

# Towards Deep Kernel Machines

Julien Mairal

Inria, Grenoble

Ohrid, September, 2016



# Part I: Scientific Context

# Adaline: a physical neural net for least square regression

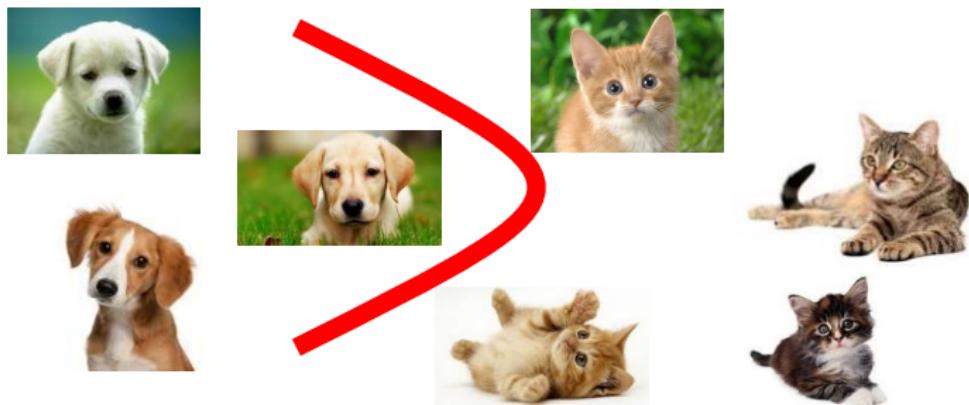


**Figure:** Adaline, [Widrow and Hoff, 1960]: A physical device that performs least square regression using stochastic gradient descent.

# A quick zoom on multilayer neural networks

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

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



# A quick zoom on multilayer neural networks

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

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

## What is specific to multilayer neural networks?

- The “neural network” space  $\mathcal{F}$  is explicitly parametrized by:

$$f(x) = \sigma_k(\mathbf{A}_k \sigma_{k-1}(\mathbf{A}_{k-1} \dots \sigma_2(\mathbf{A}_2 \sigma_1(\mathbf{A}_1 x)) \dots)).$$

- Finding the optimal  $\mathbf{A}_1, \mathbf{A}_2, \dots, \mathbf{A}_k$  yields a **non-convex** optimization problem in **huge dimension**.

# A quick zoom on convolutional neural networks

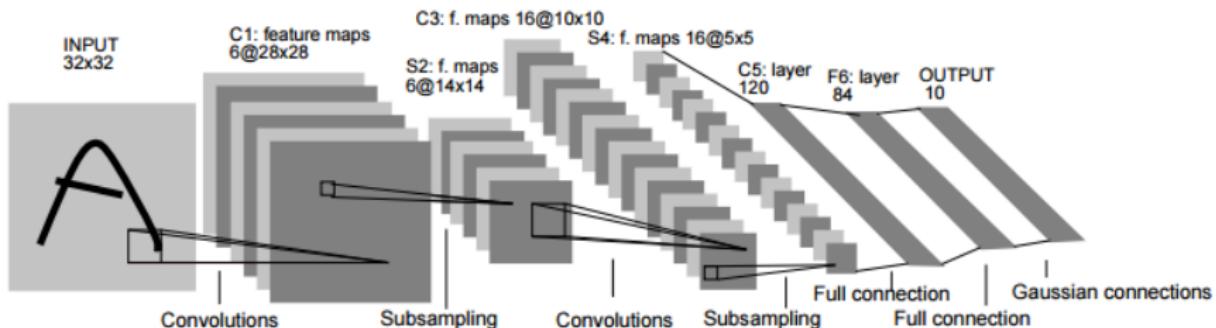


Figure: Picture from LeCun et al. [1998]

- CNNs perform “simple” operations such as convolutions, pointwise non-linearities and subsampling.
- for most successful applications of CNNs, **training is supervised**.

# A quick zoom on convolutional neural networks

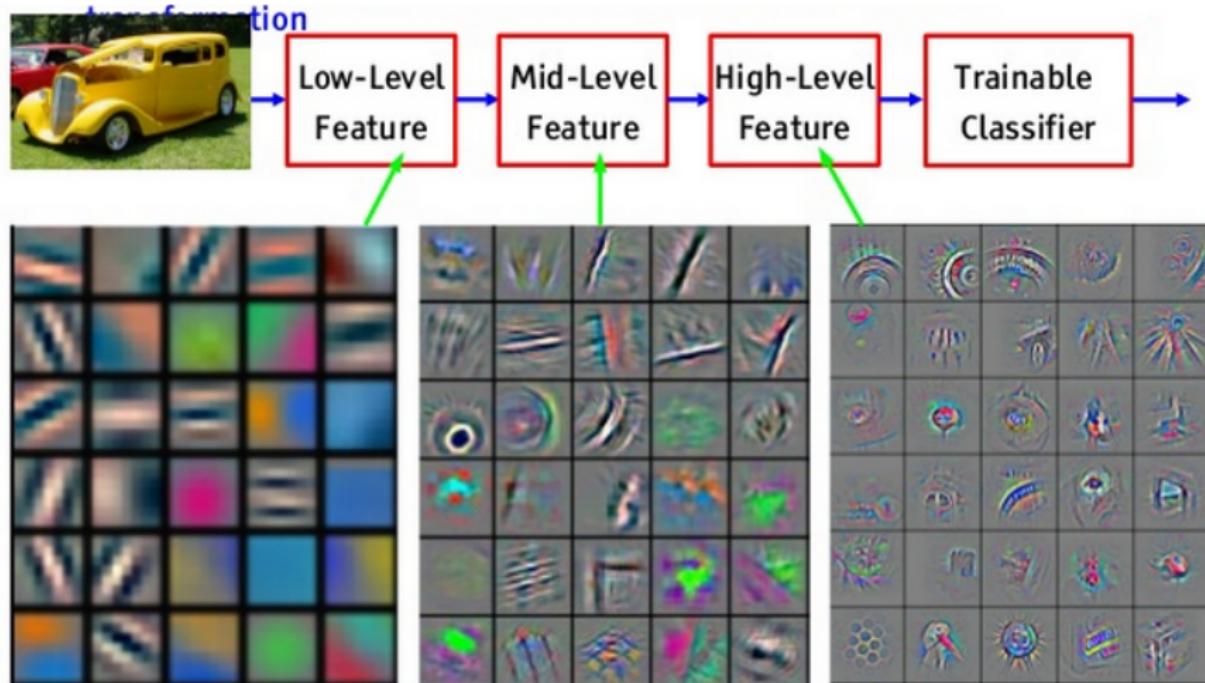


Figure: Picture from Yann LeCun's tutorial, based on Zeiler and Fergus [2014].

# A quick zoom on convolutional neural networks

What are the main features of CNNs?

- they capture **compositional** and **multiscale** structures in images;
- they provide some **invariance**;
- they model **local stationarity** of images at several scales.

# A quick zoom on convolutional neural networks

## What are the main features of CNNs?

- they capture **compositional** and **multiscale** structures in images;
- they provide some **invariance**;
- they model **local stationarity** of images at several scales.

## What are the main open problems?

- very little **theoretical understanding**;
- they require **large amounts of labeled data**;
- they require **manual design and parameter tuning**;

# A quick zoom on convolutional neural networks

## What are the main features of CNNs?

- they capture **compositional** and **multiscale** structures in images;
- they provide some **invariance**;
- they model **local stationarity** of images at several scales.

## What are the main open problems?

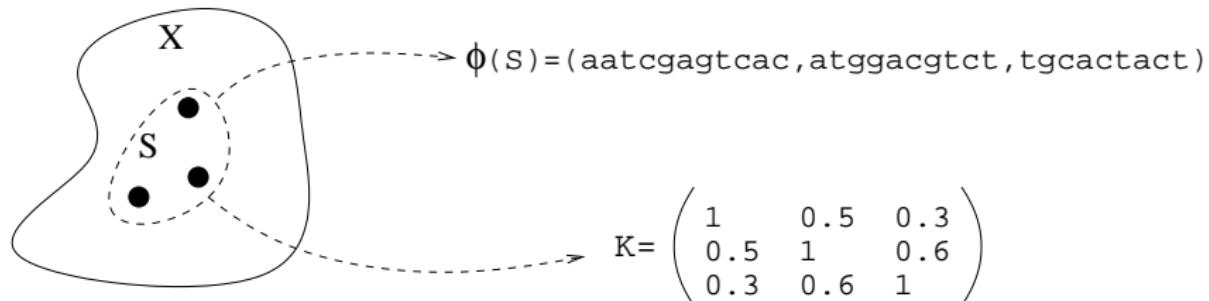
- very little **theoretical understanding**;
- they require **large amounts of labeled data**;
- they require **manual design and parameter tuning**;

Nonetheless...

- they are the focus of a **huge academic and industrial effort**;
- there is **efficient and well-documented open-source software**.

[Choromanska et al., 2015, Livni et al., 2014, Saxena and Verbeek, 2016].

