On the Benefits of Convolutional Models: a Kernel Perspective

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NYU

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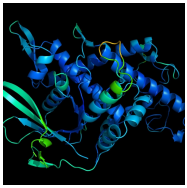
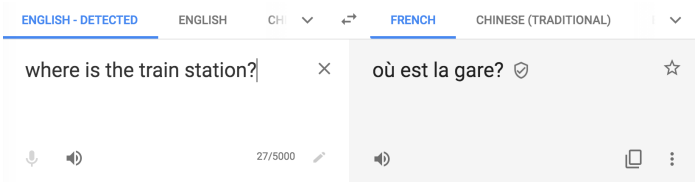
Success of Deep Learning

State-of-the-art models in various domains (images, speech, language, biology, ...)





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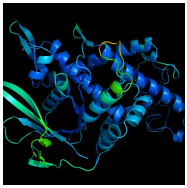
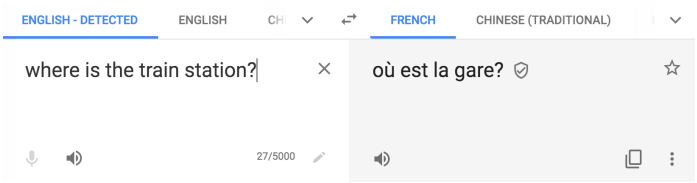
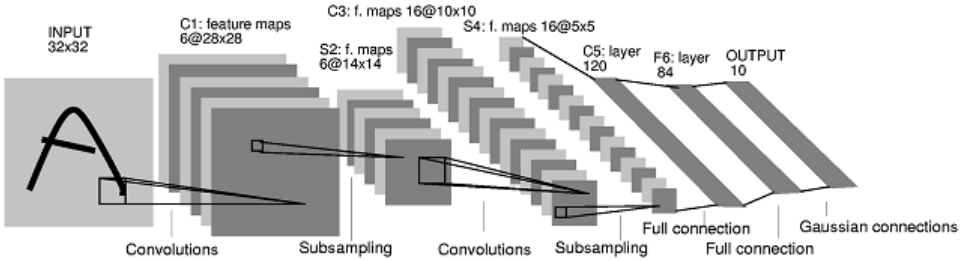




Recipe: **huge models** + **lots of data** + **compute** + **simple algorithms**

Convolutional Networks



(LeCun et al., 1998)

Exploiting the structure of natural images

- Model local information at different scales, hierarchically
- Provide some invariance through pooling
- Useful **inductive biases** for learning efficiently on natural signals

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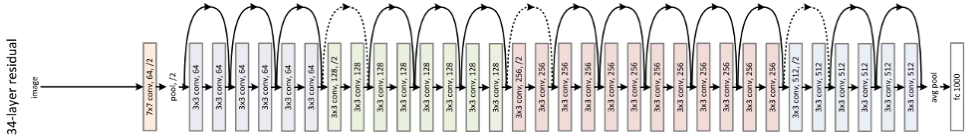

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Understanding Deep Learning

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The challenge of deep learning theory

- **Over-parameterized** (millions/billions of parameters)
- **Expressive** (can approximate any function)
- Complex **architectures** for exploiting problem structure
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A functional viewpoint

- View deep networks as functions in some functional space
- Non-parametric models, natural measures of complexity (*e.g.*, norms)
- Optimization performs **implicit regularization** towards

$$\min_f \Omega(f) \quad \text{s.t.} \quad y_i = f(x_i), \quad i = 1, \dots, n$$

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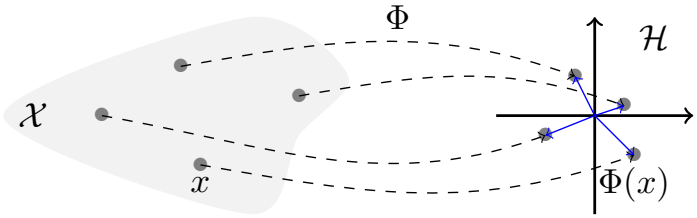
Q: What is an appropriate functional space / norm Ω?

Kernels



Kernels?

