On the Happy Marriage of Kernel Methods and Deep Learning

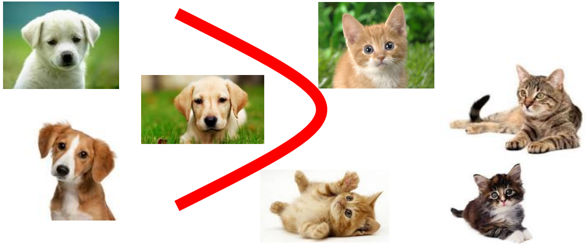
Julien Mairal

Inria Grenoble

Context of supervised learning

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

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



[Vapnik, 1995, Bottou, Curtis, and Nocedal, 2016]...

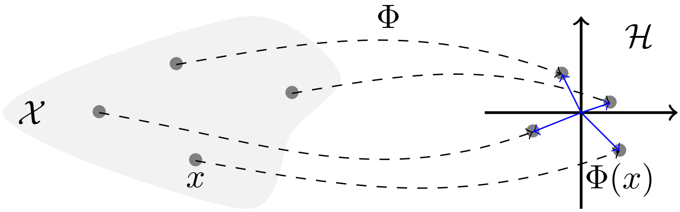
Kernel Methods 1/2

In the context of supervised learning with labels in $\mathbb{R}$,

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

- **map** data x in $\mathcal{X}$ to a Hilbert space and work with **linear forms**:

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



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

Kernel Methods 2/2

In the context of supervised learning with labels in $\mathbb{R}$,

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

- $f(x) = \langle \Phi(x), f \rangle_{\mathcal{H}}$ but $\Phi(x)$ may be very high- or infinite-dimensional.
- then, only manipulate **inner-products** $K(x, x') = \langle \Phi(x), \Phi(x') \rangle_{\mathcal{H}}$ (kernel trick).
- Alternatively, compute a finite-dimensional approximate embedding $f(x) \approx w^\top \Psi(x)$;
- **regularize** with $\|.\|_{\mathcal{H}}$ (encourages smoothness);

Kernel Methods 2/2

In the context of supervised learning with labels in $\mathbb{R}$,

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

- $f(x) = \langle \Phi(x), f \rangle_{\mathcal{H}}$ but $\Phi(x)$ may be very high- or infinite-dimensional.
- then, only manipulate **inner-products** $K(x, x') = \langle \Phi(x), \Phi(x') \rangle_{\mathcal{H}}$ (kernel trick).
- Alternatively, compute a finite-dimensional approximate embedding $f(x) \approx w^\top \Psi(x)$;
- **regularize** with $\|.\|_{\mathcal{H}}$ (encourages smoothness);

If you want to know more (24 hours course)

`http://members.cbio.mines-paristech.fr/~jvert/svn/kernelcourse/slides/master2017/master2017.pdf`

Relation with deep learning?

A functional space viewpoint: kernels for deep networks

- View deep networks as functions in some functional space;
- Non-parametric models, natural measures of complexity (*e.g.*, norms);
- Linearization $f(x) = \langle f, \Phi(x) \rangle$ decouples learning f from data representation $\Phi(x)$.

Relation with deep learning?

A functional space viewpoint: kernels for deep networks

- View deep networks as functions in some functional space;
- Non-parametric models, natural measures of complexity (*e.g.*, norms);
- Linearization $f(x) = \langle f, \Phi(x) \rangle$ decouples learning f from data representation $\Phi(x)$.

What is an appropriate functional space?

Relation with deep learning?

A functional space viewpoint: kernels for deep networks

- View deep networks as functions in some functional space;
- Non-parametric models, natural measures of complexity (*e.g.*, norms);
- Linearization $f(x) = \langle f, \Phi(x) \rangle$ decouples learning f from data representation $\Phi(x)$.

What is an appropriate functional space?

Deep learning for kernels

- Scalable learning with finite-dimensional embeddings;
- Deep networks with a geometric interpretation and regularization principles;
- End-to-end learning with kernels?

Relation with deep learning?

A functional space viewpoint: kernels for deep networks

- View deep networks as functions in some functional space;
- Non-parametric models, natural measures of complexity (*e.g.*, norms);
- Linearization $f(x) = \langle f, \Phi(x) \rangle$ decouples learning f from data representation $\Phi(x)$.

What is an appropriate functional space?

Deep learning for kernels

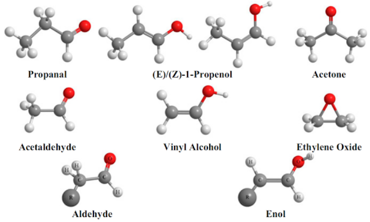
- Scalable learning with finite-dimensional embeddings;
- Deep networks with a geometric interpretation and regularization principles;
- End-to-end learning with kernels?

How do we proceed?

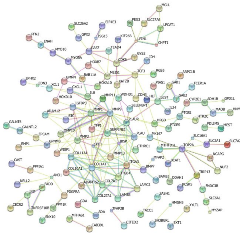
Graph Modeling

- D. Chen, L. Jacob and J. Mairal. Convolutional Kernel Networks for Graph-Structured Data. International Conference on Machine Learning (ICML). 2020.

Graph-structured data is everywhere

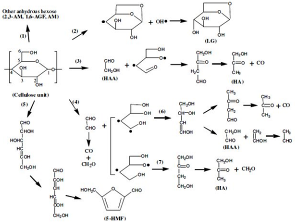


(a) molecules



(b) protein regulation

(c) social networks



(d) chemical pathways

Learning graph representations

State-of-the-art models for representing graphs:

- **Deep learning for graphs**: graph neural networks (GNNs);
- **Graph kernels**: Weisfeiler-Lehman (WL) graph kernels;
- **Hybrid models** attempt to bridge both worlds: graph neural tangent kernels (GNTK).

Learning graph representations

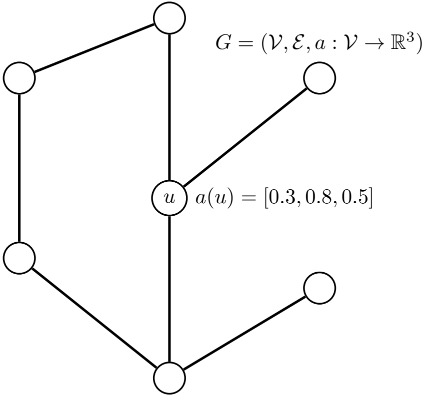
State-of-the-art models for representing graphs:

- **Deep learning for graphs**: graph neural networks (GNNs);
- **Graph kernels**: Weisfeiler-Lehman (WL) graph kernels;
- **Hybrid models** attempt to bridge both worlds: graph neural tangent kernels (GNTK).

Our model:

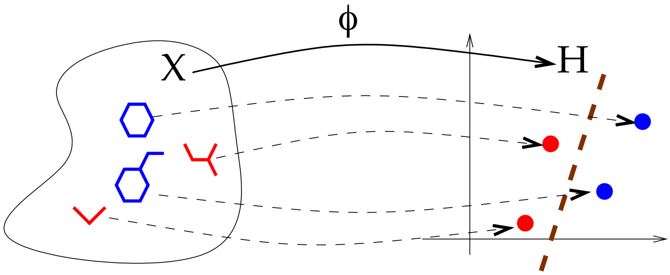
- A new type of **multilayer** graph kernel: more **expressive** than WL kernels;
- Learning easy-to-regularize and scalable **unsupervised** graph representations;
- Learning **supervised** graph representations like GNNs.

Graphs with node attributes



- A graph is defined as a triplet $(\mathcal{V}, \mathcal{E}, a)$;
- $\mathcal{V}$ and $\mathcal{E}$ correspond to the set of vertices and edges;
- $a : \mathcal{V} \to \mathbb{R}^d$ is a function assigning attributes to each node.

Graph kernel mappings

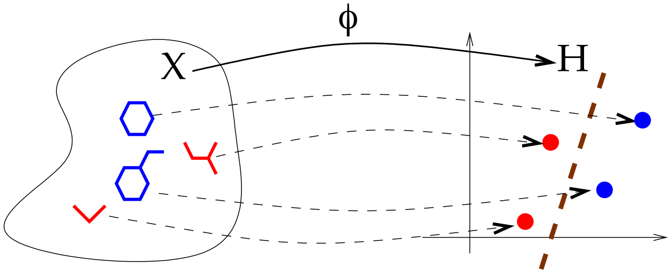


- Map each graph G in $\mathcal{X}$ to a vector $\Phi(G)$ in $\mathcal{H}$, which lends itself to learning tasks.
- A large class of graph kernel mappings can be written in the form

$$\Phi(G) := \sum_{u \in \mathcal{V}} \varphi_{\text{base}}(\ell_G(u)) \quad \text{where } \varphi_{\text{base}} \text{ embeds some local patterns } \ell_G(u) \text{ to } \mathcal{H}.$$

[Shervashidze et al., 2011, Lei et al., 2017, Kriege et al., 2019]

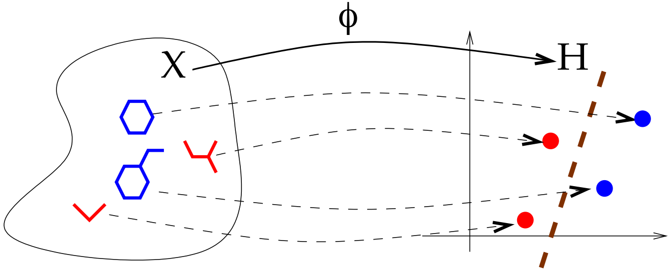
Graph kernel mappings



- Map each graph G in $\mathcal{X}$ to a vector $\Phi(G)$ in $\mathcal{H}$, which lends itself to learning tasks.
- A large class of graph kernel mappings can be written in the form

$$K(G, G') = \left\langle \underbrace{\sum_{u \in \mathcal{V}} \varphi_{\text{base}}(\ell_G(u))}_{\Phi(G)}, \underbrace{\sum_{u' \in \mathcal{V}'} \varphi_{\text{base}}(\ell_{G'}(u'))}_{\Phi(G')} \right\rangle .$$

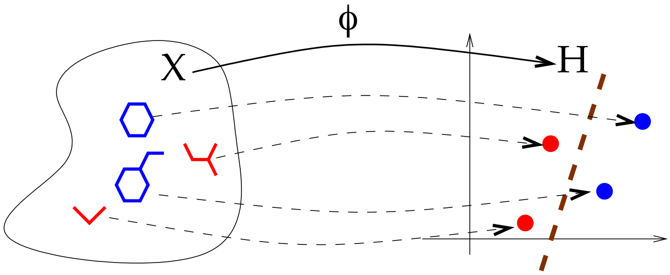
Graph kernel mappings



- Map each graph G in $\mathcal{X}$ to a vector $\Phi(G)$ in $\mathcal{H}$, which lends itself to learning tasks.
- A large class of graph kernel mappings can be written in the form

$$K(G,G') = \sum_{u \in \mathcal{V}} \sum_{u' \in \mathcal{V}'} \langle \varphi_{\text{base}}(\ell_G(u)), \varphi_{\text{base}}(\ell_{G'}(u')) \rangle.$$

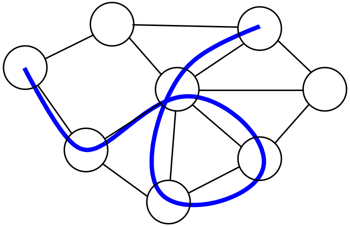
Graph kernel mappings

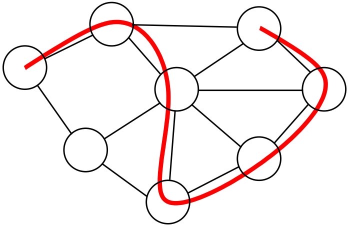


- Map each graph G in $\mathcal{X}$ to a vector $\Phi(G)$ in $\mathcal{H}$, which lends itself to learning tasks.
- A large class of graph kernel mappings can be written in the form

$$K(G, G') = \sum_{u \in \mathcal{V}} \sum_{u' \in \mathcal{V}'} \kappa_{\mathsf{base}}(\ell_G(u), \ell_{G'}(u')).$$

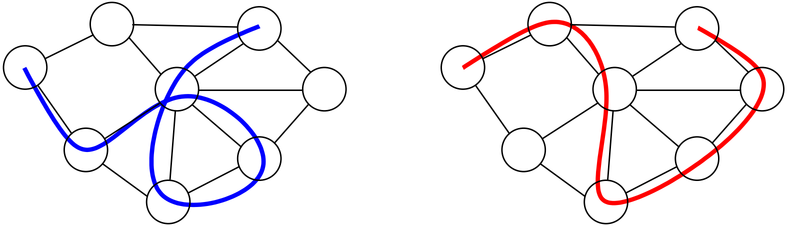
Basic kernels: walk and path kernel mappings





- Path kernels are more **expressive** than walk kernels, but less preferred for **computational** reasons.

Basic kernels: walk and path kernel mappings

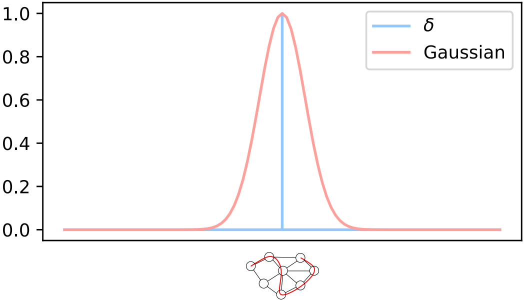


- $\mathcal{P}_k(G, u) :=$ paths of length k from node u in G. The **k-path** mapping is

$$\varphi_{\text{path}}(u) := \sum_{p \in \mathcal{P}_k(G,u)} \delta_{a(p)} \quad \Longrightarrow \quad \Phi(G) = \sum_{u \in \mathcal{V}} \sum_{p \in \mathcal{P}_k(G,u)} \delta_{a(p)}.$$

- $a(p)$: concatenated attributes in p; δ: the Dirac function;
- $\Phi(G)$ can be interpreted as a **histogram** of paths occurrences;

A relaxed path kernel

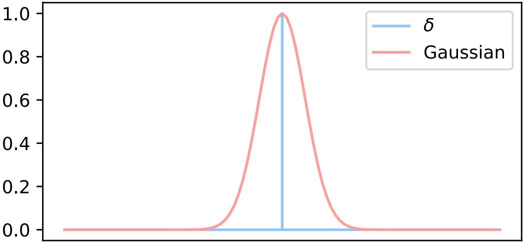


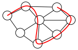
$$\varphi_{\mathsf{path}}(u) = \sum_{p \in \mathcal{P}_k(G,u)} \delta_{a(p)}(\cdot)$$

Issues of the path kernel mapping:

- δ allows hard comparison between paths thus only works for discrete attributes;
- δ is not differentiable, which cannot be "optimized" with back-propagation.