# Context of kernel methods



Idea: representation by pairwise comparisons

- Define a “comparison function”:  $K : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}$ .
- Represent a set of  $n$  data points  $\mathcal{S} = \{\mathbf{x}_1, \dots, \mathbf{x}_n\}$  by the  $n \times n$  matrix:

$$K_{ij} := K(\mathbf{x}_i, \mathbf{x}_j).$$

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

# Context of kernel methods

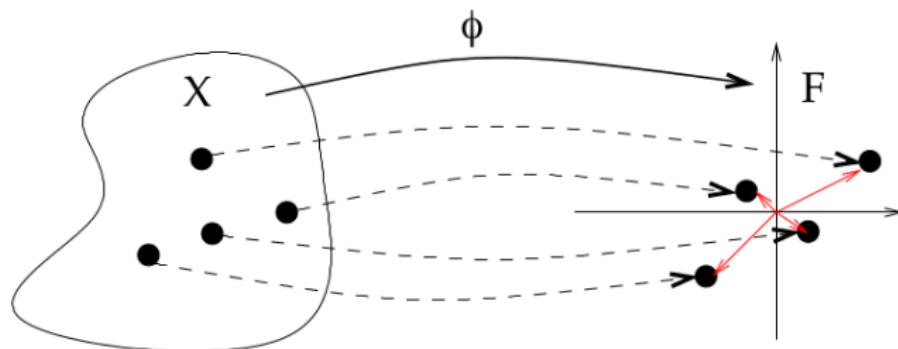
Theorem (Aronszajn, 1950)

$K : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$  is a positive definite kernel if and only if there exists a Hilbert space  $\mathcal{H}$  and a mapping

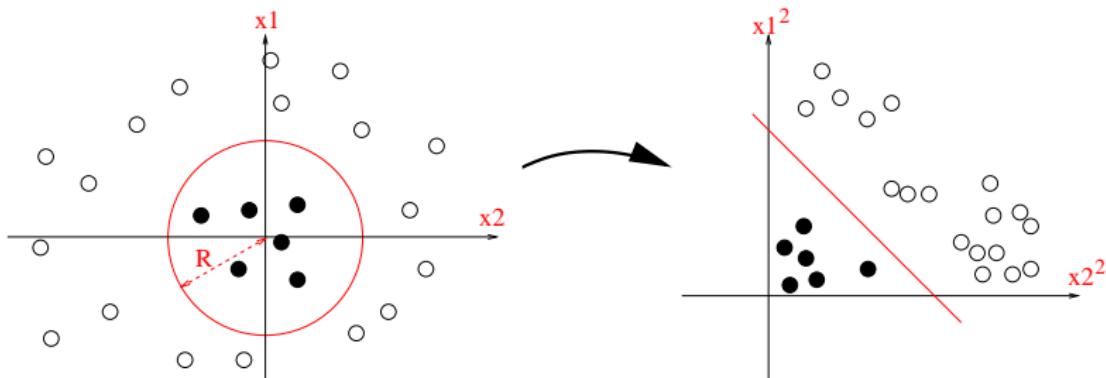
$$\varphi : \mathcal{X} \rightarrow \mathcal{H},$$

such that, for any  $\mathbf{x}, \mathbf{x}'$  in  $\mathcal{X}$ ,

$$K(\mathbf{x}, \mathbf{x}') = \langle \varphi(\mathbf{x}), \varphi(\mathbf{x}') \rangle_{\mathcal{H}}.$$



# Context of kernel methods



## The classical challenge of kernel methods

Find a kernel  $K$  such that

- the data in the feature space  $\mathcal{H}$  has **nice properties**, e.g., linear separability, cluster structure.
- $K$  is **fast to compute**.

# Context of kernel methods

## Mathematical details

- the only thing we require about  $K$  is **symmetry** and **positive definiteness**

$$\forall \mathbf{x}_1, \dots, \mathbf{x}_n \in \mathcal{X}, \alpha_1, \dots, \alpha_n \in \mathbb{R}, \quad \sum_{ij} \alpha_i \alpha_j K(\mathbf{x}_i, \mathbf{x}_j) \geq 0.$$

- then, there exists a Hilbert space  $\mathcal{H}$  of functions  $f : \mathcal{X} \rightarrow \mathbb{R}$ , called the **reproducing kernel Hilbert space (RKHS)** such that

$$\forall f \in \mathcal{H}, \mathbf{x} \in \mathcal{X}, \quad f(\mathbf{x}) = \langle \varphi(\mathbf{x}), f \rangle_{\mathcal{H}},$$

and the mapping  $\varphi : \mathcal{X} \rightarrow \mathcal{H}$  (from Aronszajn's theorem) satisfies

$$\varphi(\mathbf{x}) : \mathbf{y} \mapsto K(\mathbf{x}, \mathbf{y}).$$

# Context of kernel methods

Why mapping data in  $\mathcal{X}$  to the functional space  $\mathcal{H}$ ?

- it becomes feasible to learn a prediction function  $f \in \mathcal{H}$ :

$$\min_{f \in \mathcal{H}} \underbrace{\frac{1}{n} \sum_{i=1}^n L(y_i, f(\mathbf{x}_i))}_{\text{empirical risk, data fit}} + \underbrace{\lambda \|f\|_{\mathcal{H}}^2}_{\text{regularization}}.$$

(why? the solution lives in a finite-dimensional hyperplane).

- non-linear operations in  $\mathcal{X}$  become **inner-products** in  $\mathcal{H}$  since

$$\forall f \in \mathcal{H}, \mathbf{x} \in \mathcal{X}, \quad f(\mathbf{x}) = \langle \varphi(\mathbf{x}), f \rangle_{\mathcal{H}}.$$

- the norm of the RKHS is a **natural regularization function**:

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

# Context of kernel methods

What are the main features of kernel methods?

- **decoupling** of data representation and learning algorithm;
- a huge number of **unsupervised and supervised** algorithms;
- typically, **convex optimization problems** in a supervised context;
- **versatility**: applies to vectors, sequences, graphs, sets, . . . ;
- **natural regularization function** to control the learning capacity;
- **well studied theoretical framework**.

# Context of kernel methods

What are the main features of kernel methods?

- **decoupling** of data representation and learning algorithm;
- a huge number of **unsupervised and supervised** algorithms;
- typically, **convex optimization problems** in a supervised context;
- **versatility**: applies to vectors, sequences, graphs, sets, . . . ;
- **natural regularization function** to control the learning capacity;
- **well studied theoretical framework**.

But...

- **poor scalability in  $n$** , at least  $O(n^2)$ ;
- **decoupling** of data representation and learning may not be a good thing, according to recent **supervised** deep learning success.

# Context of kernel methods

## Challenges

- **Scaling-up kernel methods** with approximate feature maps;

$$K(\mathbf{x}, \mathbf{x}') \approx \langle \psi(\mathbf{x}), \psi(\mathbf{x}') \rangle.$$

[e.g., Williams and Seeger, 2001, Rahimi and Recht, 2007, Vedaldi and Zisserman, 2012]

- Design **data-adaptive and task-adaptive kernels**;
- Build **kernel hierarchies** to capture **compositional** structures.

# Context of kernel methods

## Challenges

- Scaling-up kernel methods with approximate feature maps;

$$K(\mathbf{x}, \mathbf{x}') \approx \langle \psi(\mathbf{x}), \psi(\mathbf{x}') \rangle.$$

[e.g., Williams and Seeger, 2001, Rahimi and Recht, 2007, Vedaldi and Zisserman, 2012]

- Design data-adaptive and task-adaptive kernels;
- Build kernel hierarchies to capture compositional structures.

We need deep kernel  
machines!

# Context of kernel methods

## Challenges

- **Scaling-up kernel methods** with approximate feature maps;

$$K(\mathbf{x}, \mathbf{x}') \approx \langle \psi(\mathbf{x}), \psi(\mathbf{x}') \rangle.$$

[e.g., Williams and Seeger, 2001, Rahimi and Recht, 2007, Vedaldi and Zisserman, 2012]

- Design **data-adaptive and task-adaptive kernels**;
- Build **kernel hierarchies** to capture **compositional** structures.

## Remark

- there exists already successful **data-adaptive** kernels that rely on probabilistic models, e.g., Fisher kernel.

[Jaakkola and Haussler, 1999, Perronnin and Dance, 2007].

## Part II: Convolutional Kernel Networks

# Convolutional kernel networks

## In a nutshell...

- the (happy?) **marriage** of kernel methods and CNNs;
- a hierarchy of kernels for **local image neighborhoods**;
- kernel approximations with **unsupervised or supervised training**;
- applications to **image retrieval and image super-resolution**.

## First proof of concept with unsupervised learning

- J. Mairal, P. Koniusz, Z. Harchaoui and C. Schmid. Convolutional Kernel Networks. NIPS 2014.

## More mature model, compatible with supervised learning

- J. Mairal. End-to-End Kernel Learning with Supervised Convolutional Kernel Networks. NIPS 2016.

**This presentation follows the NIPS'16 paper.**

# Convolutional kernel networks

Idea 1

use the kernel trick to represent image neighborhoods in a RKHS.

Consider an image  $I_0 : \Omega_0 \rightarrow \mathbb{R}^{p_0}$  with  $p_0$  channels. Given **two image patches**  $\mathbf{x}, \mathbf{x}'$  of size  $e_0 \times e_0$ , represented as vectors in  $\mathbb{R}^{p_0 e_0^2}$ , define

$$K_1(\mathbf{x}, \mathbf{x}') = \|\mathbf{x}\| \|\mathbf{x}'\| \kappa_1 \left( \left\langle \frac{\mathbf{x}}{\|\mathbf{x}\|}, \frac{\mathbf{x}'}{\|\mathbf{x}'\|} \right\rangle \right) \quad \text{if } \mathbf{x}, \mathbf{x}' \neq 0 \quad \text{and 0 otherwise,}$$

To ensure positive-definiteness,  $\kappa_1$  needs to be smooth and its Taylor expansion have non-negative coefficients (exercise)

# Convolutional kernel networks

## Idea 1

use the kernel trick to represent image neighborhoods in a RKHS.