- Map data $x \in \mathcal{X}$ to high-dimensional space, $\Phi(x) \in \mathcal{H}$ ($\mathcal{H}$: "RKHS")
- Functions $f \in \mathcal{H}$ are linear in features: $f(x) = \langle f, \Phi(x) \rangle_{\mathcal{H}}$ (f can be non-linear in x!)

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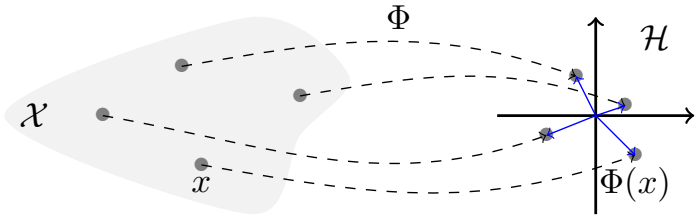

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- Learning with a positive definite kernel $K(x, x') = \langle \Phi(x), \Phi(x') \rangle_{\mathcal{H}}$
  - $\mathcal{H}$ can be infinite-dimensional! (*kernel trick*)
  - Use a kernel matrix $K = [K(x_i, x_j)]_{ij} \in \mathbb{R}^{N \times N}$ or its approximations

Kernels for Convolutional Models

My work (B. and Mairal, 2019a,b; B. et al., 2021b; B., 2022):

- Formal study of **convolutional kernels** and their RKHS
- **Benefits** of (deep) convolutional structure

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Locality
Long-range interactions

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Deformation stability
Multi-scale structure

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Clean and well-developed theory

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- Benefits of depth (*e.g.*, Eldan and Shamir, 2016; Mhaskar and Poggio, 2016): no algorithms
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A starting point to understand CNNs

- Understand the **features** $\Phi(x)$ provided by architectures
- $\approx$ study least squares before the Lasso

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A starting point to understand CNNs

- Understand the **features** $\Phi(x)$ provided by architectures
- $\approx$ study least squares before the Lasso
- Good performance on standard vision datasets (Mairal, 2016; Shankar et al., 2020; B., 2022)

Outline

1. Invariance and Stability (B., Venturi, and Bruna, 2021b)
2. Locality and Depth (B., 2022)
3. Multi-Scale Structure and Stability (B. and Mairal, 2019a,b)
4. Concluding Remarks and Research Directions

Outline

Invariance and Geometric Stability

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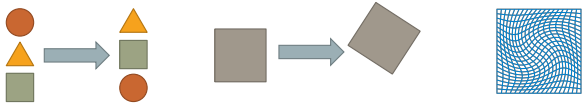
Q: Does invariance improve learning efficiency?

Invariance and Geometric Stability: Definitions



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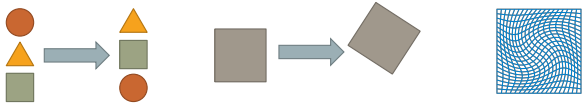

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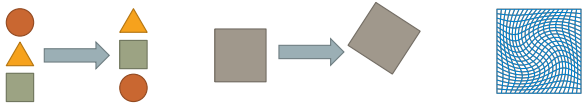

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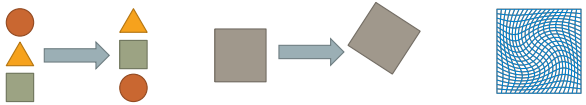

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Geometric stability: For other sets G (*e.g.*, local shifts, deformations), we want

$$f(\sigma \cdot x) \approx f(x), \quad \sigma \in G$$

Interlude: Kernels for Infinite Shallow Networks

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\begin{aligned}
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- **Random Features** (RF, Neal, 1996; Rahimi and Recht, 2007): $w_i \sim \mathcal{N}(0, I)$, learn v

$$K_{RF}(x, x') = \lim_{m \to \infty} \langle \varphi(x), \varphi(x') \rangle$$
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- Related to **Neural Tangent Kernel** (NTK, Jacot et al., 2018): train both w_i and v_i near random initialization

Group-Invariant Models through Pooling

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Convolutional network with pooling (group averaging)