A relaxed path kernel





$$\varphi_{\text{path}}(u) = \sum_{p \in \mathcal{P}_k(G,u)} \delta_{a(p)}(\cdot)$$

$$\Longrightarrow \sum_{p \in \mathcal{P}_k(G,u)} e^{-\frac{\alpha}{2}\|a(p)-\cdot\|^2}.$$

Issues of the path kernel mapping:

- δ allows hard comparison between paths thus only works for discrete attributes;
- δ is not differentiable, which cannot be "optimized" with back-propagation.

Relax it with a "soft" and differentiable mapping

- interpreted as the sum of Gaussians centered at each path from u.

One-layer GCKN: a closer look at the relaxed path kernel

- We define the one-layer GCKN as the relaxed path kernel mapping

$$\varphi_1(u) := \sum_{p \in \mathcal{P}_k(G,u)} e^{-\frac{\alpha_1}{2}\|a(p)-\cdot\|^2} = \sum_{p \in \mathcal{P}_k(G,u)} \varphi_{\mathsf{RBF}}(a(p)) \in \mathcal{H}_1.$$

- This formula can be divided into **3 steps**:
  - path extraction: enumerating all $\mathcal{P}_k(G,u)$;
  - kernel mapping: evaluating Gaussian embedding φ_{RBF} of path features;
  - path aggregation: aggregating the path embeddings.

One-layer GCKN: a closer look at the relaxed path kernel

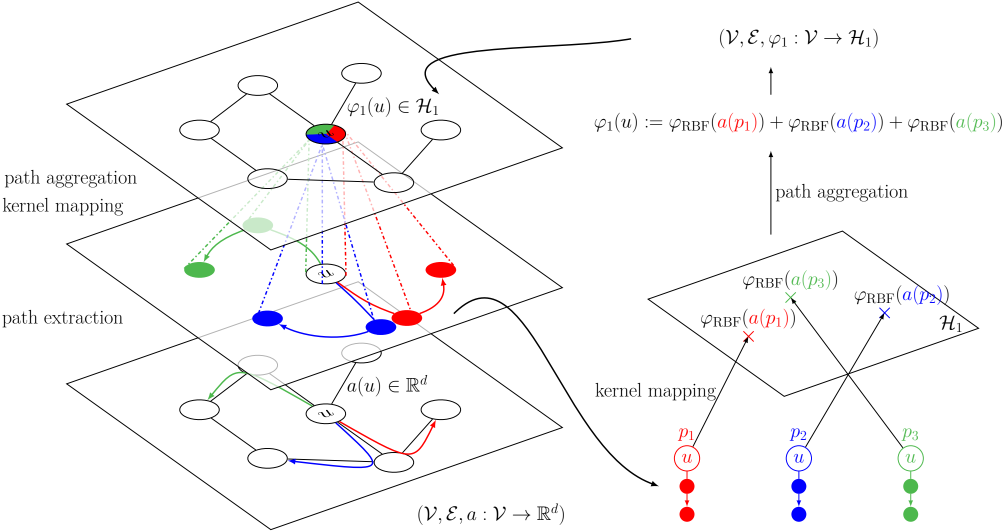
- We define the one-layer GCKN as the relaxed path kernel mapping

$$\varphi_1(u) := \sum_{p \in \mathcal{P}_k(G,u)} e^{-\frac{\alpha_1}{2}\|a(p)-\cdot\|^2} = \sum_{p \in \mathcal{P}_k(G,u)} \varphi_{\mathsf{RBF}}(a(p)) \in \mathcal{H}_1.$$

- This formula can be divided into **3 steps**:
    - path extraction: enumerating all $\mathcal{P}_k(G,u)$;
    - kernel mapping: evaluating Gaussian embedding φ_{RBF} of path features;
    - path aggregation: aggregating the path embeddings.
- We obtain a new graph with the same topology but different features

$$(\mathcal{V}, \mathcal{E}, a) \xrightarrow{\varphi_{\mathsf{path}}} (\mathcal{V}, \mathcal{E}, \varphi_1).$$

Construction of one-layer GCKN



From one-layer to multilayer GCKN

- We can repeat applying φ_{path} to the new graph

$$(\mathcal{V}, \mathcal{E}, a) \xrightarrow{\varphi_{\text{path}}} (\mathcal{V}, \mathcal{E}, \varphi_1) \xrightarrow{\varphi_{\text{path}}} (\mathcal{V}, \mathcal{E}, \varphi_2) \xrightarrow{\varphi_{\text{path}}} \dots \xrightarrow{\varphi_{\text{path}}} (\mathcal{V}, \mathcal{E}, \varphi_j).$$

- Final graph representation at layer j, $\Phi(G) = \sum_{u \in \mathcal{V}} \varphi_j(u)$.

From one-layer to multilayer GCKN

- We can repeat applying φ_{path} to the new graph

$$(\mathcal{V}, \mathcal{E}, a) \xrightarrow{\varphi_{\text{path}}} (\mathcal{V}, \mathcal{E}, \varphi_1) \xrightarrow{\varphi_{\text{path}}} (\mathcal{V}, \mathcal{E}, \varphi_2) \xrightarrow{\varphi_{\text{path}}} \ldots \xrightarrow{\varphi_{\text{path}}} (\mathcal{V}, \mathcal{E}, \varphi_j).$$

- Final graph representation at layer j, $\Phi(G) = \sum_{u \in \mathcal{V}} \varphi_j(u)$.
- Why is the multilayer model interesting ?
  - applying φ_{path} once can capture **paths**: GCKN-path;
  - applying twice can capture **subtrees**: GCKN-subtree;
  - applying more times may capture **higher-order structures**?
  - **Long paths** cannot be enumerated due to computational complexity, yet multilayer model can capture **long-range substructures**.

Scalable approximation of Gaussian kernel mapping

$$\varphi_{\text{path}}(u) = \sum_{p \in \mathcal{P}_k(G,u)} \varphi_{\text{RBF}}(a(p)).$$

- $\varphi_{\text{RBF}}(a(p)) = e^{-\frac{\alpha}{2}\|a(p)-\cdot\|^2} \in \mathcal{H}$ is infinite-dimensional;

[Chen et al., 2019a,b, Williams and Seeger, 2001]

Scalable approximation of Gaussian kernel mapping

$$\varphi_{\text{path}}(u) = \sum_{p \in \mathcal{P}_k(G,u)} \varphi_{\text{RBF}}(a(p)).$$

- $\varphi_{\text{RBF}}(a(p)) = e^{-\frac{\alpha}{2}\|a(p)-\cdot\|^2} \in \mathcal{H}$ is infinite-dimensional;
- **Nyström** provides a **finite-dimensional** approximation $\Psi(a(p))$ by orthogonally projecting $\varphi_{\text{RBF}}(a(p))$ onto some finite-dimensional subspace:

$$\text{Span}(\varphi_{\text{RBF}}(z_1), \dots, \varphi_{\text{RBF}}(z_q)) \text{ parametrized by } Z = \{z_1, \dots, z_q\},$$

where $z_j \in \mathbb{R}^{dk}$ can be interpreted as path features.

[Chen et al., 2019a,b, Williams and Seeger, 2001]

Scalable approximation of Gaussian kernel mapping

$$\varphi_{\text{path}}(u) = \sum_{p \in \mathcal{P}_k(G,u)} \varphi_{\text{RBF}}(a(p)).$$

- $\varphi_{\text{RBF}}(a(p)) = e^{-\frac{\alpha}{2}\|a(p)-\cdot\|^2} \in \mathcal{H}$ is infinite-dimensional;
- **Nyström** provides a **finite-dimensional** approximation $\Psi(a(p))$ by orthogonally projecting $\varphi_{\text{RBF}}(a(p))$ onto some finite-dimensional subspace:

$$\text{Span}(\varphi_{\text{RBF}}(z_1), \ldots, \varphi_{\text{RBF}}(z_q)) \text{ parametrized by } Z = \{z_1, \ldots, z_q\},$$

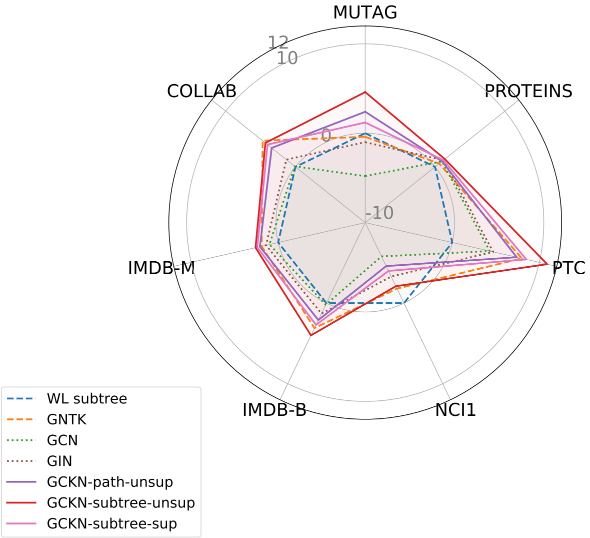
  where $z_j \in \mathbb{R}^{dk}$ can be interpreted as path features.
- The parameters Z can be learned by
  - (unsupervised) K-means on the set of path features;
  - (supervised) end-to-end learning with back-propagation.

[Chen et al., 2019a,b, Williams and Seeger, 2001]

Comparison of GCKN and GNN

GCKN	vs.	GNN
$f_{\mathsf{GCKN}}(G) = \sum_{u \in G} \psi_k(u)$		$f_{\mathsf{GNN}}(G) = \sum_{u \in G} f_k(u)$
$\psi_k(u) = \sum_{p \in \mathcal{P}_k(G,u)} \kappa(Z^\top Z)^{-\frac{1}{2}} \kappa(Z^\top \psi_{k-1}(p))$		$f_k(u) = \sum_{v \in \mathcal{N}(u)} \mathsf{ReLU}(Z^\top f_{k-1}(v))$
local path aggregation		neighborhood aggregation
projection in a known RKHS		?
supervised and unsupervised		supervised

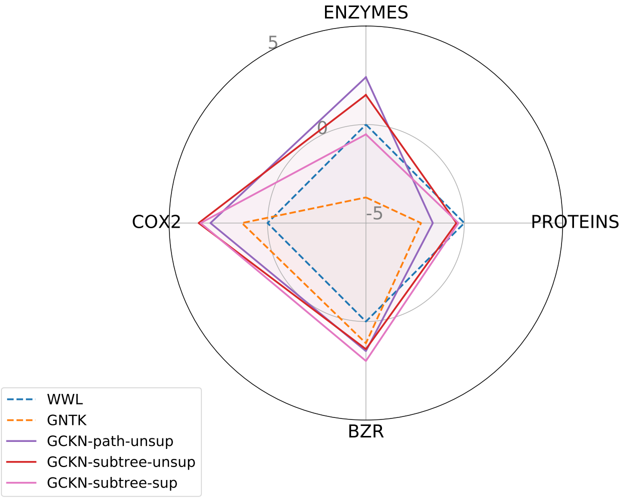
Experiments on graphs with discrete attributes



- Accuracy improvement with respect to the WL subtree kernel.
- GCKN-path already outperforms the baselines.
- Increasing number of layers brings larger improvement.
- Supervised learning does not improve performance, but leads to more compact representations.

[Shervashidze et al., 2011, Du et al., 2019, Xu et al., 2019, Kipf and Welling, 2017]

Experiments on graphs with continuous attributes

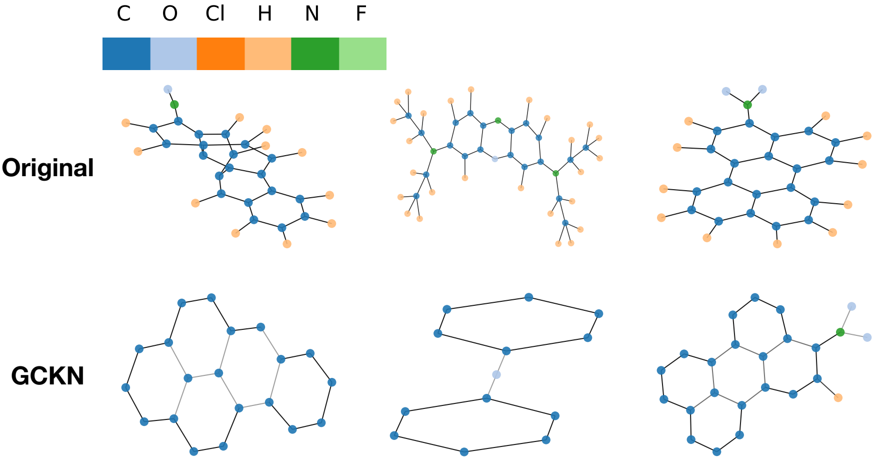


- Accuracy improvement with respect to the WWL kernel.
- Results similar to discrete case.
- Path features seem presumably predictive enough.

[Du et al., 2019, Togninalli et al., 2019]

Model interpretation for Mutagenicity prediction

- Idea: find the minimal connected component that preserves the prediction.



[Ying et al., 2019]

Take-home messages

- GCKN is a **multilayer kernel** for graphs based on **paths**, which allows to control the trade-off between **computation** and **expressiveness**.
- Its graph representations can be learned in both **supervised** and **unsupervised** fashions. Unsupervised models are **easy-to-regularize** and **scalable**.
- A straightforward model **interpretation** is also provided.
- **Our code is freely available at** `https://github.com/claying/GCKN`.

Take-home messages

- GCKN is a **multilayer kernel** for graphs based on **paths**, which allows to control the trade-off between **computation** and **expressiveness**.
- Its graph representations can be learned in both **supervised** and **unsupervised** fashions. Unsupervised models are **easy-to-regularize** and **scalable**.
- A straightforward model **interpretation** is also provided.
- **Our code is freely available at** `https://github.com/claying/GCKN`.

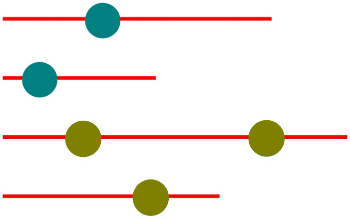
Future (on-going) work

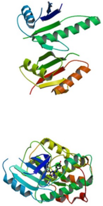
- working with real people dealing with real data (protein folding prediction).

Biological Sequence Modeling

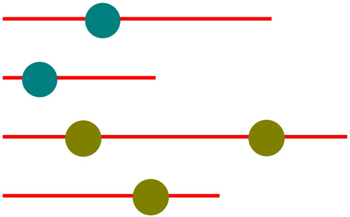
- D. Chen, L. Jacob and J. Mairal. Recurrent Kernel Networks. Adv. Neural Information Processing Systems (NeurIPS). 2019.
- D. Chen, L. Jacob and J. Mairal. Biological Sequence Modeling with Convolutional Kernel Networks. Bioinformatics. 2019.