Consider an image  $I_0 : \Omega_0 \rightarrow \mathbb{R}^{p_0}$  with  $p_0$  channels. Given **two image patches**  $\mathbf{x}, \mathbf{x}'$  of size  $e_0 \times e_0$ , represented as vectors in  $\mathbb{R}^{p_0 e_0^2}$ , define

$$K_1(\mathbf{x}, \mathbf{x}') = \|\mathbf{x}\| \|\mathbf{x}'\| \kappa_1 \left( \left\langle \frac{\mathbf{x}}{\|\mathbf{x}\|}, \frac{\mathbf{x}'}{\|\mathbf{x}'\|} \right\rangle \right) \quad \text{if } \mathbf{x}, \mathbf{x}' \neq 0 \quad \text{and 0 otherwise,}$$

To ensure positive-definiteness,  $\kappa_1$  needs to be smooth and its Taylor expansion have non-negative coefficients (exercise), e.g.,

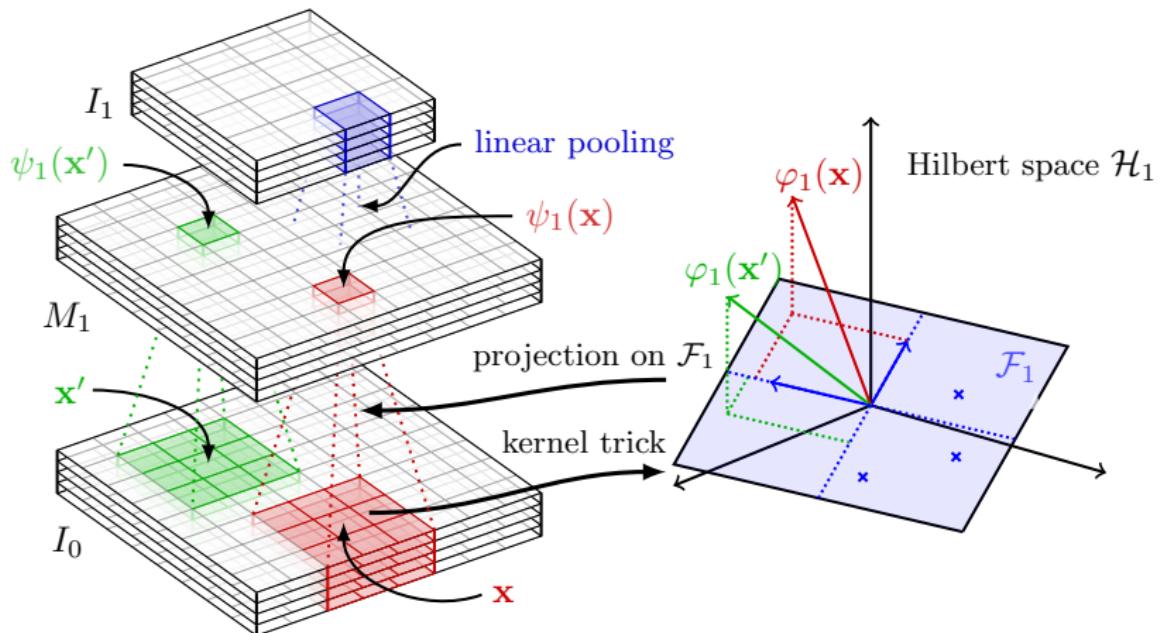
$$\kappa_1(\langle \mathbf{y}, \mathbf{y}' \rangle) = e^{\alpha_1(\langle \mathbf{y}, \mathbf{y}' \rangle - 1)} = e^{-\frac{\alpha_1}{2} \|\mathbf{y} - \mathbf{y}'\|_2^2}.$$

Then, we have implicitly defined the RKHS  $\mathcal{H}_1$  associated to  $K_1$  and a mapping  $\varphi_1 : \mathbb{R}^{p_0 e_0^2} \rightarrow \mathcal{H}_1$ .

# Convolutional kernel networks

Idea 1

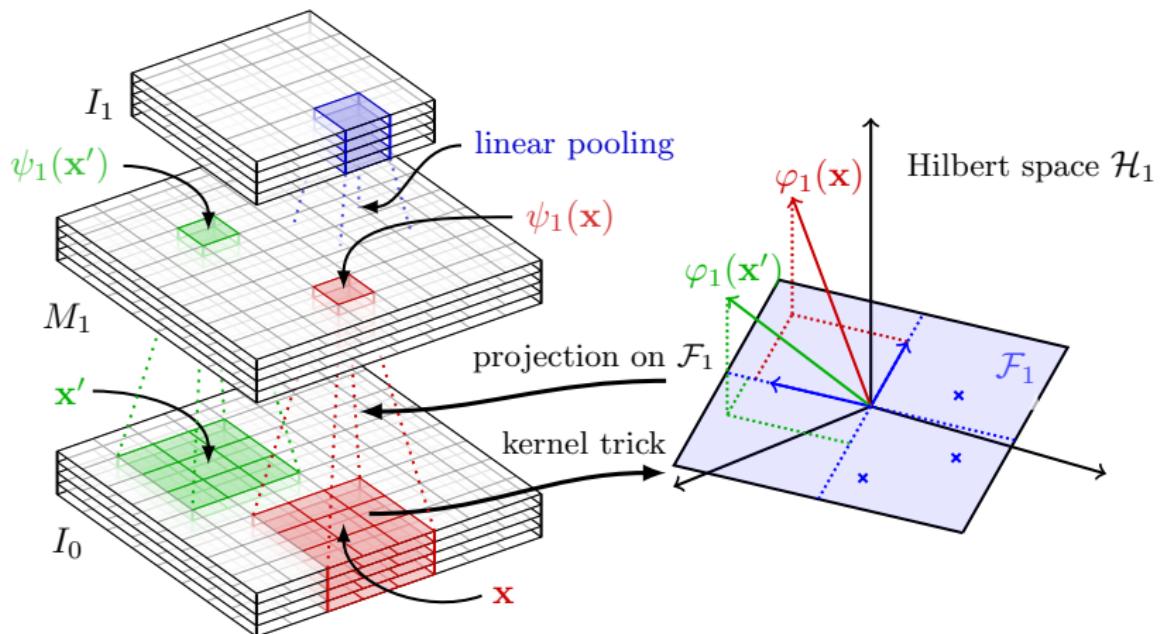
use the kernel trick to represent image neighborhoods in a RKHS.



# Convolutional kernel networks

Idea 2

project onto a finite-dimensional subspace  $\mathcal{F}_1$  of the RKHS  $\mathcal{H}_1$



# Convolutional kernel networks

## Idea 2

project onto a finite-dimensional subspace  $\mathcal{F}_1$  of the RKHS  $\mathcal{H}_1$

- $\mathcal{F}_1$  is defined as the span of  $p_1$  anchor points:

$$\mathcal{F}_1 = \text{Span}(\varphi_1(\mathbf{z}_1), \dots, \varphi_1(\mathbf{z}_{p_1})).$$

The  $\mathbf{z}_j$ 's are vectors in  $\mathbb{R}^{p_0 e_0^2}$  with unit  $\ell_2$ -norm;

- the orthogonal projection of  $\varphi_1(\mathbf{x})$  onto  $\mathcal{F}_1$  is defined as

$$f_{\mathbf{x}} := \arg \min_{f \in \mathcal{F}_1} \|\varphi_1(\mathbf{x}) - f\|_{\mathcal{H}_1}^2,$$

- which is equivalent to

$$f_{\mathbf{x}} := \sum_{j=1}^{p_1} \alpha_j^* \varphi_1(\mathbf{z}_j) \quad \text{with} \quad \boldsymbol{\alpha}^* \in \arg \min_{\boldsymbol{\alpha} \in \mathbb{R}^{p_1}} \left\| \varphi_1(\mathbf{x}) - \sum_{j=1}^{p_1} \alpha_j \varphi_1(\mathbf{z}_j) \right\|_{\mathcal{H}_1}^2.$$

# Convolutional kernel networks

## Idea 2

project onto a finite-dimensional subspace  $\mathcal{F}_1$  of the RKHS  $\mathcal{H}_1$

- for normalized patches  $\mathbf{x}$ , we have  $\boldsymbol{\alpha}^* = \kappa_1(\mathbf{Z}^\top \mathbf{Z})^{-1} \kappa_1(\mathbf{Z}^\top \mathbf{x})$
- we can define a mapping  $\psi_1 : \mathbb{R}^{p_0 e_0^2} \rightarrow \mathbb{R}^{p_1}$  such that

$$\langle f_{\mathbf{x}}, f_{\mathbf{x}'} \rangle_{\mathcal{H}_1} = \langle \psi_1(\mathbf{x}), \psi_1(\mathbf{x}') \rangle,$$

with

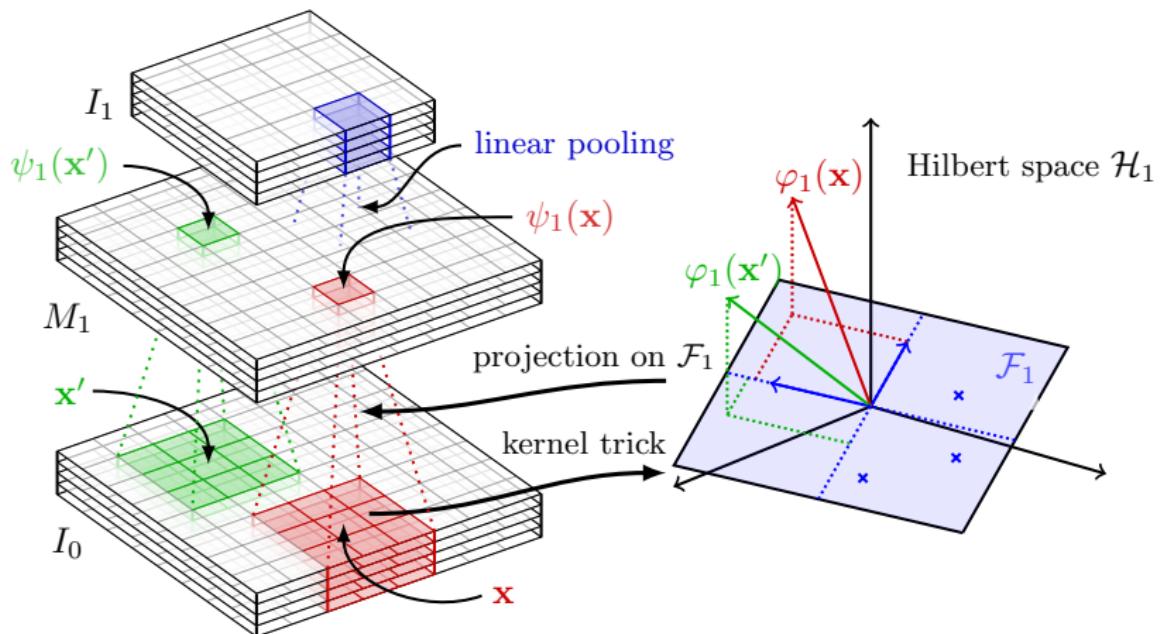
$$\psi_1(\mathbf{x}) := \|\mathbf{x}\| \kappa_1(\mathbf{Z}^\top \mathbf{Z})^{-1/2} \kappa_1 \left( \mathbf{Z}^\top \frac{\mathbf{x}}{\|\mathbf{x}\|} \right) \text{ if } \mathbf{x} \neq 0 \text{ and } 0 \text{ otherwise,}$$