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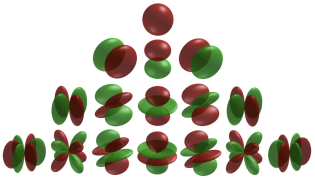
- $|G|$ can be exponential in d for some groups! (*e.g.*, the full permutation group)
- Rate β depends on d and smoothness of f^* (minimax optimal)

Key Technical Ingredient: Counting Invariant Harmonics



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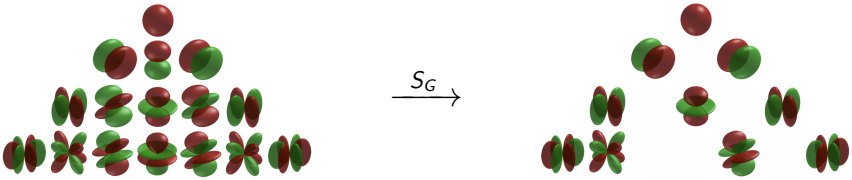

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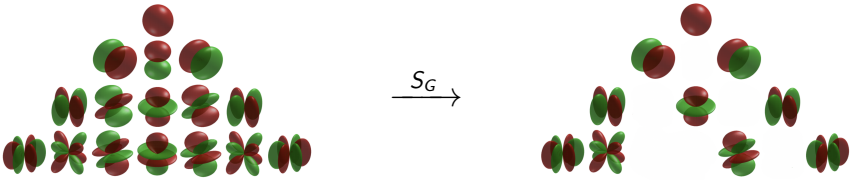

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- Key result: decrease in **effective dimensionality** by a factor $|G|$

Theorem (Invariant harmonics (B., Venturi, and Bruna, 2021b))

As $k \to \infty$, we have

$$\frac{\overline{N}_k}{N_k} \to \frac{1}{|G|}$$

Extension to Stability and Discussion

Geometric stability: G is not a group (*e.g.*, local shifts/deformations)

- Pooling operation is no longer a projection, but leads to natural stability assumption
- Similar bounds with effective sample size $n|G|$
- $|G|$ is exponential in d for a simple toy model of deformations!

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Curse of dimensionality

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Q: How can we break this curse?

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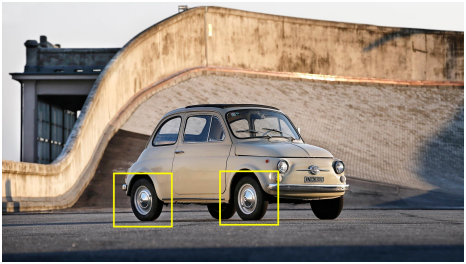
Locality



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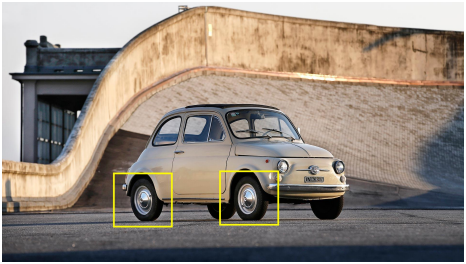
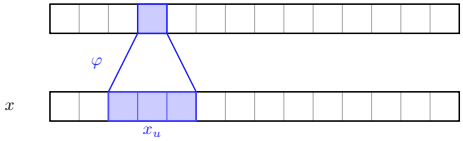


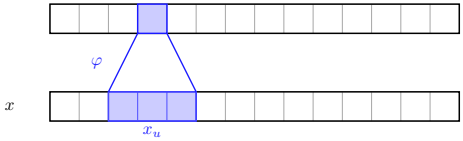
Q: Can locality improve sample complexity?

One-Layer Convolutional Kernels on Patches



- **Patches**: $x_u \in \mathbb{R}^p$ at positions $u \in \Omega$
- **Features**: $\varphi(x_u) = \frac{1}{\sqrt{m}}\rho(Wx_u)$, $m \to \infty$, **patch kernel**: $k(z, z') = \langle \varphi(z), \varphi(z') \rangle$

One-Layer Convolutional Kernels on Patches



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$$f(x) = \sum_{u \in \Omega} \langle v_u, \varphi(x_u) \rangle =: \langle v, \Phi(x) \rangle$$