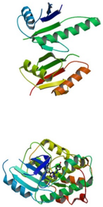
Sequence modeling as a supervised learning problem





Sequence modeling as a supervised learning problem





- Biological sequences $x_1, \ldots x_n \in \mathcal{X}$ and their associated labels $y_1, \ldots, y_n$.
- Goal: learning a **predictive** and **interpretable** function $f : \mathcal{X} \to \mathbb{R}$

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

- How do we define the functional space $\mathcal{F}$?

String kernels

A classical approach for modeling biological sequences over alphabet $\mathcal{A}$ relies on string kernels.

$$K(x, x') = \sum_{u \in \mathcal{A}^k} \delta_u(x)\delta_u(x') \qquad ,$$

where u is a k-mer over an alphabet $\mathcal{A}$ and $\delta_u(x)$ can be:

- the number of occurrences of u in x: **spectrum kernel** [Leslie et al., 2002];
- the number of occurrences of u in x up to m mismatches: **mismatch kernel** [Leslie and Kuang, 2004];
- the number of occurrences of u in x allowing gaps, with a weight decaying exponentially with the number of gaps : **substring kernel** [Lodhi et al., 2002].

What is $\Phi(x)$?

It can be interpreted as a histogram of pattern occurences.

String kernels

A classical approach for modeling biological sequences over alphabet $\mathcal{A}$ relies on string kernels.

$$K(x, x') = \sum_{u \in \mathcal{A}^k} \delta_u(x)\delta_u(x') = \langle \Phi(x), \Phi(x') \rangle,$$

where u is a k-mer over an alphabet $\mathcal{A}$ and $\delta_u(x)$ can be:

- the number of occurrences of u in x: **spectrum kernel** [Leslie et al., 2002];
- the number of occurrences of u in x up to m mismatches: **mismatch kernel** [Leslie and Kuang, 2004];
- the number of occurrences of u in x allowing gaps, with a weight decaying exponentially with the number of gaps : **substring kernel** [Lodhi et al., 2002].

What is $\Phi(x)$?

It can be interpreted as a histogram of pattern occurences.

Convolutional kernel networks for sequence modeling

Define a continuous relaxation of the mismatch kernel [Chen et al., 2019a, Morrow et al., 2017]

$$K_{\mathsf{CKN}}(x,x') = \sum_{i=1}^{|x|-k+1} \sum_{j=1}^{|x'|-k+1} K_0(\underbrace{x_{[i:i+k]}}_{\text{one k-mer}}, x'_{[j:j+k]}).$$

- Use one-hot encoding

$$x_{[i:i+5]} := \mathrm{TTGAG} \mapsto \begin{array}{c} \mathrm{A} \\ \mathrm{T} \\ \mathrm{C} \\ \mathrm{G} \end{array} \begin{bmatrix} 0 & 0 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 \end{bmatrix}.$$

- K_0 is a Gaussian kernel over **one-hot** representations of k-mers (in $\mathbb{R}^{k \times d}$).

Convolutional kernel networks for sequence modeling

Define a continuous relaxation of the mismatch kernel [Chen et al., 2019a, Morrow et al., 2017]

$$K_{\mathsf{CKN}}(x, x') = \sum_{i=1}^{|x|-k+1} \sum_{j=1}^{|x'|-k+1} \langle \varphi_0(\underbrace{x_{[i:i+k]}}_{\text{one k-mer}}), \varphi_0(x'_{[j:j+k]}) \rangle.$$

- Use one-hot encoding

$$x_{[i:i+5]} := \mathrm{TTGAG} \mapsto \begin{array}{c} \mathrm{A} \\ \mathrm{T} \\ \mathrm{C} \\ \mathrm{G} \end{array} \begin{bmatrix} 0 & 0 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 \end{bmatrix}.$$

- K_0 is a Gaussian kernel over **one-hot** representations of k-mers (in $\mathbb{R}^{k \times d}$).

Convolutional kernel networks for sequence modeling

Define a continuous relaxation of the mismatch kernel [Chen et al., 2019a, Morrow et al., 2017]

$$K_{\mathsf{CKN}}(x,x') = \Big\langle \underbrace{\sum_{i=1}^{|x|-k+1} \varphi_0(x_{[i:i+k]})}_{\Phi(x)}, \underbrace{\sum_{j=1}^{|x'|-k+1} \varphi_0(x'_{[j:j+k]})}_{\Phi(x')} \Big\rangle.$$

- Use one-hot encoding

$$x_{[i:i+5]} := \mathrm{TTGAG} \mapsto \begin{array}{c} \mathrm{A} \\ \mathrm{T} \\ \mathrm{C} \\ \mathrm{G} \end{array} \begin{bmatrix} 0 & 0 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 \end{bmatrix}.$$

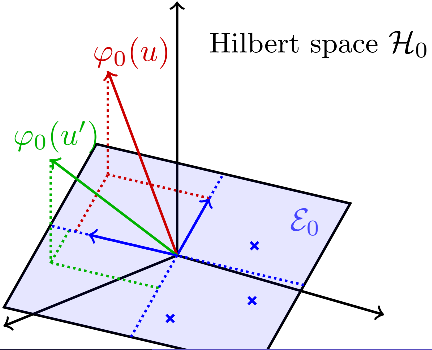
- K_0 is a Gaussian kernel over **one-hot** representations of k-mers (in $\mathbb{R}^{k \times d}$).

Scalable Approximation of Kernel Mapping (with more details this time)

$$K_0(u, u') = \langle \varphi_0(u), \varphi_0(u') \rangle_{\mathcal{H}_0} \approx \langle \psi_0(u), \psi_0(u') \rangle_{\mathbb{R}^q}.$$

- **Nyström** provides a **finite-dimensional** approximation $\psi_0(u)$ in $\mathbb{R}^q$ by orthogonally projecting $\varphi_0(u)$ onto some finite-dimensional subspace:

$$\mathcal{E}_0 = \mathsf{Span}(\varphi_0(z_1), \ldots, \varphi_0(z_q)) \text{ parametrized by } Z = \{z_1, \ldots, z_q\}.$$



Scalable Approximation of Kernel Mapping (with more details this time)

$$K_0(u, u') = \langle \varphi_0(u), \varphi_0(u') \rangle_{\mathcal{H}_0} \approx \langle \psi_0(u), \psi_0(u') \rangle_{\mathbb{R}^q}.$$

- **Nyström** provides a **finite-dimensional** approximation $\psi_0(u)$ in $\mathbb{R}^q$ by orthogonally projecting $\varphi_0(u)$ onto some finite-dimensional subspace:

$$\mathcal{E}_0 = \mathsf{Span}(\varphi_0(z_1), \ldots, \varphi_0(z_q)) \text{ parametrized by } Z = \{z_1, \ldots, z_q\}.$$

- **General case:**

$$\psi_0(u) = [K_0(z_i, z_j)]_{ij}^{-1/2} [K_0(z_1, u), \ldots, K_0(z_q, u)]^T = K_0(Z, Z)^{-1/2} K_0(Z, u).$$

Scalable Approximation of Kernel Mapping (with more details this time)

$$K_0(u,u') = \langle \varphi_0(u), \varphi_0(u') \rangle_{\mathcal{H}_0} \approx \langle \psi_0(u), \psi_0(u') \rangle_{\mathbb{R}^q}.$$

- **Nyström** provides a **finite-dimensional** approximation $\psi_0(u)$ in $\mathbb{R}^q$ by orthogonally projecting $\varphi_0(u)$ onto some finite-dimensional subspace:

$$\mathcal{E}_0 = \text{Span}(\varphi_0(z_1), \ldots, \varphi_0(z_q)) \text{ parametrized by } Z = \{z_1, \ldots, z_q\}.$$

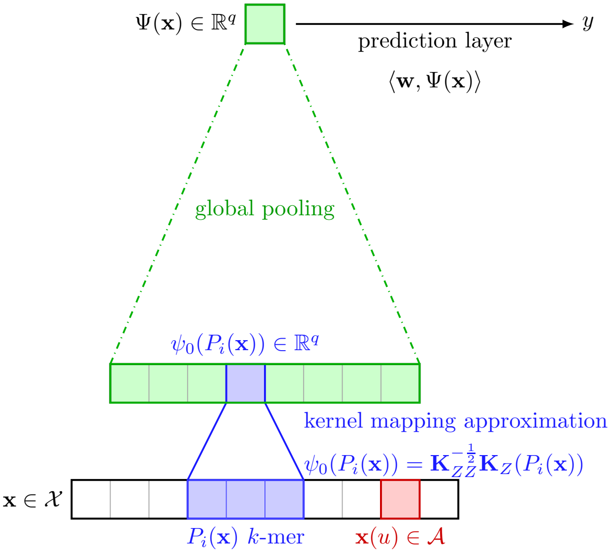
- Case of **dot-product kernels** $K_0(u,u') = \kappa(\langle u, u' \rangle)$:

$$\psi_0(u) = \kappa(Z^\top Z)^{-1/2} \kappa(Z^\top u).$$

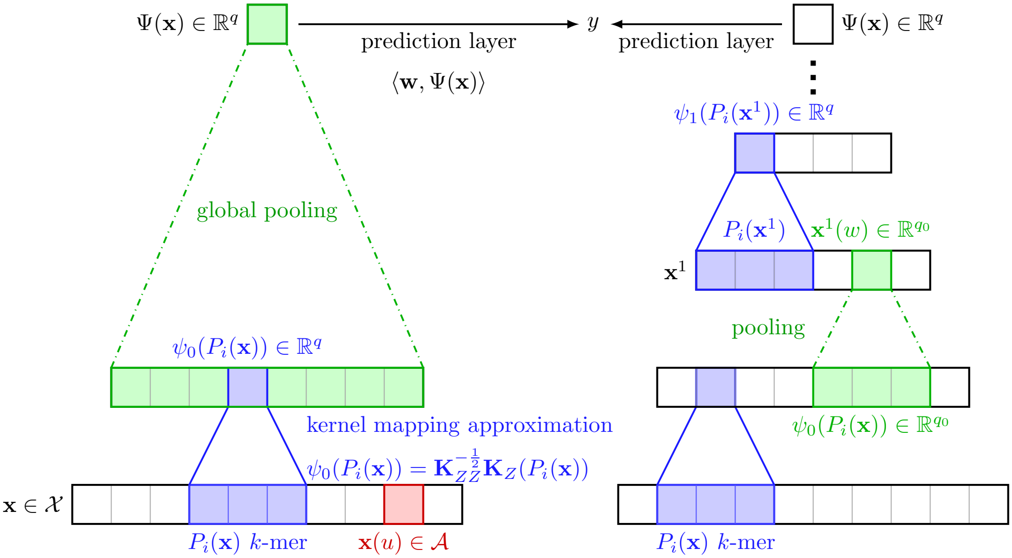
linear operation - pointwise nonlinearity - linear operation (subject to interpretation)

Ex: $\kappa(\beta) = e^{\beta - 1}$, polynomial, inverse polynomial, arc-cosine kernels....

Single-Layer CKN for sequence modeling



Multilayer CKN for sequence modeling



How to learn the anchor points Z?

with no supervision?

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

- we **extract a large number**—say $100\,000$ k-mers from the previous layer computed on a sequence database;
- perform a **K-means algorithm** to learn the anchor points;
- **compute the projection matrix** $\kappa(Z^\top Z)^{-1/2}$ (case of a dot-product kernel).

How to learn the anchor points Z?

with no supervision?

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

- we **extract a large number**—say $100\,000$ k-mers from the previous layer computed on a sequence database;
- perform a **K-means algorithm** to learn the anchor points;
- **compute the projection matrix** $\kappa(Z^\top Z)^{-1/2}$ (case of a dot-product kernel).

with supervision?

- by using **back-propagation** on a supervised loss function;
- all it requires is differentiating $\kappa(Z^\top Z)^{-1/2}$ which requires an eigenvalue decomposition;
- use the unsupervised learning procedure as initialization.

From k-mers to gapped k-mers

k-mers with gaps

- For a sequence $x = x_1 \ldots x_n \in \mathcal{X}$ of length n and a sequence of ordered indices $\mathbf{i} = (i_1, \ldots, i_k)$ in $I(k, n)$, we define a k-substring as:

$$x_{[\mathbf{i}]} = x_{i_1} x_{i_2} \ldots x_{i_k}.$$

- We introduce the quantity

$$\text{gaps}(\mathbf{i}) = \text{number of gaps in index sequence.}$$

- Example: $x =$ ABRACADABRA

$$\mathbf{i} = (4, 5, 8, 9, 11) \quad x_{[\mathbf{i}]} = \text{RADAR} \quad \text{gaps}(\mathbf{i}) = 3.$$

Recurrent kernel networks

Comparing all the k-mers between a pair of sequences (single layer models)

$$K_{\mathsf{CKN}}(x, x') = \sum_{i=1}^{|x|-k+1} \sum_{j=1}^{|x'|-k+1} K_0\left(x_{[i:i+k]}, x'_{[j:j+k]}\right).$$

- The kernel mapping is $\Phi(x) = \sum_{i=1}^{|x|-k+1} \varphi_0(x_{[i:i+k]})$.

Recurrent kernel networks

Comparing all the gapped k-mers between a pair of sequences (single layer models)

$$K_{\mathsf{RKN}}(x,x') = \sum_{\mathbf{i}\in I(k,|x|)} \sum_{\mathbf{j}\in I(k,|x'|)} \lambda^{\mathsf{gaps}(\mathbf{i})} \lambda^{\mathsf{gaps}(\mathbf{j})} K_0\left(x_{[\mathbf{i}]}, x'_{[\mathbf{j}]}\right).$$

- The kernel mapping is $\Phi(x) = \sum_{\mathbf{i}\in I(k,|x|)} \lambda^{\mathsf{gaps}(\mathbf{i})} \varphi_0(x_{[\mathbf{i}]})$.
- This is a differentiable relaxation of the substring kernel.

But enumerating all possible substrings is costly...

Approximation and recursive computation of RKN

Approximate feature map of RKN kernel

The approximate feature map of K_{RKN} via Nyström approximation is

$$\Psi(x) = \sum_{\mathbf{i} \in I(k,t)} \lambda^{\mathsf{gaps}(\mathbf{i})} \psi_0(x_{[\mathbf{i}]}) \in \mathbb{R}^q,$$

where, as usual with a dot-product kernel, $\psi_0(x_{[\mathbf{i}]}) = \kappa(Z^\top Z)^{-1/2}\kappa(Z^\top x_{[\mathbf{i}]})$.

- The sum can be computed by using **dynamic programming** [Lodhi et al., 2002],
- which leads to a **particular** recurrent neural network [see Lei et al., 2017].

A feature map for the single-layer RKN

When K_0 is a Gaussian kernel, the feature map of RKN is a mixture of Gaussians centered at $x_{[\mathbf{i}]}$, weighted by the corresponding penalization $\lambda^{\text{gaps}(\mathbf{i})}$.