- and subsequently define the map  $M_1 : \Omega_0 \rightarrow \mathbb{R}^{p_1}$  that encodes patches from  $I_0$  centered at positions in  $\Omega_0$ .
- interpretation: **convolution, point-wise non-linearities,  $1 \times 1$  convolution, contrast normalization.**

# Convolutional kernel networks

Idea 2

project onto a finite-dimensional subspace  $\mathcal{F}_1$  of the RKHS  $\mathcal{H}_1$



# Convolutional kernel networks

## Idea 2

project onto a finite-dimensional subspace  $\mathcal{F}_1$  of the RKHS  $\mathcal{H}_1$

- with kernels, we map **patches in infinite dimension**; with the projection, we **manipulate finite-dimensional objects**.
- the projection is classical in kernel approximation techniques (Nyström method [Williams and Seeger, 2001]). The goal is to **align the subspace  $\mathcal{F}_1$  with the data**, or minimize residuals.

Then,

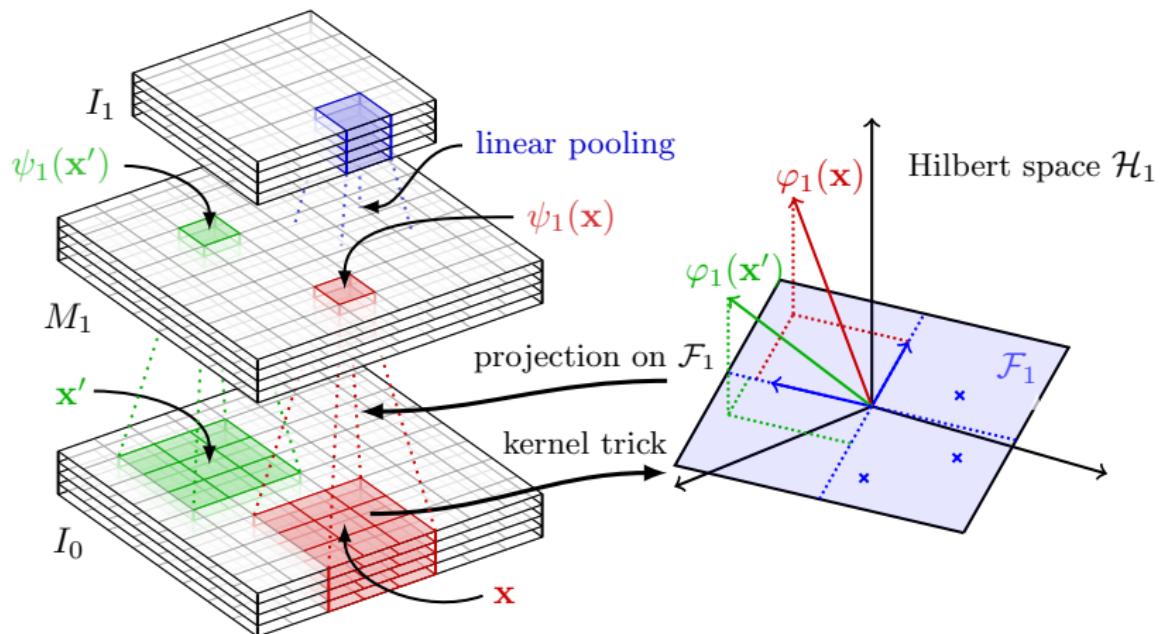
$$K_1(\mathbf{x}, \mathbf{x}') = \langle \varphi_1(\mathbf{x}), \varphi_1(\mathbf{x}') \rangle_{\mathcal{H}_1} \approx \langle f_{\mathbf{x}}, f_{\mathbf{x}'} \rangle_{\mathcal{H}_1} = \langle \psi_1(\mathbf{x}), \psi_1(\mathbf{x}') \rangle.$$

- this provides us simple techniques for **unsupervised learning** of  $\mathbf{Z}$ , e.g., K-means algorithm [Zhang et al., 2008].
- for **supervised learning**, things are a bit more involved (see later).

# Convolutional kernel networks

Idea 3

Linear pooling on  $M_1$  is equivalent to pooling on  $\mathcal{F}_1$ .



# Convolutional kernel networks

## Idea 3

Linear pooling on  $M_1$  is equivalent to pooling on  $\mathcal{F}_1$ .

- like in classical CNNs, we need subsampling to **reduce the dimension of feature maps**.
- we compute  $I_1 : \Omega_1 \rightarrow \mathbb{R}^{p_1}$  as:

$$I_1(z) = \sum_{z' \in \Omega_0} M_1(z') e^{-\beta_1 \|z' - z\|_2^2}.$$

- linear pooling does not break the interpretation in terms of **subspace learning** in  $\mathcal{H}_1$ : a linear combinations of points in  $\mathcal{F}_1$  is still a point in  $\mathcal{F}_1$ .

# Convolutional kernel networks

## Idea 4

Build a multilayer image representation by stacking and composing kernels.

- we obtain a hierarchy of feature maps  $I_0, I_1, \dots, I_k$ , similar to CNNs;
- we define a hierarchy of kernels  $K_1, \dots, K_k$  for increasing sizes of image neighborhoods (receptive fields);
- A kernel  $K_k$  is defined on  $e_k \times e_k$  patches of the map  $I_{k-1}$ , equivalently it is defined on the Cartesian product space  $\mathcal{H}_{k-1}^{e_k \times e_k}$ .

# Convolutional kernel networks

## Remark on input image pre-processing

CKNs seem to be sensitive to pre-processing; we have experimented with

- RAW RGB input;
- local **centering** of every color channel;
- local **whitening** of each color channel;
- 2D **image gradients**.



(a) RAW RGB



(b) centering

# Convolutional kernel networks

## Remark on input image pre-processing

CKNs seem to be sensitive to pre-processing; we have experimented with

- RAW RGB input;
- local **centering** of every color channel;
- local **whitening** of each color channel;
- 2D **image gradients**.



(c) RAW RGB



(d) whitening

# Convolutional kernel networks

## Remark on pre-processing with image gradients and $1 \times 1$ patches

- Every pixel/patch can be represented as a two dimensional vector

$$\mathbf{x} = \rho[\cos(\theta), \sin(\theta)],$$

where  $\rho = \|\mathbf{x}\|$  is the gradient intensity and  $\theta$  is the orientation.

- A natural choice of filters  $\mathbf{Z}$  would be

$$\mathbf{z}_j = [\cos(\theta_j), \sin(\theta_j)] \quad \text{with} \quad \theta_j = 2j\pi/p_0.$$

- Then, the vector  $\psi(\mathbf{x}) = \|\mathbf{x}\|\kappa_1(\mathbf{Z}^\top \mathbf{Z})^{-1/2}\kappa_1\left(\mathbf{Z}^\top \frac{\mathbf{x}}{\|\mathbf{x}\|}\right)$ , can be interpreted as a “soft-binning” of the gradient orientation.
- After pooling, the representation of this first layer is very close to SIFT/HOG descriptors.

Idea borrowed from the kernel descriptors of Bo et al. [2010].

# Convolutional kernel networks

How do we learn the filters **with no supervision?**

we learn one layer at a time, starting from the bottom one.

- We **extract a large number**—say 1 000 000 patches from layers  $k - 1$  computed on an image database and normalize them;
- perform a **spherical K-means algorithm** to learn the filters  $\mathbf{Z}_k$ ;
- **compute the projection matrix**  $\kappa_k(\mathbf{Z}_k^\top \mathbf{Z}_k)^{-1/2}$ .

Remember that every patch is encoded with the formula

$$\psi_k(\mathbf{x}) = \|\mathbf{x}\| \kappa_k (\mathbf{Z}_k^\top \mathbf{Z}_k)^{-1/2} \kappa_k \left( \mathbf{Z}_k^\top \frac{\mathbf{x}}{\|\mathbf{x}\|} \right).$$

# Convolutional kernel networks

How do we learn the filters **with** supervision?

