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

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- Leads to margin bound $O(\|\hat{f}_n\|R/\gamma\sqrt{N})$ 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)

Deep convolutional representations: conclusions

Study of generic properties

- Deformation stability with small patches, adapted to resolution
- Signal preservation when subsampling \leq patch size
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Applies to learned models

- Same quantity $\|f\|$ controls stability and generalization:
 - ▶ “higher capacity” is needed to discriminate small deformations
 - ▶ Learning is “easier” with stable functions
- Questions:
 - ▶ Better regularization?
 - ▶ How does SGD control capacity in CNNs?

AI Summer School in Grenoble! July 2-6

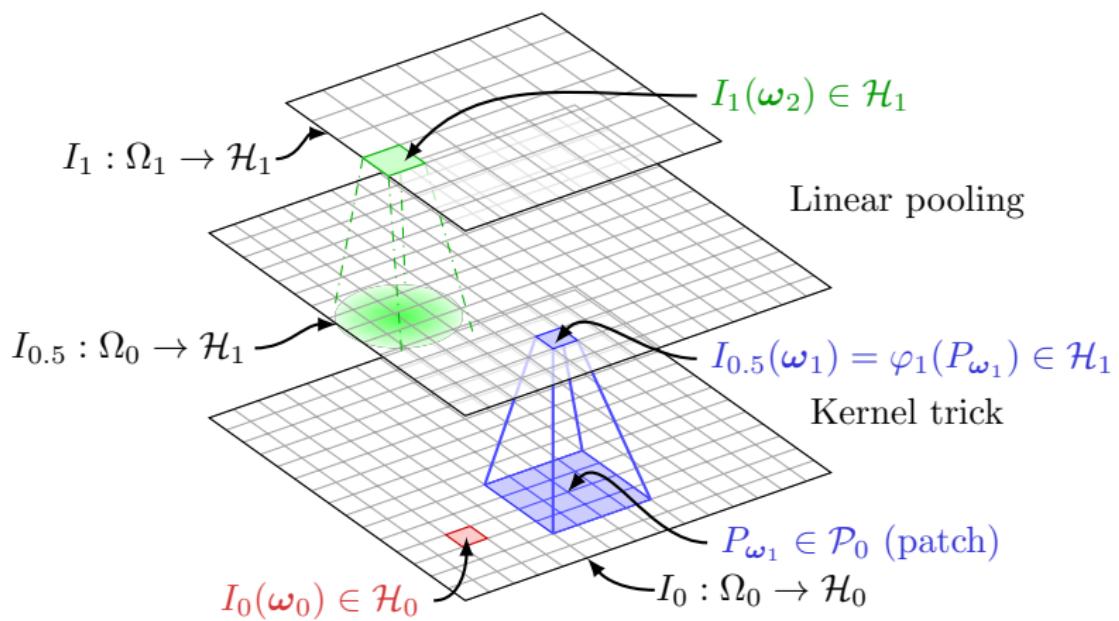
PAISS - <https://project.inria.fr/paiss/>



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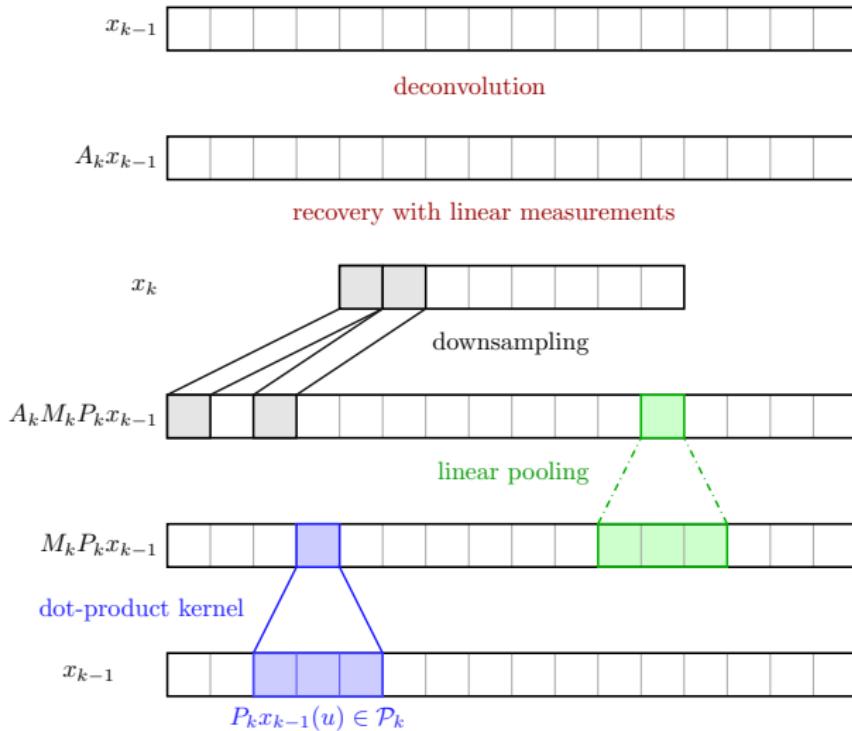
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- **How?** Kernels! Recover patches with **linear functions** (contained in RKHS)

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

Signal recovery: example in 1D



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)

G -equivariant layer construction

- Feature maps $x(u)$ defined on $u \in G$ (G : locally compact group)
- **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

- Stability analysis should work on “compact Lie groups” (similar to Mallat, 2012), e.g., rotations only
- For more complex groups (e.g., roto-translations):
 - ▶ Stability only w.r.t. subgroup (translations) is enough?
 - ▶ Inner layers: only pool on translation group
 - ▶ Last layer: global pooling on rotations
 - ▶ Cohen and Welling (2016): rotation pooling in inner layers hurts performance on Rotated MNIST