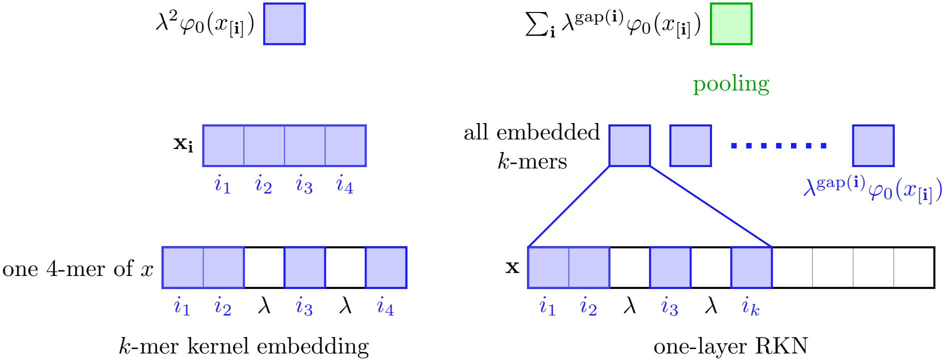


Figure: Example of K_{RKN} for $k = 4$

Results

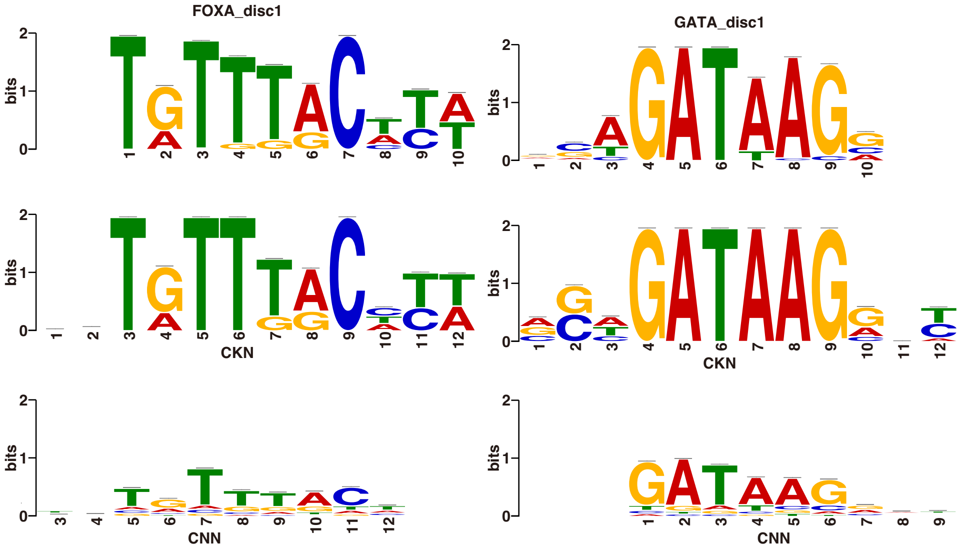
Protein fold classification on SCOP 2.06 [Hou et al., 2017] (using more informative sequence features including PSSM, secondary structure and solvent accessibility)

Method	♯Params	Accuracy		Level-stratified accuracy (top1/top5)		
		top 1	top 5	family	superfamily	fold
PSI-BLAST	-	84.53	86.48	82.20/84.50	86.90/88.40	18.90/35.100
DeepSF	920k	73.00	90.25	75.87/91.77	72.23/90.08	51.35/67.57
CKN (128 filters)	211k	76.30	92.17	83.30/94.22	74.03/91.83	43.78/67.03
CKN (512 filters)	843k	84.11	94.29	**90.24**/**95.77**	82.33/94.20	45.41/69.19
RKN (128 filters)	211k	77.82	92.89	76.91/93.13	78.56/92.98	60.54/83.78
RKN (512 filters)	843k	**85.29**	**94.95**	84.31/94.80	**85.99**/**95.22**	**71.35**/**84.86**

Note: More experiments with statistical tests have been conducted in our paper.

[Hou et al., 2017, Chen et al., 2019a]

Logos, by finding pre-image of each filter



Results

Protein fold recognition on SCOP 1.67 (widely used in the past)

Method	pooling	one-hot		BLOSUM62	
		auROC	auROC50	auROC	auROC50
SVM-pairwise		0.724	0.359		
Mismatch		0.814	0.467		
LA-kernel		–	–	0.834	0.504
LSTM		0.830	0.566	–	–
CKN		0.837	0.572	0.866	0.621
RKN	mean	0.829	0.541	0.840	0.571
RKN	max	**0.844**	**0.587**	**0.871**	**0.629**
RKN (unsup)	mean	0.805	0.504	0.833	0.570

[Liao and Noble, 2003, Leslie et al., 2003, Vert et al., 2004, Hochreiter et al., 2007, Chen et al., 2019a]

Take-home messages

- CKN and RKNs are **multilayer kernels** for sequences, achieving state-of-the-art results for biological sequence modeling (see other tasks in papers).
- RKN is able to model gaps with a recurrent neural network structure.
- These models can be used without supervision, providing effective, but **high-dimensional** embeddings.
- With supervision, models trained with backpropagation are much more compact.
- For biological sequences, best results were obtained with a single layer.

Take-home messages

- CKN and RKNs are **multilayer kernels** for sequences, achieving state-of-the-art results for biological sequence modeling (see other tasks in papers).
- RKN is able to model gaps with a recurrent neural network structure.
- These models can be used without supervision, providing effective, but **high-dimensional** embeddings.
- With supervision, models trained with backpropagation are much more compact.
- For biological sequences, best results were obtained with a single layer.

Our code in Pytorch is freely available at

`https://gitlab.inria.fr/dchen/CKN-seq`

`https://github.com/claying/RKN`

Image Modeling

- J. Mairal. End-to-End Kernel Learning with Supervised Convolutional Kernel Networks. Adv. Neural Information Processing Systems (NIPS), 2016.
- J. Mairal, P. Koniusz, Z. Harchaoui and C. Schmid. Convolutional Kernel Networks. Adv. Neural Information Processing Systems (NIPS). 2014.

Construction of the RKHS for continuous signals

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

$x_0 : \Omega \to \mathcal{H}_0$: **continuous** input signal, with $\Omega = \mathbb{R}^d$: 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).

Construction of the RKHS for continuous signals

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

$x_0 : \Omega \to \mathcal{H}_0$: **continuous** input signal, with $\Omega = \mathbb{R}^d$: 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).

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).

Construction of the RKHS for continuous signals

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

$x_0 : \Omega \to \mathcal{H}_0$: **continuous** input signal, with $\Omega = \mathbb{R}^d$: 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).

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

$$M_k P_k x_{k-1}.$$

- 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).
- M_k: **non-linear mapping** operator, maps each patch to a new Hilbert space $\mathcal{H}_k$ with a **pointwise** non-linear function $\varphi_k(\cdot)$.

Construction of the RKHS for continuous signals

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

$x_0 : \Omega \to \mathcal{H}_0$: **continuous** input signal, with $\Omega = \mathbb{R}^d$: 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).

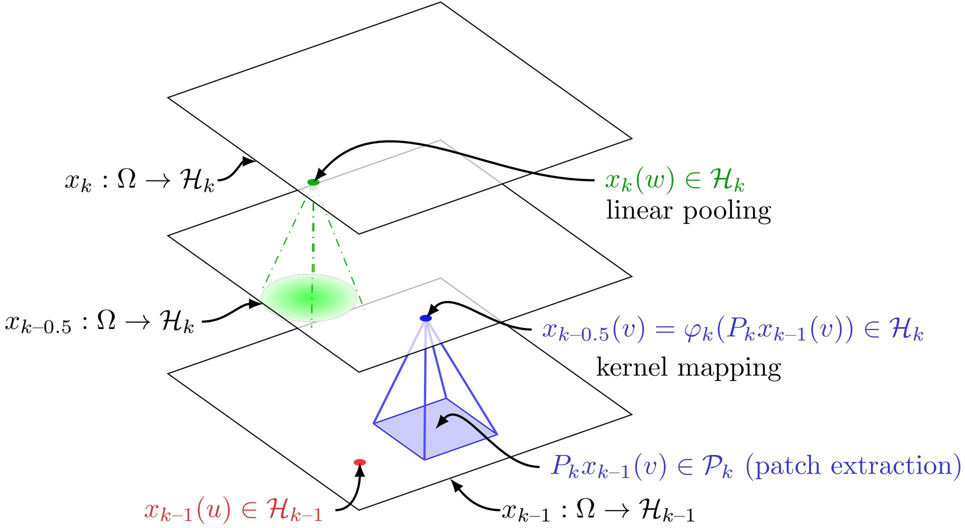
Building map x_k in $L^2(\Omega, \mathcal{H}_k)$ from x_{k-1} in $L^2(\Omega, \mathcal{H}_{k-1})$

$x_k : \Omega \to \mathcal{H}_k$: **feature map** at layer k

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

- 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).
- M_k: **non-linear mapping** operator, maps each patch to a new Hilbert space $\mathcal{H}_k$ with a **pointwise** non-linear function $\varphi_k(\cdot)$.
- A_k: (linear) **pooling** operator at scale σ_k.

Construction of the RKHS for continuous signals



Construction of the RKHS for continuous signals

Kernel mapping for patches

- We use a homogeneous dot-product kernel for image patches

$$K(z, z') = \|z\| \|z'\| \kappa \left(\frac{\langle z, z' \rangle}{\|z\| \|z'\|} \right).$$

Multilayer representation

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

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

Construction of the RKHS for continuous signals

Kernel mapping for patches

- We use a homogeneous dot-product kernel for image patches

$$K(z, z') = \|z\| \|z'\| \kappa \left(\frac{\langle z, z' \rangle}{\|z\| \|z'\|} \right).$$

Multilayer representation

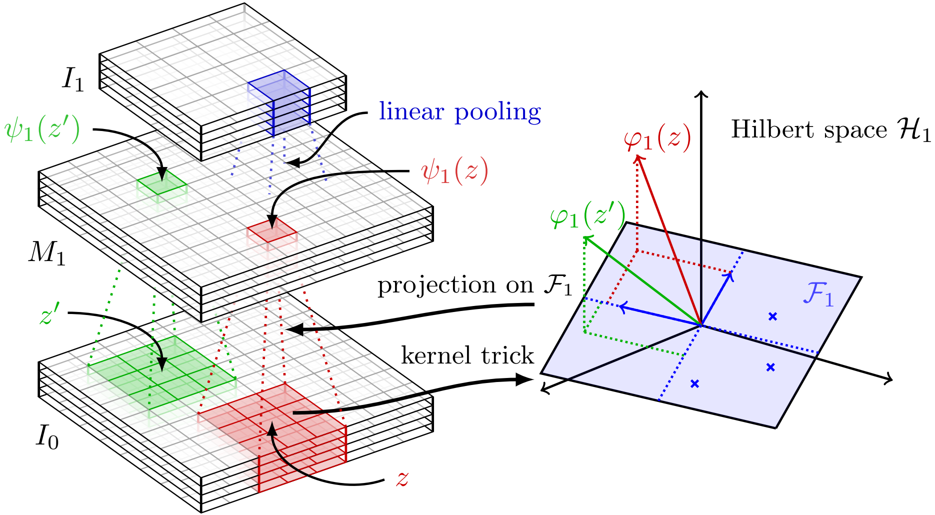
$$\Phi_n(x) = A_n M_n P_n A_{n-1} M_{n-1} P_{n-1} \cdots A_1 M_1 P_1 x_0 \ \in \ L^2(\Omega, \mathcal{H}_n).$$

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

Prediction layer

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

Convolutional Kernel Networks in practice



Learning mechanism of CKNs between layers 0 and 1.

Convolutional Kernel Networks in Practice

What is the difference with a CNN?

- Given a patch x, a CNN computes $\psi_{CNN}(x) = \sigma(Z^\top x)$ (+batch norm?)
- Given a patch x, a CKN computes $\psi_{CKN}(x) = \|x\|\kappa(Z^\top Z)^{-1/2}\kappa(Z^\top x/\|x\|)$.

Convolutional Kernel Networks in Practice

What is the difference with a CNN?

- Given a patch x, a CNN computes $\psi_{CNN}(x) = \sigma(Z^\top x)$ (+batch norm?)
- Given a patch x, a CKN computes $\psi_{CKN}(x) = \|x\|\kappa(Z^\top Z)^{-1/2}\kappa(Z^\top x/\|x\|)$.

Consequences

- we have a geometric interpretation in terms of subspace learning.
- it provides unsupervised learning mechanisms (kernel approximation with Nyström).
- supervised learning is still feasible (backpropagating through $\kappa(Z^\top Z)^{-1/2}$ is fun).
- the kernel interpretation provides regularization mechanisms.
- kernel representations can possibly be used in other contexts (statistical testing? kernel PCA? CCA? K-means?).

Experiments

- Briefly state-of-the-art for image retrieval [Paulin et al., 2015];
- Briefly state-of-the-art for image super-resolution [Mairal, 2016a];

Interesting findings from CIFAR-10

- about 92% with supervision, mild data augmentation, 14 layers, 256 anchor points per layers (no need for batch norm, vanilla SGD+momentum).
- about 86% **with no supervision** for a two-layer model with a huge number of anchor points (1024-16384) and no data augmentation.
- with no supervision, **the performance monotonically increases with the dimension** (better kernel approximation).
- computing the exact kernel does not make sense in practice for computational reasons, but it is feasible with lots of CPUs; it yields about 90% with three layers (unpublished, by A. Bietti), which is consistent with [Shankar et al., 2020].

Take-home messages

- unsupervised representations are shallow and high-dimensional;
- supervised representations may be deep and compact;
- **Our code is freely available at** `https://gitlab.inria.fr/mairal/ckn-cudnn-matlab`.
- **and** `https://github.com/claying/CKN-Pytorch-image`.

Take-home messages

- unsupervised representations are shallow and high-dimensional;
- supervised representations may be deep and compact;
- **Our code is freely available at** `https://gitlab.inria.fr/mairal/ckn-cudnn-matlab`.
- **and** `https://github.com/claying/CKN-Pytorch-image`.

Open

- how to close the gap between the approximate embedding and the exact kernel?

Theory for Deep Learning Models

- A. Bietti and J. Mairal. On the Inductive Bias of Neural Tangent Kernels. Adv. Neural Information Processing Systems (NeurIPS). 2019.
- A. Bietti and J. Mairal. Group Invariance, Stability to Deformations, and Complexity of Deep Convolutional Representations. Journal of Machine Learning Research (JMLR). 2019.