- Given a kernel  $K$  and RKHS  $\mathcal{H}$ , the ERM objective is

$$\min_{f \in \mathcal{H}} \underbrace{\frac{1}{n} \sum_{i=1}^n L(y_i, f(\mathbf{x}_i))}_{\text{empirical risk, data fit}} + \underbrace{\frac{\lambda}{2} \|f\|_{\mathcal{H}}^2}_{\text{regularization}}.$$

- here, we use the parametrized kernel

$$K_{\mathcal{Z}}(I_0, I'_0) = \sum_{z \in \Omega_k} \langle f_k(z), f'_k(z) \rangle_{\mathcal{H}_k} = \sum_{z \in \Omega_k} \langle I_k(z), I'_k(z) \rangle,$$

- and we obtain the simple formulation

$$\min_{\mathbf{W} \in \mathbb{R}^{p_k \times |\Omega_k|}} \frac{1}{n} \sum_{i=1}^n L(y_i, \langle \mathbf{W}, I_k^i \rangle) + \frac{\lambda}{2} \|\mathbf{W}\|_{\text{F}}^2. \quad (1)$$

# Convolutional kernel networks

## How do we learn the filters **with supervision?**

- we **alternate** between the optimization of the filters  $\mathcal{Z}$  and of  $\mathbf{W}$ ;
- for  $\mathbf{W}$ , the problem is strongly-convex and can be tackled with recent algorithms that are much faster than SGD;
- for  $\mathcal{Z}$ , we derive **backpropagation rules** and use classical tricks for learning CNNs (one pass of SGD+momentum);
- we also use a **pre-conditioning heuristic on the sphere**;
- we can also learn the **kernel hyper-parameters**.

The main originality compared to CNN is the **subspace learning interpretation**, due to the projection matrix.

We also use a heuristic for automatically choosing the learning rate of SGD, which was used in all experiments (was never tuned by hand).

# Convolutional kernel networks

Remark on the NIPS'14 paper (older model)

The first paper used a different principle for the kernel approximation:

$$e^{-\frac{1}{2\sigma^2} \|\mathbf{x}-\mathbf{x}'\|_2^2} = \left( \frac{2}{\pi\sigma^2} \right)^{\frac{m}{2}} \int_{\mathbf{w} \in \mathbb{R}^m} e^{-\frac{1}{\sigma^2} \|\mathbf{x}-\mathbf{w}\|_2^2} e^{-\frac{1}{\sigma^2} \|\mathbf{x}'-\mathbf{w}\|_2^2} d\mathbf{w},$$

and a non-convex cost function is formulated to learn the mapping

$$\psi(\mathbf{x}) = [\sqrt{\eta_l} e^{-(1/\sigma^2) \|\mathbf{x}-\mathbf{w}_l\|_2^2}]_{l=1}^p \in \mathbb{R}^p,$$

# Convolutional kernel networks

## Remark on the NIPS'14 paper (older model)

The first paper used a different principle for the kernel approximation:

$$e^{-\frac{1}{2\sigma^2} \|\mathbf{x}-\mathbf{x}'\|_2^2} = \left( \frac{2}{\pi\sigma^2} \right)^{\frac{m}{2}} \int_{\mathbf{w} \in \mathbb{R}^m} e^{-\frac{1}{\sigma^2} \|\mathbf{x}-\mathbf{w}\|_2^2} e^{-\frac{1}{\sigma^2} \|\mathbf{x}'-\mathbf{w}\|_2^2} d\mathbf{w},$$

and a non-convex cost function is formulated to learn the mapping

$$\psi(\mathbf{x}) = [\sqrt{\eta_l} e^{-(1/\sigma^2) \|\mathbf{x}-\mathbf{w}_l\|_2^2}]_{l=1}^p \in \mathbb{R}^p,$$

This is an **approximation scheme**; the mapping  $\psi$  **does not live in the RKHS**. Approximation errors accumulate from one layer to another.

The new scheme (NIPS'16) is **faster to train**, provides **better results** in the unsupervised context, and is **compatible with supervised learning**.

## Related work

- first proof of concept for combining kernels and deep learning [Cho and Saul, 2009];
- hierarchical kernel descriptors [Bo et al., 2011];
- other multilayer models [Bouvie et al., 2009, Montavon et al., 2011, Anselmi et al., 2015];
- deep Gaussian processes [Damianou and Lawrence, 2013]...
- RBF networks [Broomhead and Lowe, 1988].

# Convolutional kernel networks

## Short summary of features

We obtain a particular type of CNN with

- a novel **unsupervised** learning principle;
- a **regularization function** (the norm  $\|\cdot\|_{\mathcal{H}_k}$ ), effective at least in the unsupervised context;
- also compatible with **supervised learning**;
- learning the filters corresponds to **learning linear subspaces**.

## Some perspectives

- use similar principles for **graph-structured data**;
- connect with deep Gaussian processes;
- leverage the literature about **subspace learning**;
- use **union of subspaces**, introduce **sparsity**...

## Part III: Applications

# Image classification

Experiments were conducted on classical “deep learning” datasets, on CPUs only (at the moment).

Dataset	# classes	im. size	$n_{\text{train}}$	$n_{\text{test}}$
CIFAR-10	10	$32 \times 32$	50 000	10 000
SVHN	10	$32 \times 32$	604 388	26 032

We use the following 9-layer network with 512 filters per layer.

Subsampling	$\sqrt{2}$	1	$\sqrt{2}$	1	$\sqrt{2}$	1	$\sqrt{2}$	1	3
Size patches	3	1	3	1	3	1	3	1	3

- we use the squared hinge loss in a one-vs-all setting;
- we use the **supervised** CKNs;
- The regularization parameter  $\lambda$  and the number of epochs are set by first running the algorithm on a 80/20% validation split.

# Image classification

	Stoch P. [29]	MaxOut [9]	NiN [17]	DSN [15]	Gen P. [14]	SCKN (Ours)
CIFAR-10	15.13	11.68	10.41	9.69	<b>7.62</b>	10.20
SVHN	2.80	2.47	2.35	1.92	<b>1.69</b>	2.04

**Figure:** Figure from the NIPS'16 paper (preprint arXiv). Error rates in percents for single models with no data augmentation.

## Remarks on CIFAR-10

- simpler model (5 layers, with integer subsampling factors) also performs well  $\approx 12\%$ ;
- the original model of Krizhevsky et al. [2012] does  $\approx 18\%$ ;
- the best **unsupervised** architecture has two layers, is wide (1024-16384 filters), and achieves 14.2%;
- the **unsupervised** model reported in the NIPS'14 was 21.7% (same model here 19.3%).

## Image super-resolution

The task is to predict a high-resolution  $y$  image from low-resolution one  $x$ . This may be formulated as a **multivariate regression problem**.



(a) Low-resolution  $y$



(b) High-resolution  $x$

## Image super-resolution

The task is to predict a high-resolution  $y$  image from low-resolution one  $x$ . This may be formulated as a **multivariate regression problem**.



(c) Low-resolution  $y$



(d) Bicubic interpolation

## Image super-resolution

Following classical approaches based on CNNs [Dong et al., 2016], we want to predict high-resolution images from bicubic interpolations.

- we use the **square loss** instead of a classification loss;
- models are trained to **up-scale by a factor 2**, using a database of 200 000 pairs of high/low-res patches of size  $32 \times 32$  and  $16 \times 16$ ;
- we also use a 9-layer network with  $3 \times 3$  patches, 128 filters at every layer, no pooling, no zero-padding;
- to perform  $x3$  upscaling, we simply apply  $x2$  twice, and downsample by  $3/4$ ;

# Image super-resolution

Fact.	Dataset	Bicubic	SC	CNN	CSCN	SCKN
x2	Set5	33.66	35.78	36.66	36.93	<b>37.07</b>
	Set14	30.23	31.80	32.45	32.56	<b>32.76</b>
	Kodim	30.84	32.19	32.80	32.94	<b>33.21</b>
x3	Set5	30.39	31.90	32.75	<b>33.10</b>	33.08
	Set14	27.54	28.67	29.29	29.41	<b>29.50</b>
	Kodim	28.43	29.21	29.64	29.76	<b>29.88</b>

**Table:** Reconstruction accuracy for super-resolution in PSNR (the higher, the better). All CNN approaches are without data augmentation at test time.

## Remarks

- CNN is a “vanilla CNN”;
- Kim et al. [2016] from CVPR’16 does better by using very deep CNNs and residual learning;
- CSCN combines ideas from sparse coding and CNNs;

[Zeyde et al., 2010, Dong et al., 2016, Wang et al., 2015, Kim et al., 2016].

# Image super-resolution



Bicubic

Sparse coding

CNN

SCKN (Ours)

Figure: Results for x3 upscaling.