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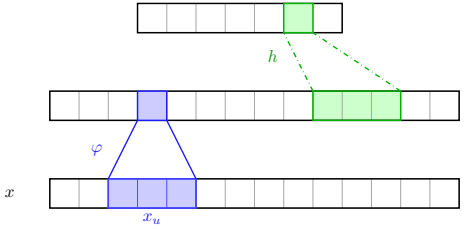

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$$f_h(x) = \sum_{u \in \Omega} \langle v_u, \sum_v h[u - v] \varphi(x_v) \rangle$$

- **Convolutional kernel**:

$$K_h(x, x') = \sum_{u \in \Omega} \sum_{v, v'} h[u - v] h[u - v'] k(x_v, x'_{v'})$$

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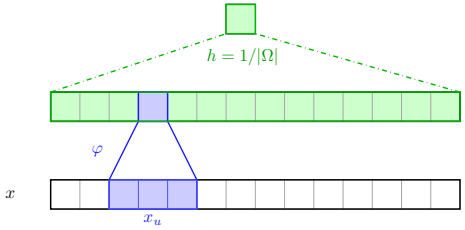

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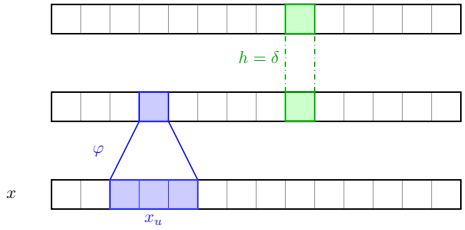

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Benefits of Locality and Pooling

- Assume **additive**, **invariant** target $f^*(x) = \sum_{u \in \Omega} g^*(x_u)$
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Assume non-overlapping patches on $\mathbb{S}^{p-1}$. Learning with K_h yields

$$\mathbb{E}\, R(\hat{f}_{g,n}) - R(f^*) \lesssim \left(\frac{1}{n}\right)^\beta \quad \textit{vs} \quad \mathbb{E}\, R(\hat{f}_{\delta,n}) - R(f^*) \lesssim \left(\frac{|\Omega|}{n}\right)^\beta$$

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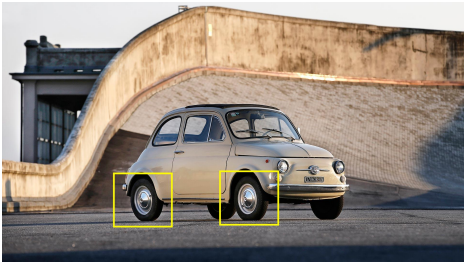
- Rate β only depends on $p \ll d = p|\Omega|$ (**breaks the curse of dimensionality**!)
- With local pooling, we can also learn $f^*(x) = \sum_{u \in \Omega} g^*_u(x_u)$ with different g^*_u

Long-Range Interactions



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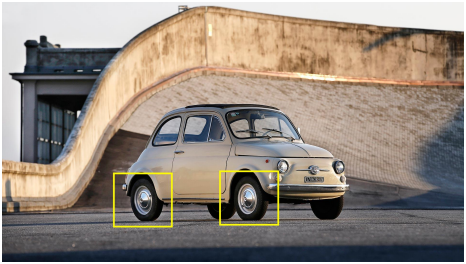

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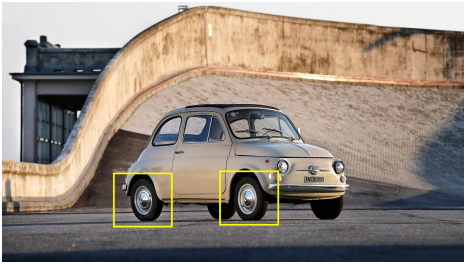

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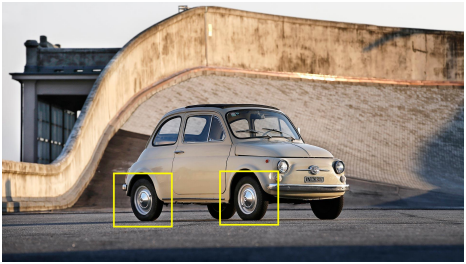