Kernels for deep models: deep kernel machines

Hierarchical kernels [Cho and Saul, 2009]

- Kernels can be constructed **hierarchically**

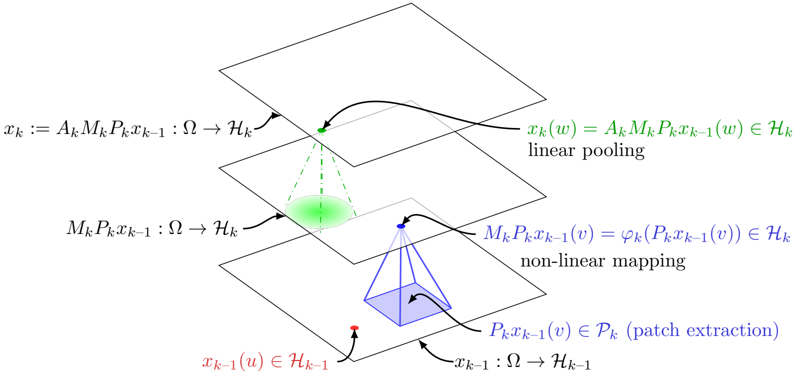
$$K(x,x') = \langle \Phi(x), \Phi(x') \rangle \text{ with } \Phi(x) = \varphi_2(\varphi_1(x))$$

- *e.g.*, dot-product kernels on the sphere

$$K(x,x') = \kappa_2(\langle \varphi_1(x), \varphi_1(x') \rangle) = \kappa_2(\kappa_1(x^\top x'))$$

Kernels for deep models: deep kernel machines

Convolutional kernels networks (CKNs) for images [Mairal et al., 2014, Mairal, 2016b]



- Good empirical performance with tractable approximations (Nyström)

Kernels for deep models: infinite-width networks

$$f_\theta(x) = \frac{1}{\sqrt{m}} \sum_{i=1}^{m} v_i \sigma(w_i^\top x), \qquad m \to \infty$$

Random feature kernels [RF, Neal, 1996, Rahimi and Recht, 2007]

- $\theta = (v_i)_i$, fixed random weights $w_i \sim N(0, I)$

$$K_{RF}(x, x') = \mathbb{E}_{w \sim N(0,I)}[\sigma(w^\top x)\sigma(w^\top x')]$$

Kernels for deep models: infinite-width networks

$$f_\theta(x) = \frac{1}{\sqrt{m}} \sum_{i=1}^{m} v_i \sigma(w_i^\top x), \qquad m \to \infty$$

Random feature kernels [RF, Neal, 1996, Rahimi and Recht, 2007]

- $\theta = (v_i)_i$, fixed random weights $w_i \sim N(0, I)$

$$K_{RF}(x, x') = \mathbb{E}_{w \sim N(0,I)}[\sigma(w^\top x)\sigma(w^\top x')]$$

Neural tangent kernels [NTK, Jacot et al., 2018]

- $\theta = (v_i, w_i)_i$, initialization $\theta_0 \sim N(0, I)$
- **Lazy training** [Chizat et al., 2019]: θ stays close to θ_0 when training with large m

$$f_\theta(x) \approx f_{\theta_0}(x) + \langle \theta - \theta_0, \nabla_\theta f_\theta(x)|_{\theta=\theta_0} \rangle.$$

Kernels for deep models: infinite-width networks

$$f_\theta(x) = \frac{1}{\sqrt{m}} \sum_{i=1}^{m} v_i \sigma(w_i^\top x), \qquad m \to \infty$$

Random feature kernels [RF, Neal, 1996, Rahimi and Recht, 2007]

- $\theta = (v_i)_i$, fixed random weights $w_i \sim N(0, I)$

$$K_{RF}(x, x') = \mathbb{E}_{w\sim N(0,I)}[\sigma(w^\top x)\sigma(w^\top x')]$$

Neural tangent kernels [NTK, Jacot et al., 2018]

- $\theta = (v_i, w_i)_i$, initialization $\theta_0 \sim N(0, I)$
- **Lazy training** [Chizat et al., 2019]: θ stays close to θ_0 when training with large m

$$f_\theta(x) \approx f_{\theta_0}(x) + \langle \theta - \theta_0, \nabla_\theta f_\theta(x)|_{\theta=\theta_0} \rangle.$$

- Gradient descent for $m \to \infty$ $\approx$ kernel ridge regression with **neural tangent kernel**

$$K_{NTK}(x, x') = \lim_{m\to\infty} \langle \nabla_\theta f_{\theta_0}(x), \nabla_\theta f_{\theta_0}(x') \rangle$$

Other relations between kernels and deep learning

- hierarchical kernel descriptors [Bo et al., 2011];
- other multilayer models [Bouvrie et al., 2009, Montavon et al., 2011, Anselmi et al., 2015];
- deep Gaussian processes [Damianou and Lawrence, 2013].
- multilayer PCA [Schölkopf et al., 1998].
- old kernels for images [Scholkopf, 1997], related to one-layer CKN.
- RBF networks [Broomhead and Lowe, 1988].
- ...

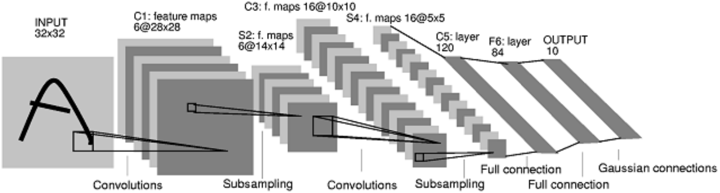
Objectives

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**.



Focus on convolutional kernel networks (CKNs)

What is the relation?

- it is possible to design functional spaces $\mathcal{H}$ for deep neural networks [Mairal, 2016b].

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

- we call the construction "**convolutional kernel networks**" (in short, replace $u \mapsto \sigma(\langle a, u \rangle)$ by a kernel mapping $u \mapsto \varphi_k(u)$.

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?

Focus on convolutional kernel networks (CKNs)

What is the relation?

- it is possible to design functional spaces $\mathcal{H}$ for deep neural networks [Mairal, 2016b].

$$f(x) = \sigma_k(W_k\sigma_{k-1}(W_{k-1}\ldots\sigma_2(W_2\sigma_1(W_1x))\ldots)) = \langle f, \Phi(x)\rangle_{\mathcal{H}}.$$

- we call the construction "**convolutional kernel networks**" (in short, replace $u \mapsto \sigma(\langle a, u\rangle)$ by a kernel mapping $u \mapsto \varphi_k(u)$.

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?

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

Summary of the results from Bietti and Mairal [2019a]

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

- Contains CNNs with smooth homogeneous activations functions.

Summary of the results from Bietti and Mairal [2019a]

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

- Contains CNNs with smooth homogeneous activations functions.

Signal representation: Conditions for

- **Signal preservation** of the multi-layer kernel mapping Φ.
- **Stability to deformations and non-expansiveness** for Φ.
- Constructions to achieve **group invariance**.

Summary of the results from Bietti and Mairal [2019a]

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

- Contains CNNs with smooth homogeneous activations functions.

Signal representation: Conditions for

- **Signal preservation** of the multi-layer kernel mapping Φ.
- **Stability to deformations and non-expansiveness** for Φ.
- Constructions to achieve **group invariance**.

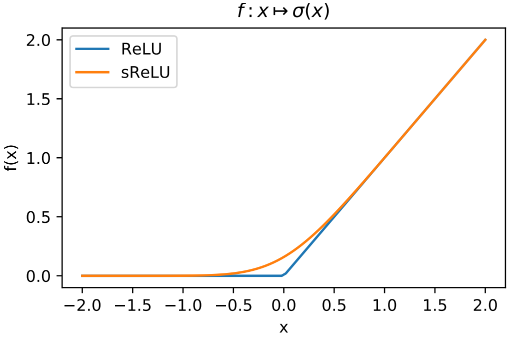
On learning

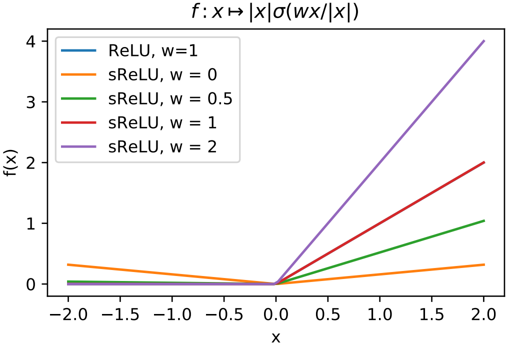
- Bounds on the RKHS norm $\|.\|_{\mathcal{H}}$ to control **stability and generalization** of a predictive model f.

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

Smooth homogeneous activations functions

$$z \mapsto \mathsf{ReLU}(w^\top z) \qquad \Longrightarrow \qquad z \mapsto \|z\|\sigma(w^\top z/\|z\|).$$





Recap: Construction of the RKHS for continuous signals

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

$x_0 : \Omega \to \mathcal{H}_0$: **continuous** input signal, with $\Omega = \mathbb{R}^d$: 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).

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: **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).
- M_k: **non-linear mapping** operator, maps each patch to a new Hilbert space $\mathcal{H}_k$ with a **pointwise** non-linear function $\varphi_k(\cdot)$.
- A_k: (linear) **pooling** operator at scale σ_k.

Recap: Construction of the RKHS for continuous signals

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

$x_0 : \Omega \rightarrow \mathcal{H}_0$: **continuous** input signal, with $\Omega = \mathbb{R}^d$: 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).

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).
- M_k: **non-linear mapping** operator, maps each patch to a new Hilbert space $\mathcal{H}_k$ with a **pointwise** non-linear function $\varphi_k(\cdot)$.
- A_k: (linear) **pooling** operator at scale σ_k.

Recap: Construction of the RKHS for continuous signals

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

$x_0 : \Omega \to \mathcal{H}_0$: **continuous** input signal, with $\Omega = \mathbb{R}^d$: 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).

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

$$M_k P_k x_{k-1}.$$

- 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).
- M_k: **non-linear mapping** operator, maps each patch to a new Hilbert space $\mathcal{H}_k$ with a **pointwise** non-linear function $\varphi_k(\cdot)$.
- A_k: (linear) **pooling** operator at scale σ_k.

Recap: Construction of the RKHS for continuous signals

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

$x_0 : \Omega \rightarrow \mathcal{H}_0$: **continuous** input signal, with $\Omega = \mathbb{R}^d$: 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).

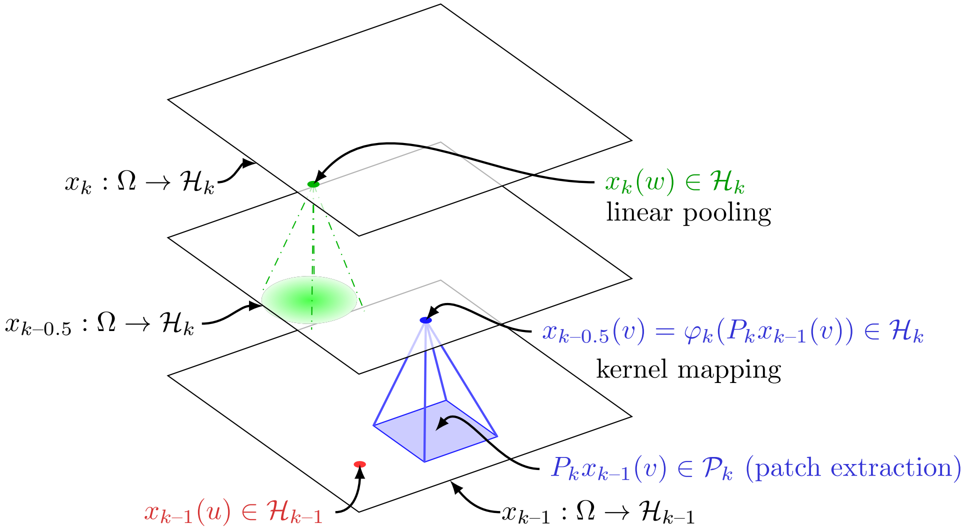
Building map x_k in $L^2(\Omega, \mathcal{H}_k)$ from x_{k-1} in $L^2(\Omega, \mathcal{H}_{k-1})$

$x_k : \Omega \rightarrow \mathcal{H}_k$: **feature map** at layer k

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

- 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).
- M_k: **non-linear mapping** operator, maps each patch to a new Hilbert space $\mathcal{H}_k$ with a **pointwise** non-linear function $\varphi_k(\cdot)$.
- A_k: (linear) **pooling** operator at scale σ_k.

Construction of the RKHS for continuous signals



Construction of the RKHS for continuous signals

Multilayer representation

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

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

Construction of the RKHS for continuous signals

Multilayer representation

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

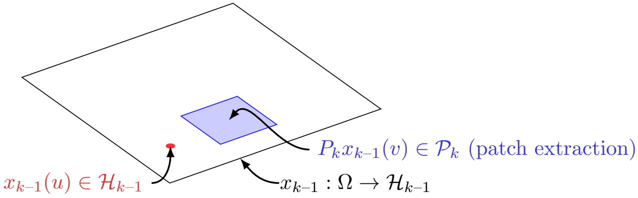
- σ_k grows exponentially in practice (i.e., fixed with subsampling).