# Image super-resolution

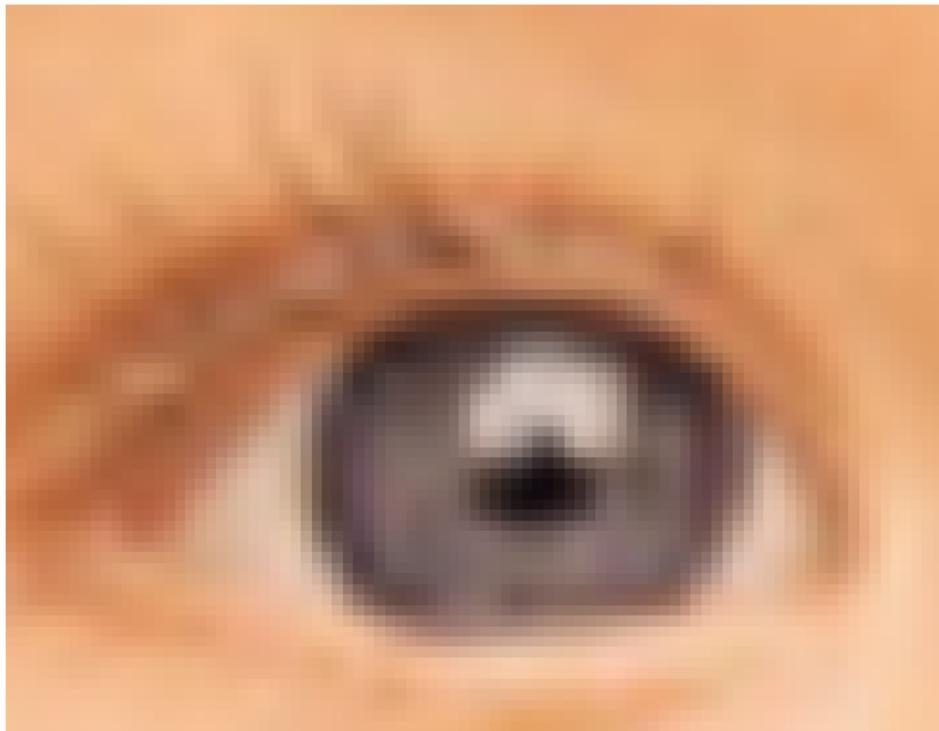


Figure: Bicubic

## Image super-resolution

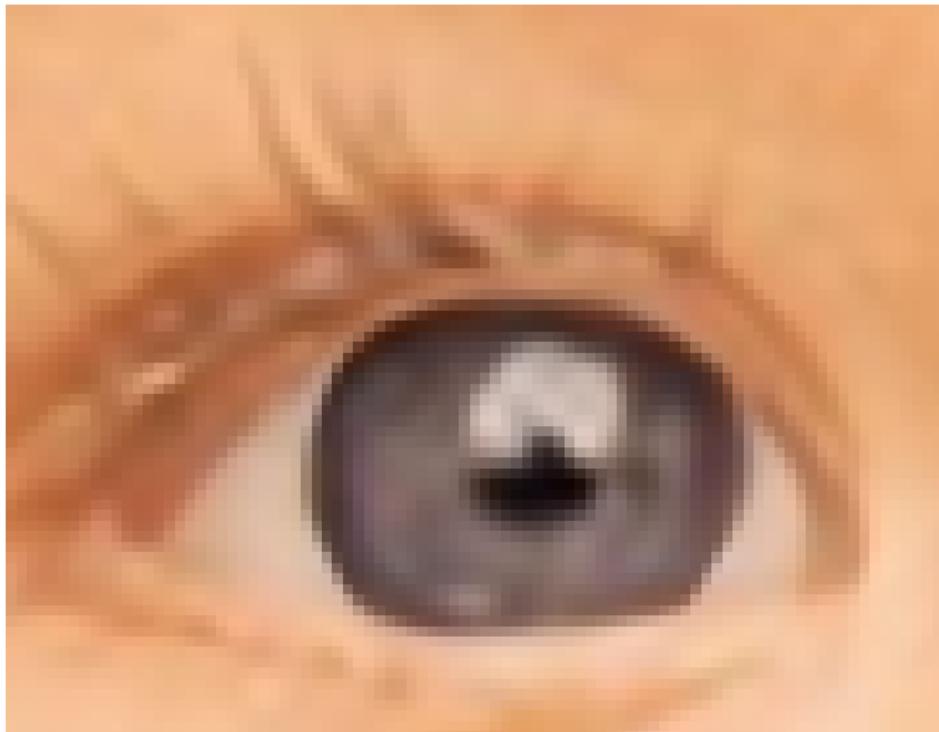
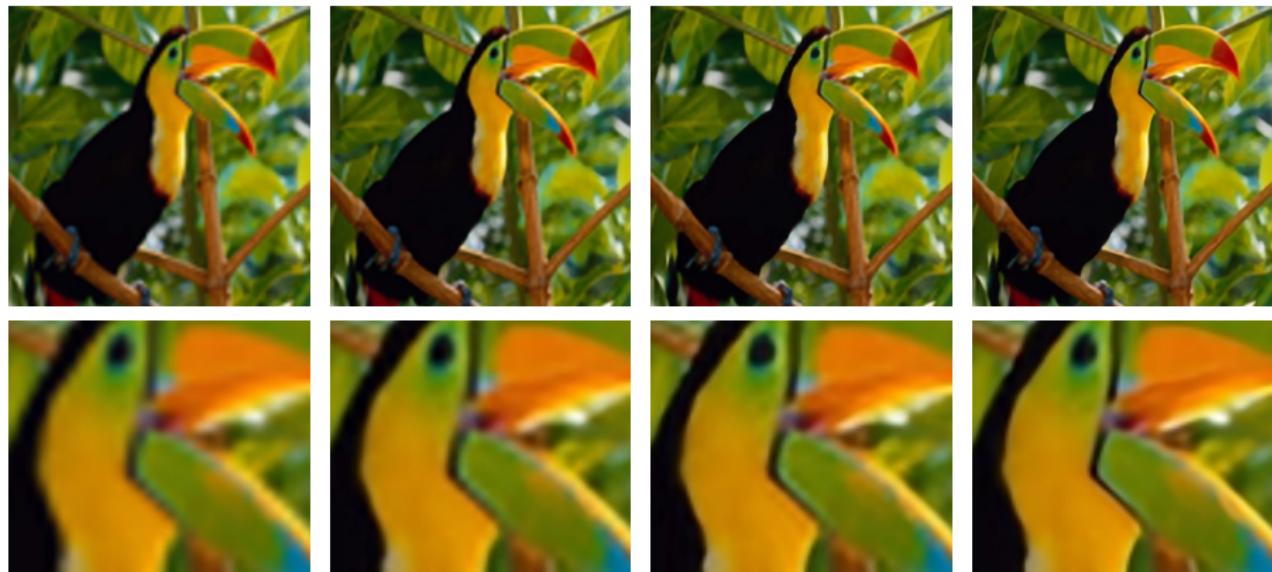


Figure: SCKN

# Image super-resolution



Bicubic

Sparse coding

CNN

SCKN (Ours)

Figure: Results for x3 upscaling.