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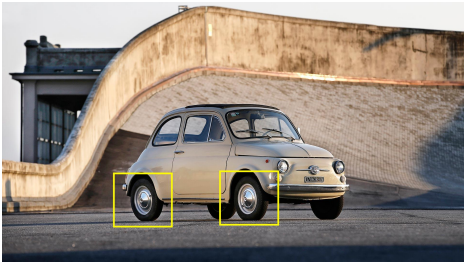

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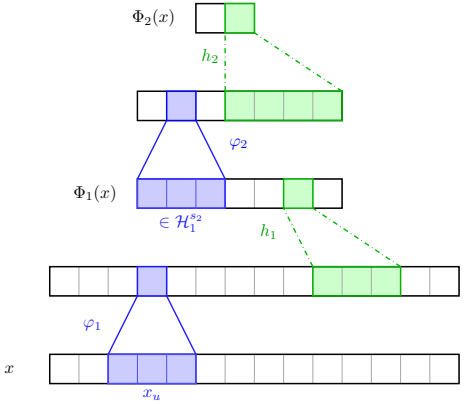

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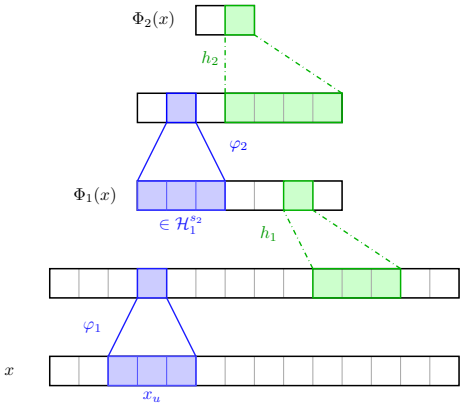

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- Take $\kappa_2(u) = u^2$. RKHS contains

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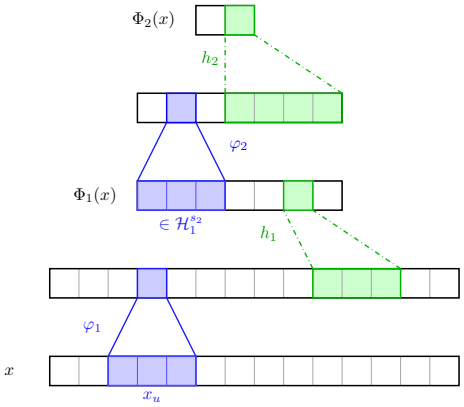

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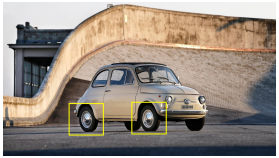

- Pooling h_1: invariance to **relative** position
- Pooling h_2: invariance to **global** position

Is it a Good Model for Cifar10? (B., 2022)

Compute $50\,000 \times 50\,000$ kernel matrix and run Kernel Ridge Regression.[1]

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2-layers, patch sizes (3, 5), Gaussian pooling factors (2,5).

κ_1	κ_2	Test acc.
Gauss	Gauss	88.3%
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- **Polynomial kernels at second layer suffice!**
- **State-of-the-art for kernels on Cifar10**
  - Shankar et al. (2020): 88.2% with 10 layers (90% with data augmentation)

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Generalization Benefits with Two Layers (B., 2022)

- Consider **invariant** $f^*(x) = \sum_{u,v \in \Omega} g^*(x_u, x_v)$
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Polynomial gains in $|\Omega|$ when using the right architecture![2]

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Q: Can more layers help with multi-scale structure?

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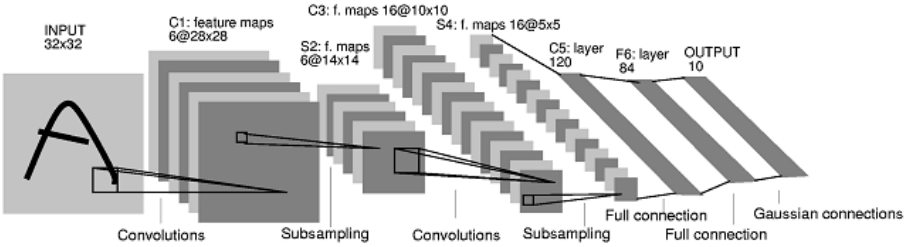
Outline

Beyond Translation Invariance



Convolutional architectures:

- Capture **multi-scale** structure in natural signals
- Provide near-**translation invariance**

Q: Beyond translation invariance using multi-scale structure?