Prediction layer

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

Patch extraction operator P_k

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



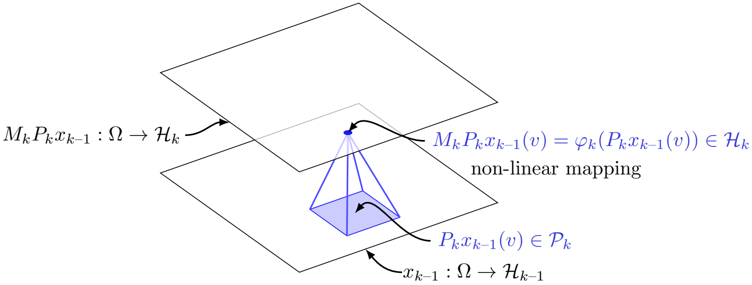
Patch extraction operator P_k

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

- S_k: patch shape, e.g. box

Non-linear mapping operator M_k

$$M_k P_k x_{k\text{–}1}(u) := \varphi_k(P_k x_{k\text{–}1}(u)) \in \mathcal{H}_k$$



Non-linear mapping operator M_k

$$M_k P_k x_{k-1}(u) := \varphi_k(P_k x_{k-1}(u)) \in \mathcal{H}_k$$

Kernel mapping of **homogeneous dot-product kernels**:

$$K_k(z, z') = \|z\|\|z'\|\kappa_k\left(\frac{\langle z, z'\rangle}{\|z\|\|z'\|}\right) = \langle \varphi_k(z), \varphi_k(z')\rangle.$$

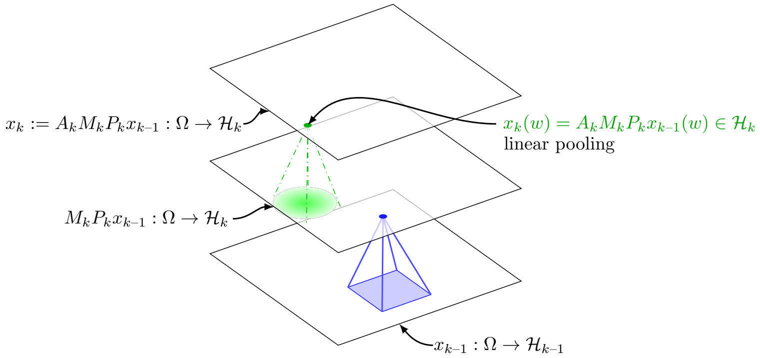
$\kappa_k(u) = \sum_{j=0}^{\infty} b_j u^j$ with $b_j \geq 0$, $\kappa_k(1) = 1$

Examples

- $\kappa_{\text{exp}}(\langle z, z'\rangle) = e^{\langle z, z'\rangle - 1}$ (Gaussian kernel on the sphere)
- $\kappa_{\text{inv-poly}}(\langle z, z'\rangle) = \frac{1}{2 - \langle z, z'\rangle}$

Pooling operator A_k

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



Pooling operator A_k

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

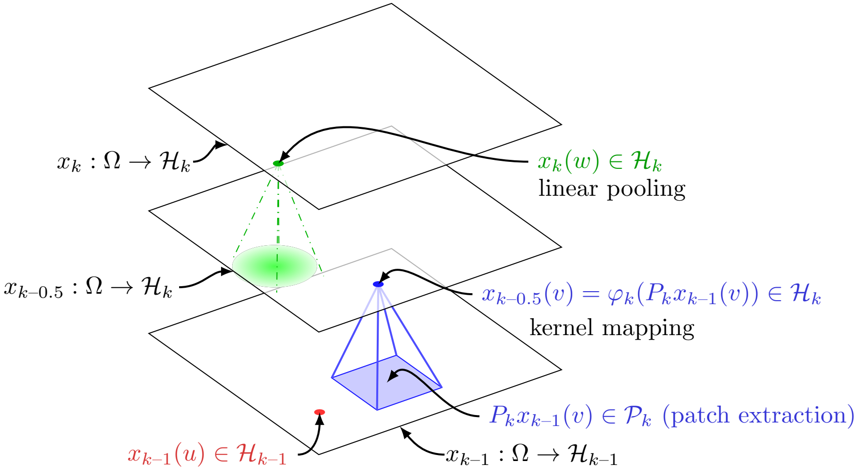
- h_{σ_k}: pooling filter at scale σ_k
- $h_{\sigma_k}(u) := \sigma_k^{-d} h(u/\sigma_k)$ with $h(u)$ **Gaussian**
- **linear, non-expansive operator**: $\|A_k\| \leq 1$

Pooling operator A_k

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

- 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**: $\|A_k\| \leq 1$
- In practice: **discretization**, sampling at resolution σ_k after pooling
- "Preserves information" when **subsampling** $\leq$ **patch size**

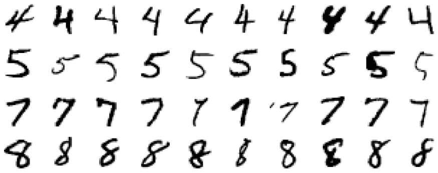
Recap: P_k, M_k, A_k



Stability to deformations

Deformations

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



- Studied for wavelet-based scattering transform [Mallat, 2012, Bruna and Mallat, 2013]

Stability to deformations

Deformations

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

Definition of stability

- Representation $\Phi(\cdot)$ is **stable** [Mallat, 2012] if:

$$\|\Phi(L_\tau x) - \Phi(x)\| \leq (C_1 \|\nabla \tau\|_\infty + C_2 \|\tau\|_\infty)\|x\|$$

- $\|\nabla \tau\|_\infty = \sup_u \|\nabla \tau(u)\|$ controls deformation
- $\|\tau\|_\infty = \sup_u |\tau(u)|$ controls translation
- $C_2 \to 0$: translation invariance

Smoothness and stability with kernels

Geometry of the kernel mapping: $f(x) = \langle f, \Phi(x) \rangle$

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

- $\|f\|_{\mathcal{H}}$ controls **complexity** of the model
- $\Phi(x)$ encodes CNN **architecture** independently of the model (smoothness, invariance, stability to deformations)

Smoothness and stability with kernels

Geometry of the kernel mapping: $f(x) = \langle f, \Phi(x) \rangle$

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

- $\|f\|_{\mathcal{H}}$ controls **complexity** of the model
- $\Phi(x)$ encodes CNN **architecture** independently of the model (smoothness, invariance, stability to deformations)

Useful kernels in practice:

- Convolutional kernel networks [**CKNs**, Mairal, 2016b] with efficient approximations
- Extends to neural tangent kernels [**NTKs**, Jacot et al., 2018] of infinitely wide CNNs [Bietti and Mairal, 2019b]

Recap: multilayer construction

Multilayer representation

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

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

Recap: multilayer construction

Multilayer representation

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

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

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**).

Recap: multilayer construction

Multilayer representation

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

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

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**).

Final kernel

$$K_{CKN}(x, x') = \langle \Phi(x), \Phi(x') \rangle_{L^2(\Omega)} = \int_\Omega \langle x_n(u), x'_n(u) \rangle du$$

Warmup: translation invariance

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 translation invariance?

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

Warmup: translation invariance

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 translation invariance?

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

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

Warmup: translation invariance

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 translation invariance?

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

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

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

Warmup: translation invariance

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 translation invariance?

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

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

- 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!

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

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

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

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!
- $\|[A_k, L_\tau]\| \leq C_1 \|\nabla \tau\|_\infty$ [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}:

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

Stability to deformations

Representation

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

How to achieve stability to deformations?

- Patch extraction P_k and pooling A_k **do not commute** with L_τ!
- $\|[A_k, L_\tau]\| \leq C_1 \|\nabla \tau\|_\infty$ [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}:

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

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

Stability to deformations

Theorem (Stability of CKN [Bietti and Mairal, 2019a])

Let $\Phi_n(x) = \Phi(A_0 x)$ *and assume* $\|\nabla\tau\|_\infty \leq 1/2$,

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

- Translation invariance: large σ_n
- Stability: small patch sizes ($\beta \approx$ patch size, $C_\beta = O(\beta^3)$ for images)
- Signal preservation: subsampling factor $\approx$ patch size

$\Longrightarrow$ need several layers with small patches $\quad n = O(\log(\sigma_n/\sigma_0)/\log\beta)$

Stability to deformations

Theorem (Stability of CKN [Bietti and Mairal, 2019a])

Let $\Phi_n(x) = \Phi(A_0 x)$ *and assume* $\|\nabla \tau\|_\infty \leq 1/2$*,*

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

- Translation invariance: large σ_n
- Stability: small patch sizes ($\beta \approx$ patch size, $C_\beta = O(\beta^3)$ for images)
- Signal preservation: subsampling factor $\approx$ patch size

$\Longrightarrow$ need several layers with small patches $\quad n = O(\log(\sigma_n/\sigma_0)/\log \beta)$

- Achieved by controlling norm of **commutator** $[L_\tau, P_k A_{k-1}]$
  - Extend result by Mallat [2012] for controlling $\|[L_\tau, A]\|$
  - Need patches S_k adapted to resolution σ_{k-1}: diam $S_k \leq \beta \sigma_{k-1}$

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).

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).

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]...

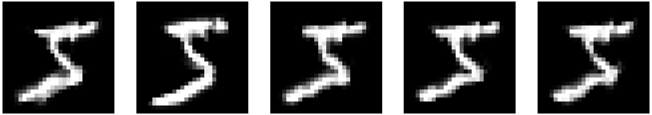
Stability to deformations for convolutional NTK

Theorem (Stability of NTK [Bietti and Mairal, 2019b])

Let $\Phi_n(x) = \Phi^{NTK}(A_0 x)$, *and assume* $\|\nabla\tau\|_\infty \leq 1/2$

$$\begin{aligned}&\|\Phi_n(L_\tau x) - \Phi_n(x)\| \\ &\leq \left(C_\beta n^{7/4} \|\nabla\tau\|_\infty^{1/2} + C'_\beta n^2 \|\nabla\tau\|_\infty + \sqrt{n+1}\frac{C}{\sigma_n}\|\tau\|_\infty \right) \|x\|,\end{aligned}$$

Comparison with random feature CKN on deformed MNIST digits:



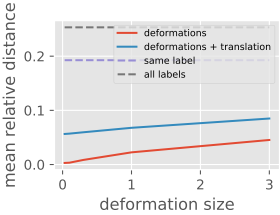
Stability to deformations for convolutional NTK

Theorem (Stability of NTK [Bietti and Mairal, 2019b])

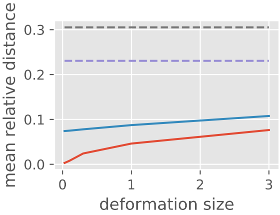
Let $\Phi_n(x) = \Phi^{NTK}(A_0 x)$, *and assume* $\|\nabla\tau\|_\infty \leq 1/2$

$$\|\Phi_n(L_\tau x) - \Phi_n(x)\| \leq \left(C_\beta n^{7/4} \|\nabla\tau\|_\infty^{1/2} + C'_\beta n^2 \|\nabla\tau\|_\infty + \sqrt{n+1}\frac{C}{\sigma_n}\|\tau\|_\infty \right) \|x\|,$$

Comparison with random feature CKN on deformed MNIST digits:



(a) CKN



(b) NTK

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 $\sigma_k \approx s_k$:

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

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 $\sigma_k \approx s_k$:

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

- Claim: We can recover $\bar{x}_{k-1}$ from $\bar{x}_k$ if factor $s_k \leq$ **patch size**.

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 $\sigma_k \approx s_k$:

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

- Claim: We can recover $\bar{x}_{k-1}$ from $\bar{x}_k$ if factor $s_k \leq$ **patch size**.
- 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

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

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 $\sigma_k \approx s_k$:

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

- Claim: We can recover $\bar{x}_{k-1}$ from $\bar{x}_k$ if factor $s_k \leq$ **patch size**.
- How? Recover patches with **linear functions** (contained in $\bar{\mathcal{H}}_k$)

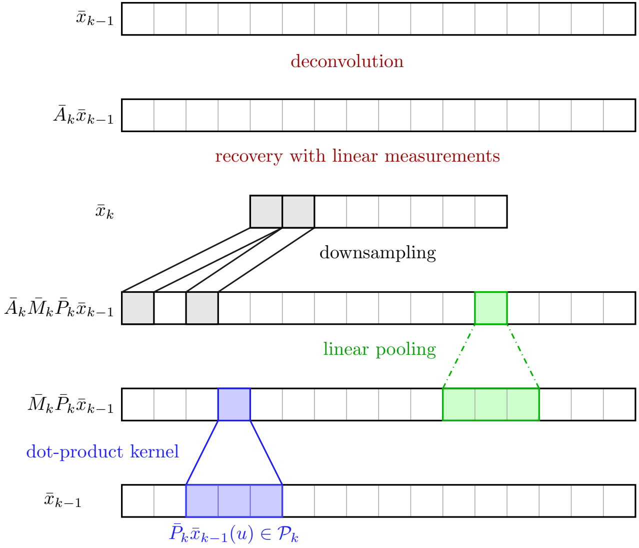
$$\langle f_w, \bar{M}_k \bar{P}_k \bar{x}_{k-1}(u) \rangle = f_w(\bar{P}_k \bar{x}_{k-1}(u)) = \langle w, \bar{P}_k \bar{x}_{k-1}(u) \rangle,$$

and

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

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

Discretization and signal preservation: example in 1D



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]

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?

- RKHS contains **homogeneous functions**:

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

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

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?

- RKHS contains **homogeneous functions**:

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

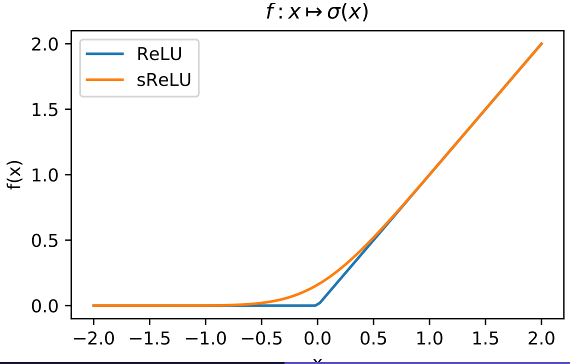
- **Smooth activations**: $\sigma(u) = \sum_{j=0}^{\infty} a_j u^j$ with $a_j \geq 0$.
- Norm: $\|f\|_{\mathcal{H}_k}^2 \leq C_\sigma^2(\|g\|^2) = \sum_{j=0}^{\infty} \frac{a_j^2}{b_j}\|g\|^2 < \infty$.

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 $\mathcal{H}_{\mathcal{K}}$

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

$$f(x) = \sigma_k(W_k\sigma_{k-1}(W_{k-1}\ldots\sigma_2(W_2\sigma_1(W_1x))\ldots)) = \langle f, \Phi(x)\rangle_{\mathcal{H}}.$$

- 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):

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

- 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.

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.

Applies to learned models

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

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.

Applies to learned models

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

Questions:

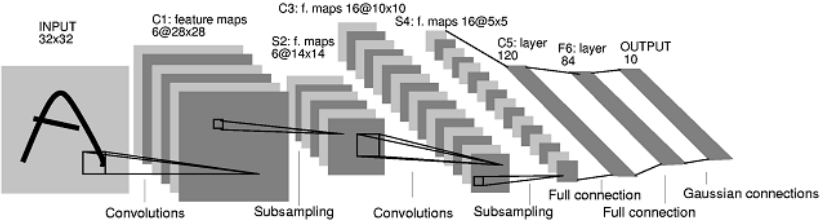
- Better regularization?
- How does SGD control capacity in CNNs?
- What about networks with no pooling layers? ResNet?

Robust Deep Learning Models with Kernels

- A. Bietti, G. Mialon, D. Chen, and J. Mairal. A Kernel Perspective for Regularizing Deep Neural Networks. International Conference on Machine Learning (ICML). 2019.

Convolutional Neural Networks

Picture from LeCun et al. [1998]

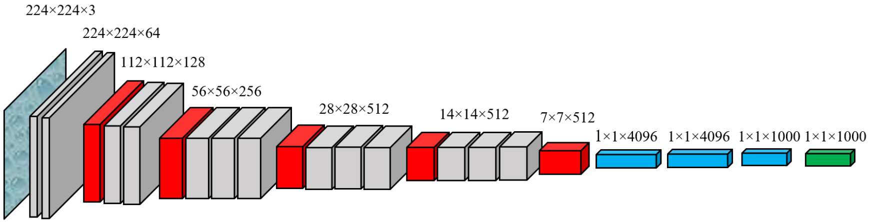


What are the main features of CNNs?