# Image super-resolution

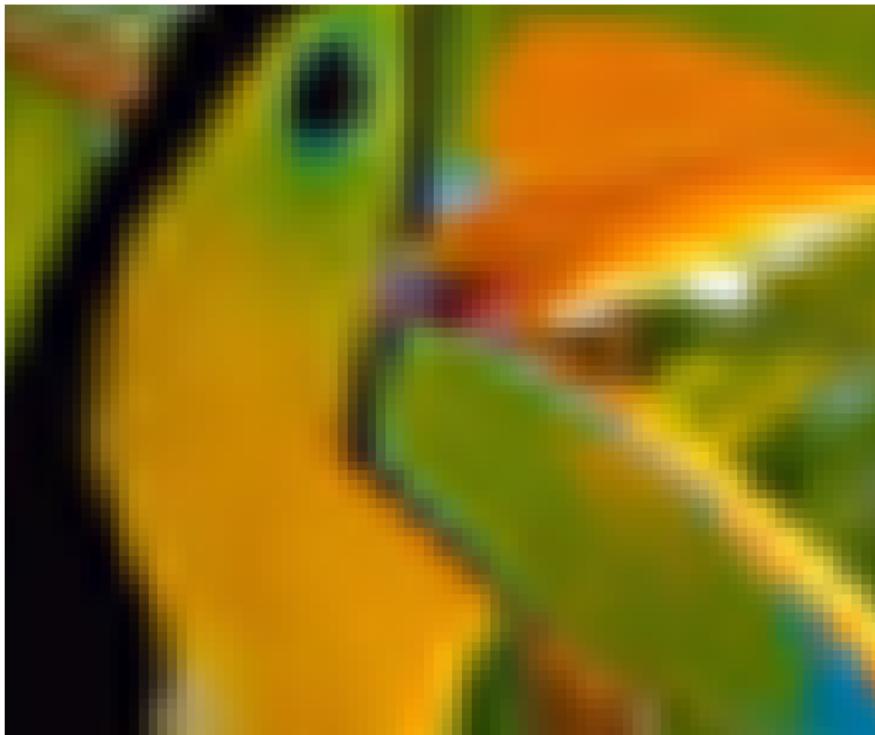


Figure: Bicubic

# Image super-resolution

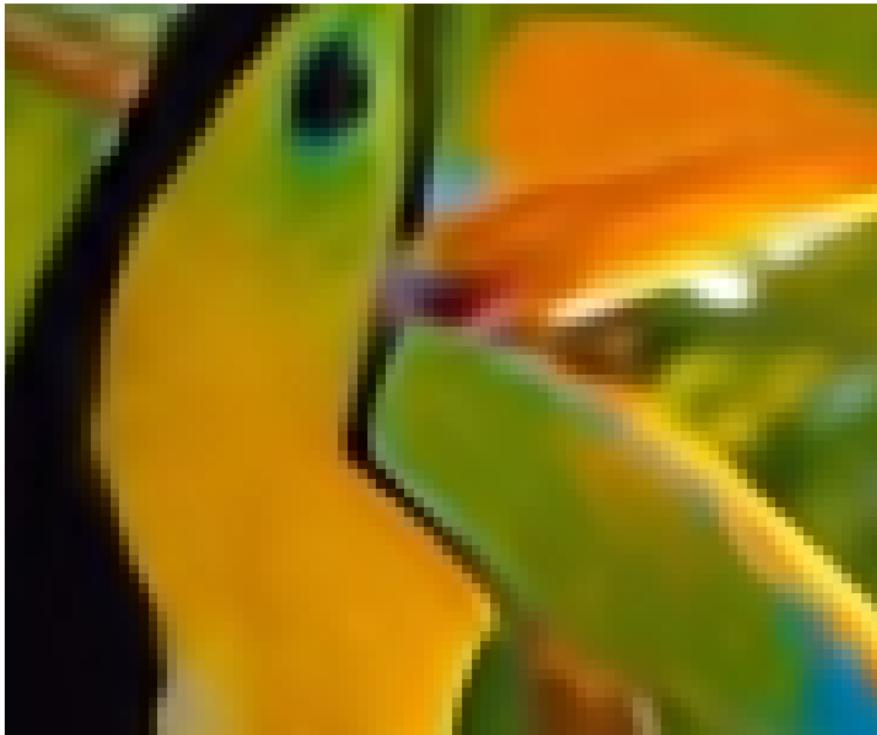


Figure: SCKN

# Image super-resolution

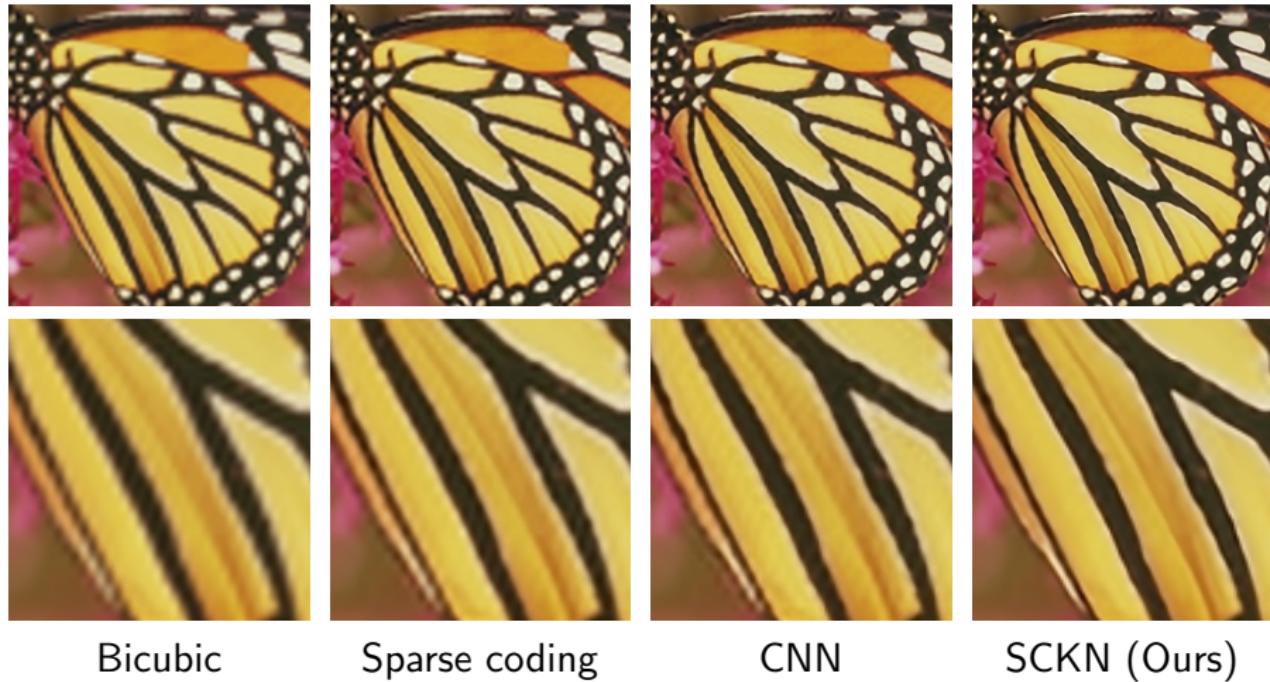


Figure: Results for x3 upscaling.

# Image super-resolution

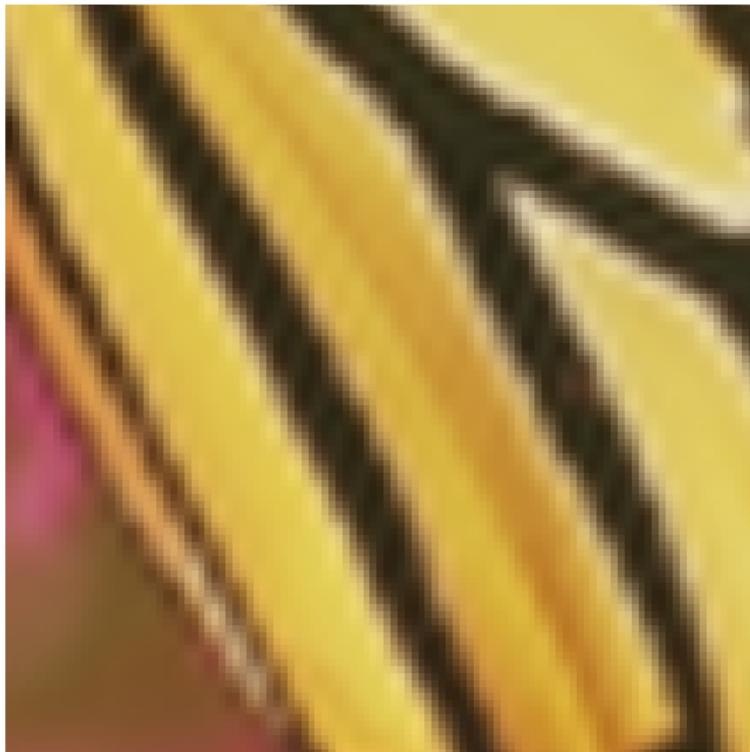


Figure: Bicubic

# Image super-resolution

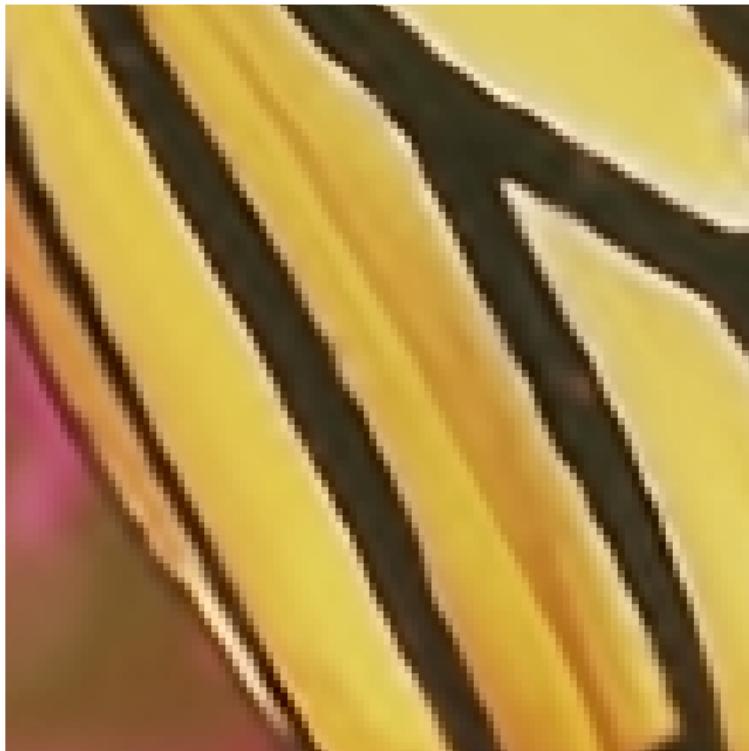


Figure: SCKN

# Image super-resolution



Bicubic

CNN

SCKN (Ours)

Figure: Results for x3 upscaling.

# Image super-resolution



Figure: Bicubic

## Image super-resolution



Figure: SCKN

# Image retrieval

## Collaborators



Zaid  
Harchaoui



Cordelia  
Schmid



Florent  
Perronnin



Matthijs  
Douze



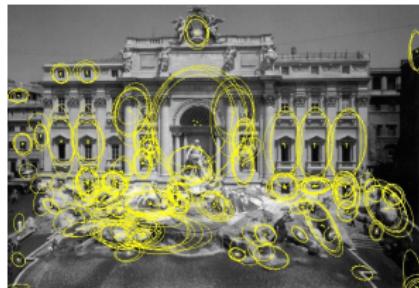
Mattis  
Paulin

## Publications

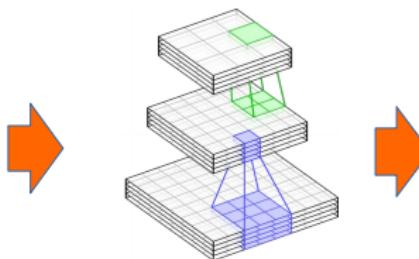
- M. Paulin, J. Mairal, M. Douze, Z. Harchaoui, F. Perronnin and C. Schmid. Convolutional Patch Representations for Image Retrieval: an Unsupervised Approach. IJCV 2016.
- M. Paulin, M. Douze, Z. Harchaoui, J. Mairal, F. Perronnin and C. Schmid. Local Convolutional Features with Unsupervised Training for Image Retrieval. ICCV 2015.

These publications use the older model of the CKN (NIPS'14).

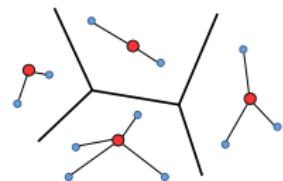
# Image retrieval



Keypoint detection  
*Hessian-affine*



Patch description  
*Deep Network*



Aggregation  
*VLAD*

## Remarks

- possibly followed by PCA to **reduce the dimension**;
- retrieval is performed by **simple inner-product evaluations**;
- here, we evaluate only the **patch representation**.

# Image retrieval

From patches...



# Image retrieval

To images...



## Remarks

- We benchmark both tasks at the same time;
- retrieval **differs significantly from classification**; Training a CNN for retrieval **with supervision** is hard;
- results using supervision have been mitigated until CVPR/ECCV'16.

[Babenko et al., 2014, Babenko and Lempitsky, 2015, Gong et al., 2014, Fischer et al., 2014, Zagoruyko and Komodakis, 2015, Radenović et al., 2016, Gordo et al., 2016].