Stability to Deformations

Deformations

- $\tau : \Omega \to \Omega$: smooth vector field
- $\tau \cdot x(u) = x(u - \tau(u))$: deformation operator
- Much richer group of transformations than translations

- Studied for wavelet-based scattering transform (Mallat, 2012; Bruna and Mallat, 2013)

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Definition of stability

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

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Q: Can we achieve this along with approximation using kernels?

Stability with Kernels (B. and Mairal, 2019a)

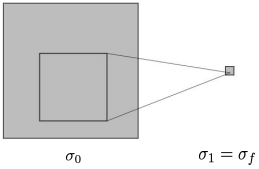
Geometry of the kernel mapping: $f(x) = \langle f, \Phi(x) \rangle_{\mathcal{H}}$

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

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

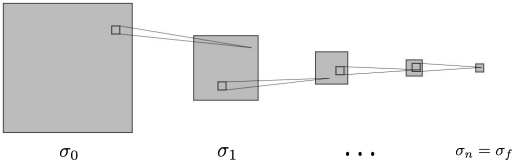
Deep vs Shallow Convolutional Models

Shallow



- $n = 1$
- $s \approx \sigma_f / \sigma_0$

Deep



- $s = O(1)$
- $n \approx \log(\sigma_f / \sigma_0) / \log s$

- n layers, multiple scales $\sigma_0, \ldots, \sigma_n = \sigma_f$
- Patch size $s \approx \sigma_k / \sigma_{k-1}$ = pooling/downsampling factor
  - Ensures **universal approximation** and **invariance**

Stability of Convolutional Kernels

Theorem (Stability of Convolutional Kernel (B. and Mairal, 2019a))

Let Φ be a n-layer conv kernel with scales $\sigma_0, \dots, \sigma_f$, and patch size s.

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Q: What about stability of predictions?

Stability and Regularization in Deep Learning Practice

Two common issues with deep learning models:

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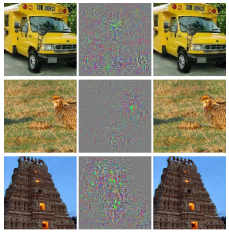

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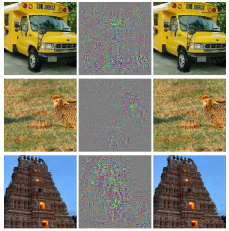

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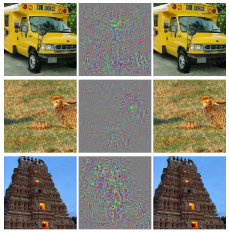

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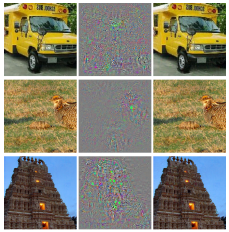

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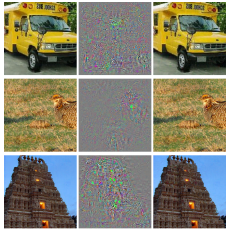

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- **New practical regularizers**, outperform existing ones on:
  - Small data problems (vision, biology)
  - Adversarial robustness (**state-of-the-art** on Cifar10)

Outline

Concluding Remarks

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Kernels can help us understand deep learning architectures

Deep Learning Structure Beyond Kernels

Convolutional networks beyond kernels

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Generative models, representation learning

- How do DL algorithms discover structure without labels?
- Feature learning in energy-based models (Domingo-Enrich et al., 2021b,a)
- Role of transformations in contrastive self-supervised learning

Understanding Architectures

Graph Neural Networks

- Graph data are rich and varied (*e.g.*, social networks, chemistry, drug discovery, graphics)
- B. et al. (2020); Keriven et al. (2021): we show **stability** and **approximation** benefits for GNNs on large random graph models
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Interpretability

- Use insights from kernels to understand mechanisms behind trained networks?

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- Stochastic and private optimization
  - (B. et al., 2022; B. and Mairal, 2017)

Thank you!

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