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

Convolutional Neural Networks

[Simonyan and Zisserman, 2014]



What are the main features of CNNs?

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

Convolutional neural networks for biological sequences

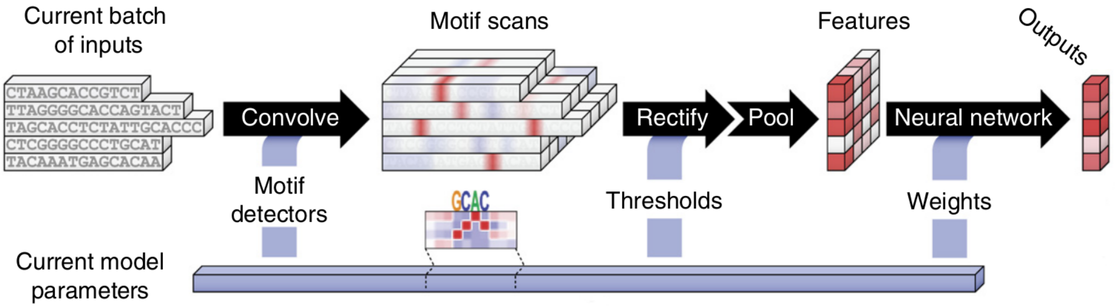
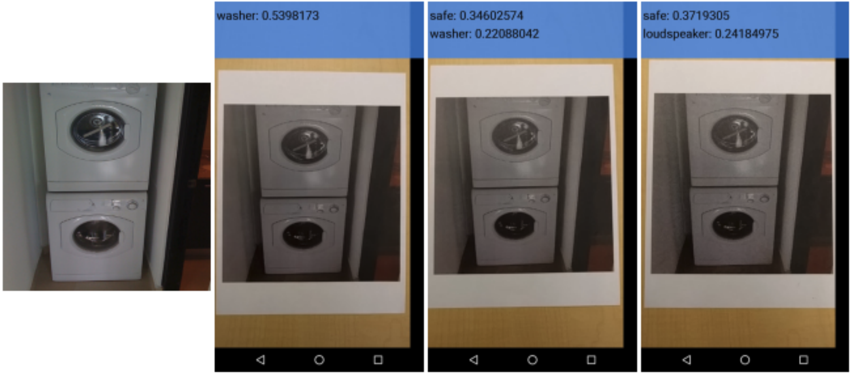


Figure: two-layer CNN architecture from Alipanahi et al. [2015]

- Sequences are represented by one-hot encoding (A=(1,0,0,0),C=(0,1,0,0),...).
- Single convolution layer followed by linear classifier.

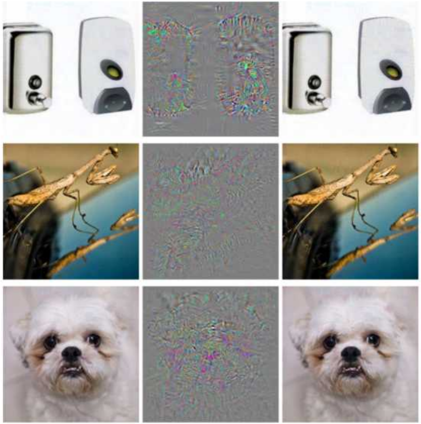
Adversarial examples, Picture from Kurakin et al. [2016]



(a) Image from dataset (b) Clean image (c) Adv. image, $\epsilon = 4$ (d) Adv. image, $\epsilon = 8$

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

Adversarial Examples



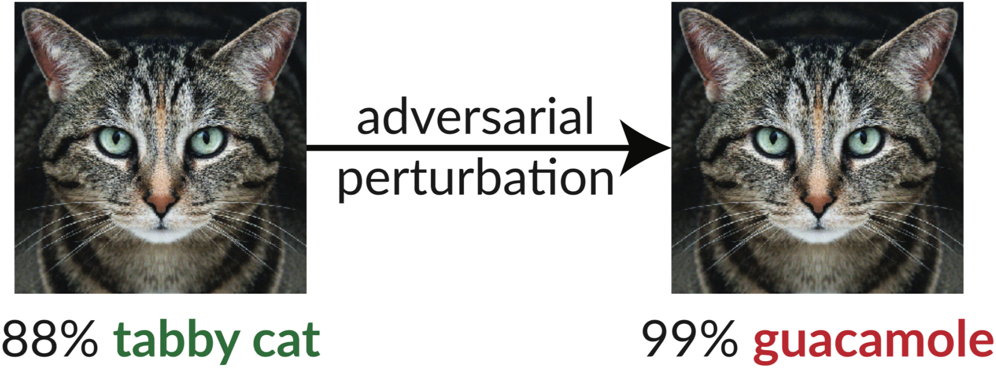
(b)

clean $+$ noise $\rightarrow$ "**ostrich**" [Szegedy et al., 2013].

Adversarial Examples

(a real ostrich)

Adversarial Examples



https://github.com/anishathalye/obfuscated-gradients

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**?

$$|f(x) - f(x')| \text{ should be close if } x \text{ and } x' \text{ are "similar".}$$

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

A kernel perspective: regularization

Assume we have an RKHS $\mathcal{H}$ for deep networks:

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

$\|.\|_{\mathcal{H}}$ encourages smoothness and stability w.r.t. the geometry induced by the kernel (which depends itself on the choice of architecture).

A kernel perspective: regularization

Assume we have an RKHS $\mathcal{H}$ for deep networks:

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

$\|.\|_{\mathcal{H}}$ encourages smoothness and stability w.r.t. the geometry induced by the kernel (which depends itself on the choice of architecture).

Problem

Multilayer kernels developed for deep networks are **typically intractable**.

One solution [Mairal, 2016a]

do kernel approximations at each layer, which leads to non-standard CNNs called convolutional kernel networks (CKNs).

A kernel perspective: regularization

Assume we have an RKHS $\mathcal{H}$ for deep networks:

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

$\|.\|_{\mathcal{H}}$ encourages smoothness and stability w.r.t. the geometry induced by the kernel (which depends itself on the choice of architecture).

Problem

Multilayer kernels developed for deep networks are **typically intractable**.

One solution [Mairal, 2016a]

do kernel approximations at each layer, which leads to non-standard CNNs called convolutional kernel networks (CKNs).
not the subject of this part.

A kernel perspective: regularization

Consider a classical CNN parametrized by θ, which live in the RKHS:

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

This is different than CKNs since f_θ admits a classical parametrization.

A kernel perspective: regularization

Consider a classical CNN parametrized by θ, which live in the RKHS:

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

This is different than CKNs since f_θ admits a classical parametrization.

Problem

$\|f_\theta\|_{\mathcal{H}}$ is **intractable**...

One solution [Bietti et al., 2019]

use approximations (lower- and upper-bounds), based on mathematical properties of $\|.\|_{\mathcal{H}}$.

A kernel perspective: regularization

Consider a classical CNN parametrized by θ, which live in the RKHS:

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

This is different than CKNs since f_θ admits a classical parametrization.

Problem

$\|f_\theta\|_{\mathcal{H}}$ is **intractable**...

One solution [Bietti et al., 2019]

use approximations (lower- and upper-bounds), based on mathematical properties of $\|.\|_{\mathcal{H}}$.

This is the subject of this part.

A kernel perspective: regularization

Another point of view: consider a classical CNN parametrized by θ, which live in the RKHS:

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

Upper-bounds

$$\|f_\theta\|_{\mathcal{H}} \leq \omega(\|W_k\|, \|W_{k-1}\|, \ldots, \|W_1\|) \quad \text{(spectral norms)}\ ,$$

where the W_j's are the convolution filters. The bound suggests controlling the spectral norm of the filters.

[Cisse et al., 2017, Miyato et al., 2018, Bartlett et al., 2017]...

A kernel perspective: regularization

Another point of view: consider a classical CNN parametrized by θ, which live in the RKHS:

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

Lower-bounds

$$\|f\|_{\mathcal{H}} = \sup_{\|u\|_{\mathcal{H}} \leq 1} \langle f, u \rangle_{\mathcal{H}} \quad \geq \quad \sup_{u \in U} \langle f, u \rangle_{\mathcal{H}} \quad \text{for} \quad U \subseteq B_{\mathcal{H}}(1).$$

We design a set U that leads to a tractable approximation, but it requires **some knowledge** about the properties of $\mathcal{H}, \Phi$.

A kernel perspective: regularization

Adversarial penalty

We know that Φ is **non-expansive** and $f(x) = \langle f, \Phi(x) \rangle$. Then,

$$U = \{\Phi(x+\delta) - \Phi(x) : x \in \mathcal{X}, \|\delta\|_2 \leq 1\}$$

leads to

$$\lambda \|f\|_\delta^2 = \sup_{x \in \mathcal{X}, \|\delta\|_2 \leq \lambda} f(x+\delta) - f(x).$$

The resulting strategy is related to **adversarial regularization** (but it is decoupled from the loss term and does not use labels).

$$\min_{\theta \in \mathbb{R}^p} \frac{1}{n} \sum_{i=1}^n L(y_i, f_\theta(x_i)) + \sup_{x \in \mathcal{X}, \|\delta\|_2 \leq \lambda} f_\theta(x+\delta) - f_\theta(x).$$

[Madry et al., 2018]

A kernel perspective: regularization

Adversarial penalty

We know that Φ is **non-expansive** and $f(x) = \langle f, \Phi(x) \rangle$. Then,

$$U = \{\Phi(x+\delta) - \Phi(x) : x \in \mathcal{X}, \|\delta\|_2 \leq 1\}$$

leads to

$$\lambda \|f\|_\delta^2 = \sup_{x \in \mathcal{X}, \|\delta\|_2 \leq \lambda} f(x+\delta) - f(x).$$

The resulting strategy is related to **adversarial regularization** (but it is decoupled from the loss term and does not use labels).
vs, for adversarial regularization,

$$\min_{\theta \in \mathbb{R}^p} \frac{1}{n} \sum_{i=1}^{n} \sup_{\|\delta\|_2 \leq \lambda} L(y_i, f_\theta(x_i + \delta)).$$

[Madry et al., 2018]

A kernel perspective: regularization

Gradient penalties

We know that Φ is non-expansive and $f(x) = \langle f, \Phi(x) \rangle$. Then,

$$U = \{\Phi(x+\delta) - \Phi(x) : x \in \mathcal{X}, \|\delta\|_2 \leq 1\}$$

leads to

$$\|\nabla f\| = \sup_{x \in \mathcal{X}} \|\nabla f(x)\|_2.$$

Related penalties have been used to stabilize the training of GANs and gradients of the **loss function** have been used to improve robustness.

[Gulrajani et al., 2017, Roth et al., 2017, 2018, Drucker and Le Cun, 1991, Lyu et al., 2015, Simon-Gabriel et al., 2018]

A kernel perspective: regularization

Adversarial deformation penalties

We know that Φ is **stable to deformations** and $f(x) = \langle f, \Phi(x) \rangle$. Then,

$$U = \{\Phi(L_\tau x) - \Phi(x) : x \in \mathcal{X}, \tau\}$$

leads to

$$\|f\|_\tau^2 = \sup_{\substack{x \in \mathcal{X} \\ \tau \text{ small deformation}}} f(L_\tau x) - f(x).$$

This is related to **data augmentation** and **tangent propagation**.

[Engstrom et al., 2017, Simard et al., 1998]

Experiments with Few labeled Samples

Table: Accuracies on CIFAR10 with 1 000 examples for standard architectures VGG-11 and ResNet-18. With / without data augmentation.

Method	1k VGG-11	1k ResNet-18
No weight decay	50.70 / 43.75	45.23 / 37.12
Weight decay	51.32 / 43.95	44.85 / 37.09
SN projection	54.14 / **46.70**	47.12 / 37.28
PGD-ℓ_2	51.25 / 44.40	45.80 / 41.87
grad-ℓ_2	**55.19** / 43.88	**49.30** / **44.65**
$\|f\|_\delta^2$ penalty	51.41 / 45.07	48.73 / 43.72
$\|\nabla f\|^2$ penalty	54.80 / 46.37	**48.99** / **44.97**
PGD-ℓ_2 + SN proj	54.19 / **46.66**	47.47 / 41.25
grad-ℓ_2 + SN proj	**55.32** / **46.88**	48.73 / 42.78
$\|f\|_\delta^2$ + SN proj	54.02 / **46.72**	48.12 / 43.56
$\|\nabla f\|^2$ + SN proj	**55.24** / **46.80**	**49.06** / **44.92**

Experiments with Few labeled Samples

Table: Accuracies with 300 or 1 000 examples from MNIST, using deformations. $(*)$ indicates that random deformations were included as training examples,

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

Experiments with Few labeled Samples

Table: AUROC50 for protein homology detection tasks using CNN, with or without data augmentation (DA).

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

Experiments with Few labeled Samples

Table: AUROC50 for protein homology detection tasks using CNN, with or without data augmentation (DA).

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

Note: statistical tests have been conducted for all of these experiments (see paper).

Adversarial Robustness: Trade-offs

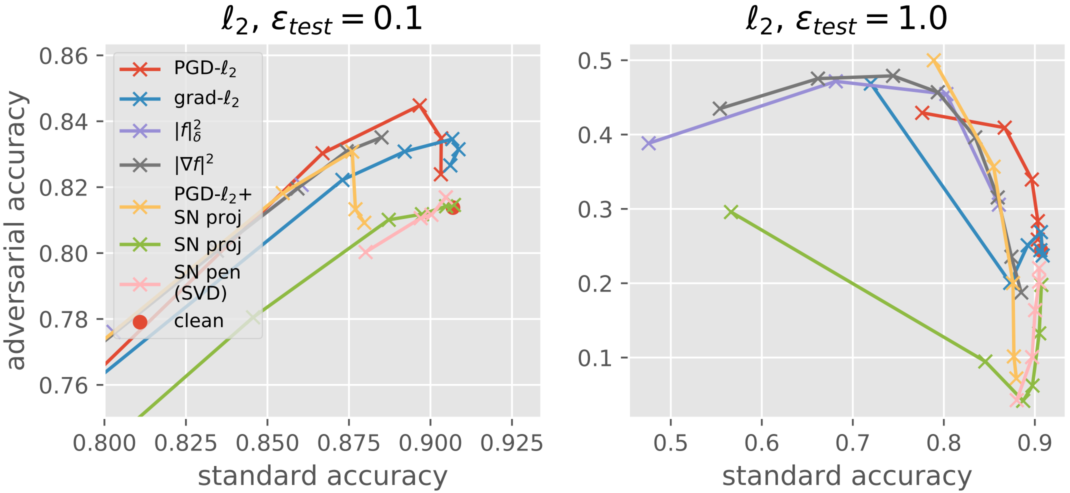


Figure: Robustness trade-off curves of different regularization methods for VGG11 on CIFAR10. Each plot shows test accuracy vs adversarial test accuracy Different points on a curve correspond to

Conclusions from this work on regularization

What the kernel perspective brings us

- gives a **unified perspective on many regularization principles**.
- useful both for **generalization and robustness**.
- related to **robust optimization**.