## Image retrieval

- we use a patch retrieval task to optimize model parameters;
- we try different input types: RGB, RGB+whitening, gradients;

Input	Layer 1	Layer 2	dim.
<b>CKN-raw</b>	5x5, 5, 512	—	41,472
<b>CKN-white</b>	3x3, 3, 128	2x2, 2, 512	32,768
<b>CKN-grad</b>	1x1, 3, 16	4x4, 2, 1024	50,176

- training is fast, 10mn on a GPU (would be about 1mn on a CPU with the NIPS'16 paper);
- dimensionality is then reduced with PCA + whitening.

# Image retrieval

## Evaluation of different patch representations for patch retrieval

Architecture	coverage	Dim	RomePatches	Miko.
			train	
SIFT	51x51	128	91.6	87.9
AlexNet-conv1	11x11	96	66.4	65.0
AlexNet-conv2	51x51	256	73.8	69.9
AlexNet-conv3	99x99	384	81.6	79.2
AlexNet-conv4	131x131	384	78.4	75.7
AlexNet-conv5	163x163	256	53.9	49.6
PhilippNet	64x64	512	86.1	81.4
PhilippNet	91x91	2048	88.0	83.7
CKN-grad	51x51	1024	<b>92.5</b>	<b>88.1</b>
CKN-raw	51x51	1024	79.3	76.3
CKN-white	51x51	1024	91.9	87.7
				<b>62.5</b>

[Krizhevsky et al., 2012, Fischer et al., 2014].

## Image retrieval

...which become, in the same pipeline, for **image** retrieval

	<b>Holidays</b>	<b>UKB</b>	<b>Oxford</b>	<b>Rome</b>	
				train	test
SIFT	64.0	3.44	43.7	52.9	62.7
AlexNet-conv1	59.0	3.33	18.8	28.9	36.8
AlexNet-conv2	62.7	3.19	12.5	36.1	21.0
AlexNet-conv3	<b>79.3</b>	3.74	33.3	47.1	54.7
AlexNet-conv4	77.1	3.73	34.3	47.9	55.4
AlexNet-conv5	75.3	3.69	33.4	45.7	53.1
PhilippNet 64x64	74.1	3.66	38.3	50.2	60.4
PhilippNet 91x91	74.7	3.67	43.6	51.4	61.3
CKN-grad	66.5	3.42	<b>49.8</b>	<b>57.0</b>	<b>66.2</b>
CKN-raw	69.9	3.54	23.0	33.0	43.8
CKN-white	78.7	3.74	41.8	51.9	62.4
CKN-mix	<b>79.3</b>	<b>3.76</b>	43.4	54.5	65.3

# Image retrieval

## Comparison with other pipelines

Method \ Dataset	Holidays	UKB	Oxford
VLAD [Jégou et al., 2012]	63.4	3.47	-
VLAD++ [Arandjelovic and Zisserman, 2013]	64.6	-	<b>55.5</b>
Global-CNN [Babenko et al., 2014]	79.3	3.56	54.5
MOP-CNN [Gong et al., 2014]	80.2	-	-
Sum-pooling OxfordNet [Babenko and Lempitsky, 2015]	80.2	3.65	53.1
Ours	79.3	3.76	49.8
Ours+PCA 4096	<b>82.9</b>	<b>3.77</b>	47.2

## Remarks

- this is a comparison with relatively high-dimensional descriptors;
- with dense feature extraction, our model does 55.5 for Oxford;
- supervised CNNs for retrieval have been mitigated until CVPR/ECCV'16 (see O. Chum's talk + [Gordo et al., 2016]);
- these results use the older NIPS'14 model and no supervision.

# Conclusion

## First achievements

- new type of convolutional networks where **learning filters amount to learning subspaces**;
- new principles for **unsupervised learning** of deep network, also compatible with **supervised learning**.
- **competitive results** for image super-resolution, classification, and patch representation in image retrieval;

## Future work

- build semi-generic models for **structured data**;
- explore novel **subspace learning models and algorithms**;
- study theoretically invariant properties of the kernels;

## Software

- coming soon (with GPU implementation)...

## References I

- Fabio Anselmi, Lorenzo Rosasco, Cheston Tan, and Tomaso Poggio.  
Deep convolutional networks are hierarchical kernel machines. *arXiv preprint arXiv:1508.01084*, 2015.
- Relja Arandjelovic and Andrew Zisserman. All about VLAD. In *IEEE Conference on Computer Vision and Pattern Recognition*, 2013.
- Artem Babenko and Victor Lempitsky. Aggregating local deep features for image retrieval. In *Proceedings of the IEEE International Conference on Computer Vision*, pages 1269–1277, 2015.
- Artem Babenko, Anton Slesarev, Alexandr Chigorin, and Victor Lempitsky. Neural codes for image retrieval. In *European Conference on Computer Vision*, 2014.
- L. Bo, X. Ren, and D. Fox. Kernel descriptors for visual recognition. In *Adv. NIPS*, 2010.

## References II

- L. Bo, K. Lai, X. Ren, and D. Fox. Object recognition with hierarchical kernel descriptors. In *Proc. CVPR*, 2011.
- J. V. Bouvrie, L. Rosasco, and T. Poggio. On invariance in hierarchical models. In *Adv. NIPS*, 2009.
- David S Broomhead and David Lowe. Radial basis functions, multi-variable functional interpolation and adaptive networks. Technical report, DTIC Document, 1988.
- Y. Cho and L. K. Saul. Kernel methods for deep learning. In *Adv. NIPS*, 2009.
- A. Choromanska, M. Henaff, M. Mathieu, G. Ben Arous, and Y. LeCun. The loss surfaces of multilayer networks. In *Proc. AISTATS*, 2015.
- A. Damianou and N. Lawrence. Deep Gaussian processes. In *Proc. AISTATS*, 2013.

## References III

- C. Dong, C. C. Loy, K. He, and X. Tang. Image super-resolution using deep convolutional networks. *IEEE T. Pattern Anal.*, 38(2):295–307, 2016.
- Philipp Fischer, Alexey Dosovitskiy, and Thomas Brox. Descriptor matching with Convolutional Neural Networks: a comparison to SIFT. arXiv Preprint, 2014.
- Yunchao Gong, Liwei Wang, Ruiqi Guo, and Svetlana Lazebnik. Multi-scale orderless pooling of deep convolutional activation features. In *European Conference on Computer Vision*, 2014.
- Albert Gordo, Jon Almazan, Jerome Revaud, and Diane Larlus. Deep image retrieval: Learning global representations for image search. *arXiv preprint arXiv:1604.01325*, 2016.
- T. Jaakkola and D. Haussler. Exploiting generative models in discriminative classifiers. *Advances in neural information processing systems*, 1999.

## References IV

- Hervé Jégou, Florent Perronnin, Matthijs Douze, Jorge Sánchez, Patrick Pérez, and Cordelia Schmid. Aggregating local image descriptors into compact codes. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 2012.
- Jiwon Kim, Jung Kwon Lee, and Kyoung Mu Lee. Accurate image super-resolution using very deep convolutional networks. In *Proc. CVPR*, 2016.
- A. Krizhevsky, I. Sutskever, and G. E. Hinton. Imagenet classification with deep convolutional neural networks. In *Adv. NIPS*, 2012.
- Y. LeCun, L. Bottou, Y. Bengio, and P. Haffner. Gradient-based learning applied to document recognition. *P. IEEE*, 86(11):2278–2324, 1998.
- Roi Livni, Shai Shalev-Shwartz, and Ohad Shamir. On the computational efficiency of training neural networks. In *Advances in Neural Information Processing Systems*, pages 855–863, 2014.

## References V

- Grégoire Montavon, Mikio L Braun, and Klaus-Robert Müller. Kernel analysis of deep networks. *Journal of Machine Learning Research*, 12 (Sep):2563–2581, 2011.
- F. Perronnin and C. Dance. Fisher kernels on visual vocabularies for image categorization. In *Proc. CVPR*, 2007.
- Filip Radenović, Giorgos Tolias, and Ondřej Chum. Cnn image retrieval learns from bow: Unsupervised fine-tuning with hard examples. *arXiv preprint arXiv:1604.02426*, 2016.
- A. Rahimi and B. Recht. Random features for large-scale kernel machines. In *Adv. NIPS*, 2007.
- Shreyas Saxena and Jakob Verbeek. Convolutional neural fabrics. *arXiv preprint arXiv:1606.02492*, 2016.
- Bernhard Schölkopf and Alexander J Smola. *Learning with kernels: support vector machines, regularization, optimization, and beyond*. MIT press, 2002.

## References VI

- J. Shawe-Taylor and N. Cristianini. *Kernel methods for pattern analysis*. 2004.
- A. Vedaldi and A. Zisserman. Efficient additive kernels via explicit feature maps. *IEEE T. Pattern Anal.*, 34(3):480–492, 2012.
- Z. Wang, D. Liu, J. Yang, W. Han, and T. Huang. Deep networks for image super-resolution with sparse prior. In *Proc. ICCV*, 2015.
- B. Widrow and M. E. Hoff. Adaptive switching circuits. In *IRE WESCON convention record*, volume 4, pages 96–104. New York, 1960.
- C. Williams and M. Seeger. Using the Nyström method to speed up kernel machines. In *Adv. NIPS*, 2001.
- Serguey Zagoruyko and Nikos Komodakis. Learning to compare image patches via convolutional neural networks. In *IEEE Conference on Computer Vision and Pattern Recognition*, 2015.

## References VII

- M. D. Zeiler and R. Fergus. Visualizing and understanding convolutional networks. In *Proc. ECCV*, 2014.
- R. Zeyde, M. Elad, and M. Protter. On single image scale-up using sparse-representations. In *Curves and Surfaces*, pages 711–730. 2010.
- K. Zhang, I. W. Tsang, and J. T. Kwok. Improved Nyström low-rank approximation and error analysis. In *Proc. ICML*, 2008.