Future work

- regularization based on kernel approximations.
- semi-supervised learning to exploit unlabeled data.
- relation with implicit regularization.

References I

Babak Alipanahi, Andrew Delong, Matthew T Weirauch, and Brendan J Frey. Predicting the sequence specificities of dna-and rna-binding proteins by deep learning. *Nature biotechnology*, 33 (8):831–838, 2015.

Fabio Anselmi, Lorenzo Rosasco, Cheston Tan, and Tomaso Poggio. Deep convolutional networks are hierarchical kernel machines. *arXiv preprint arXiv:1508.01084*, 2015.

Peter Bartlett, Dylan J Foster, and Matus Telgarsky. Spectrally-normalized margin bounds for neural networks. *arXiv preprint arXiv:1706.08498*, 2017.

Alberto Bietti and Julien Mairal. Group invariance, stability to deformations, and complexity of deep convolutional representations. *Journal of Machine Learning Research (JMLR)*, 2019a.

Alberto Bietti and Julien Mairal. On the inductive bias of neural tangent kernels. In *Advances in Neural Information Processing Systems (NeurIPS)*, 2019b.

Alberto Bietti, Grégoire Mialon, Dexiong Chen, and Julien Mairal. A kernel perspective for regularizing deep neural networks. In *Proceedings of the International Conference on Machine Learning (ICML)*, 2019.

References II

L. Bo, K. Lai, X. Ren, and D. Fox. Object recognition with hierarchical kernel descriptors. In *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition (CVPR)*, 2011.

Léon Bottou, Frank E Curtis, and Jorge Nocedal. Optimization methods for large-scale machine learning. *arXiv preprint arXiv:1606.04838*, 2016.

Stéphane Boucheron, Olivier Bousquet, and Gábor Lugosi. Theory of classification: A survey of some recent advances. *ESAIM: probability and statistics*, 9:323–375, 2005.

J. V. Bouvrie, L. Rosasco, and T. Poggio. On invariance in hierarchical models. In *Advances in Neural Information Processing Systems (NIPS)*, 2009.

David S Broomhead and David Lowe. Radial basis functions, multi-variable functional interpolation and adaptive networks. Technical report, DTIC Document, 1988.

Joan Bruna and Stéphane Mallat. Invariant scattering convolution networks. *IEEE Transactions on pattern analysis and machine intelligence (PAMI)*, 35(8):1872–1886, 2013.

Dexiong Chen, Laurent Jacob, and Julien Mairal. Biological sequence modeling with convolutional kernel networks. *Bioinformatics*, 35(18):3294–3302, 02 2019a.

References III

Dexiong Chen, Laurent Jacob, and Julien Mairal. Recurrent kernel networks. In *Advances in Neural Information Processing Systems (NeurIPS)*, 2019b.

Lenaic Chizat, Edouard Oyallon, and Francis Bach. On lazy training in differentiable programming. In *Advances in Neural Information Processing Systems (NeurIPS)*, 2019.

Youngmin Cho and Lawrence K Saul. Kernel methods for deep learning. In *Advances in Neural Information Processing Systems (NIPS)*, 2009.

Moustapha Cisse, Piotr Bojanowski, Edouard Grave, Yann Dauphin, and Nicolas Usunier. Parseval networks: Improving robustness to adversarial examples. In *Proceedings of the International Conference on Machine Learning (ICML)*, 2017.

Taco Cohen and Max Welling. Group equivariant convolutional networks. In *International Conference on Machine Learning (ICML)*, 2016.

A. Damianou and N. Lawrence. Deep Gaussian processes. In *Proceedings of the International Conference on Artificial Intelligence and Statistics (AISTATS)*, 2013.

Harris Drucker and Yann Le Cun. Double backpropagation increasing generalization performance. In *International Joint Conference on Neural Networks (IJCNN)*, 1991.

References IV

Simon S Du, Kangcheng Hou, Russ R Salakhutdinov, Barnabas Poczos, Ruosong Wang, and Keyulu Xu. Graph neural tangent kernel: Fusing graph neural networks with graph kernels. In *Advances in Neural Information Processing Systems (NeurIPS)*, 2019.

Logan Engstrom, Dimitris Tsipras, Ludwig Schmidt, and Aleksander Madry. A rotation and a translation suffice: Fooling cnns with simple transformations. *arXiv preprint arXiv:1712.02779*, 2017.

Ishaan Gulrajani, Faruk Ahmed, Martin Arjovsky, Vincent Dumoulin, and Aaron C Courville. Improved training of Wasserstein GANs. In *Advances in Neural Information Processing Systems (NIPS)*, 2017.

Sepp Hochreiter, Martin Heusel, and Klaus Obermayer. Fast model-based protein homology detection without alignment. *Bioinformatics*, 23(14):1728–1736, 2007.

Jie Hou, Badri Adhikari, and Jianlin Cheng. DeepSF: deep convolutional neural network for mapping protein sequences to folds. *Bioinformatics*, 34(8):1295–1303, 12 2017. ISSN 1367-4803. doi: 10.1093/bioinformatics/btx780. URL `https://doi.org/10.1093/bioinformatics/btx780`.

References V

Arthur Jacot, Franck Gabriel, and Clément Hongler. Neural tangent kernel: Convergence and generalization in neural networks. In *Advances in Neural Information Processing Systems (NeurIPS)*, 2018.

Thomas N Kipf and Max Welling. Semi-supervised classification with graph convolutional networks. In *Proceedings of the International Conference on Learning Representations (ICLR)*, 2017.

Nils M Kriege, Marion Neumann, Christopher Morris, Kristian Kersting, and Petra Mutzel. A unifying view of explicit and implicit feature maps of graph kernels. *Data Mining and Knowledge Discovery*, 33(6):1505–1547, 2019.

Alexey Kurakin, Ian Goodfellow, and Samy Bengio. Adversarial examples in the physical world. *arXiv preprint arXiv:1607.02533*, 2016.

Y. LeCun, L. Bottou, Y. Bengio, and P. Haffner. Gradient-based learning applied to document recognition. *P. IEEE*, 86(11):2278–2324, 1998.

Tao Lei, Wengong Jin, Regina Barzilay, and Tommi Jaakkola. Deriving neural architectures from sequence and graph kernels. In *Proceedings of the International Conference on Machine Learning (ICML)*, 2017.

References VI

C. Leslie, E. Eskin, J. Weston, and W.S. Noble. Mismatch String Kernels for SVM Protein Classification. In *Advances in Neural Information Processing Systems 15*. MIT Press, 2003. URL `http://www.cs.columbia.edu/~cleslie/papers/mismatch-short.pdf`.

Christina Leslie and Rui Kuang. Fast string kernels using inexact matching for protein sequences. *Journal of Machine Learning Research*, 5(Nov):1435–1455, 2004.

Christina S Leslie, Eleazar Eskin, and William Stafford Noble. The spectrum kernel: A string kernel for svm protein classification. In *Pacific Symposium on Biocomputing*, volume 7, pages 566–575. Hawaii, USA, 2002.

Li Liao and William Stafford Noble. Combining pairwise sequence similarity and support vector machines for detecting remote protein evolutionary and structural relationships. *Journal of computational biology*, 10(6):857–868, 2003.

Huma Lodhi, Craig Saunders, John Shawe-Taylor, Nello Cristianini, and Chris Watkins. Text classification using string kernels. *Journal of Machine Learning Research (JMLR)*, 2:419–444, 2002.

Chunchuan Lyu, Kaizhu Huang, and Hai-Ning Liang. A unified gradient regularization family for adversarial examples. In *IEEE International Conference on Data Mining (ICDM)*, 2015.

References VII

Aleksander Madry, Aleksandar Makelov, Ludwig Schmidt, Dimitris Tsipras, and Adrian Vladu. Towards deep learning models resistant to adversarial attacks. In *Proceedings of the International Conference on Learning Representations (ICLR)*, 2018.

J. Mairal. End-to-end kernel learning with supervised convolutional kernel networks. In *Advances in Neural Information Processing Systems (NIPS)*, 2016a.

Julien Mairal. End-to-End Kernel Learning with Supervised Convolutional Kernel Networks. In *Advances in Neural Information Processing Systems (NIPS)*, 2016b.

Julien Mairal, Piotr Koniusz, Zaid Harchaoui, and Cordelia Schmid. Convolutional kernel networks. In *Advances in Neural Information Processing Systems (NIPS)*, 2014.

Stéphane Mallat. Group invariant scattering. *Communications on Pure and Applied Mathematics*, 65 (10):1331–1398, 2012.

Takeru Miyato, Toshiki Kataoka, Masanori Koyama, and Yuichi Yoshida. Spectral normalization for generative adversarial networks. In *Proceedings of the International Conference on Learning Representations (ICLR)*, 2018.

References VIII

GrÃŠgoire Montavon, Mikio L Braun, and Klaus-Robert MÃÅ§ller. Kernel analysis of deep networks. *Journal of Machine Learning Research*, 12(Sep):2563–2581, 2011.

Alyssa Morrow, Vaishaal Shankar, Devin Petersohn, Anthony Joseph, Benjamin Recht, and Nir Yosef. Convolutional kitchen sinks for transcription factor binding site prediction. *arXiv preprint arXiv:1706.00125*, 2017.

Radford M Neal. *Bayesian learning for neural networks*. Springer, 1996.

Behnam Neyshabur, Srinadh Bhojanapalli, David McAllester, and Nathan Srebro. A PAC-Bayesian approach to spectrally-normalized margin bounds for neural networks. In *Proceedings of the International Conference on Learning Representations (ICLR)*, 2018.

Mattis Paulin, Matthijs Douze, Zaid Harchaoui, Julien Mairal, Florent Perronin, and Cordelia Schmid. Local convolutional features with unsupervised training for image retrieval. In *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition (CVPR)*, 2015.

Ali Rahimi and Benjamin Recht. Random features for large-scale kernel machines. In *Advances in Neural Information Processing Systems (NIPS)*, 2007.

References IX

Anant Raj, Abhishek Kumar, Youssef Mroueh, P Thomas Fletcher, and Bernhard Scholkopf. Local group invariant representations via orbit embeddings. *preprint arXiv:1612.01988*, 2016.

Kevin Roth, Aurelien Lucchi, Sebastian Nowozin, and Thomas Hofmann. Stabilizing training of generative adversarial networks through regularization. In *Advances in Neural Information Processing Systems (NIPS)*, 2017.

Kevin Roth, Aurelien Lucchi, Sebastian Nowozin, and Thomas Hofmann. Adversarially robust training through structured gradient regularization. *arXiv preprint arXiv:1805.08736*, 2018.

B. Scholkopf. *Support Vector Learning*. PhD thesis, Technischen Universität Berlin, 1997.

Bernhard Schölkopf and Alexander J Smola. *Learning with kernels: support vector machines, regularization, optimization, and beyond*. MIT press, 2002.

Bernhard Schölkopf, Alexander Smola, and Klaus-Robert Müller. Nonlinear component analysis as a kernel eigenvalue problem. *Neural Computation*, 10(5):1299–1319, 1998.

Shai Shalev-Shwartz and Shai Ben-David. *Understanding machine learning: From theory to algorithms*. Cambridge university press, 2014.

References X

Vaishaal Shankar, Alex Fang, Wenshuo Guo, Sara Fridovich-Keil, Ludwig Schmidt, Jonathan Ragan-Kelley, and Benjamin Recht. Neural kernels without tangents. *preprint arXiv:2003.02237*, 2020.

John Shawe-Taylor and Nello Cristianini. *An introduction to support vector machines and other kernel-based learning methods*. Cambridge University Press, 2004.

Nino Shervashidze, Pascal Schweitzer, Erik Jan van Leeuwen, Kurt Mehlhorn, and Karsten M Borgwardt. Weisfeiler-Lehman graph kernels. *Journal of Machine Learning Research (JMLR)*, 12: 2539–2561, 2011.

Laurent Sifre and Stéphane Mallat. Rotation, scaling and deformation invariant scattering for texture discrimination. In *Proceedings of the IEEE conference on computer vision and pattern recognition (CVPR)*, 2013.

Patrice Y Simard, Yann A LeCun, John S Denker, and Bernard Victorri. Transformation invariance in pattern recognition–tangent distance and tangent propagation. In *Neural networks: tricks of the trade*, pages 239–274. Springer, 1998.

References XI

Carl-Johann Simon-Gabriel, Yann Ollivier, Bernhard Schölkopf, Léon Bottou, and David Lopez-Paz. Adversarial vulnerability of neural networks increases with input dimension. *arXiv preprint arXiv:1802.01421*, 2018.

Karen Simonyan and Andrew Zisserman. Very deep convolutional networks for large-scale image recognition. In *Proceedings of the International Conference on Learning Representations (ICLR)*, 2014.

Christian Szegedy, Wojciech Zaremba, Ilya Sutskever, Joan Bruna, Dumitru Erhan, Ian Goodfellow, and Rob Fergus. Intriguing properties of neural networks. *arXiv preprint arXiv:1312.6199*, 2013.

Matteo Togninalli, Elisabetta Ghisu, Felipe Llinares-López, Bastian Rieck, and Karsten Borgwardt. Wasserstein Weisfeiler-Lehman graph kernels. In *Advances in Neural Information Processing Systems (NeurIPS)*, 2019.

Vladimir Vapnik. *The nature of statistical learning theory*. Springer science & business media, 1995.

Jean-Philippe Vert, Hiroto Saigo, and Tatsuya Akutsu. Convolution and local alignment kernels. *Kernel methods in computational biology*, pages 131–154, 2004.

References XII

Christopher KI Williams and Matthias Seeger. Using the Nyström method to speed up kernel machines. In *Advances in Neural Information Processing Systems (NIPS)*, 2001.

Keyulu Xu, Weihua Hu, Jure Leskovec, and Stefanie Jegelka. How powerful are graph neural networks? In *Proceedings of the International Conference on Learning Representations (ICLR)*, 2019.

Zhitao Ying, Dylan Bourgeois, Jiaxuan You, Marinka Zitnik, and Jure Leskovec. Gnnexplainer: Generating explanations for graph neural networks. In *Advances in Neural Information Processing Systems (NeurIPS)*, 2019.

Y. Zhang, P. Liang, and M. J. Wainwright. Convexified convolutional neural networks. In *International Conference on Machine Learning (ICML)*, 2017.

Yuchen Zhang, Jason D Lee, and Michael I Jordan. ℓ_1-regularized neural networks are improperly learnable in polynomial time. In *International Conference on Machine Learning (ICML)*, 2016.