On the Benefits of Convolutional Models: a Kernel Perspective

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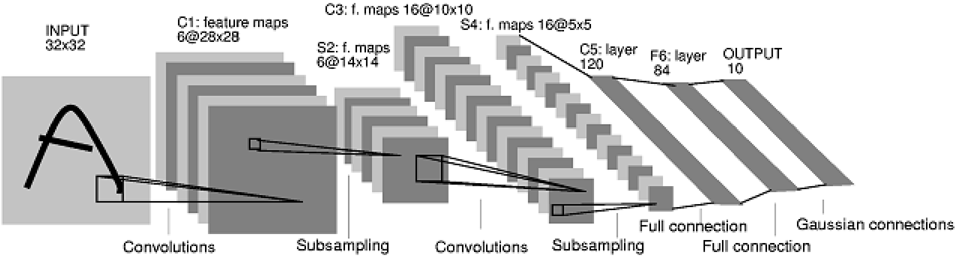
NYU

BIRS. May 26, 2022.

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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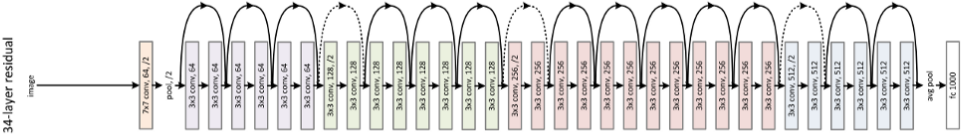

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Setup

Nonparametric regression with kernels

- Data model: $y = f^*(x) + \epsilon$
- Kernel ridge regression with kernel K (with RKHS $\mathcal{H}$)

$$\hat{f}_n = \arg\min_{f \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} (y_i - f(x_i))^2 + \lambda \|f\|_{\mathcal{H}}^2$$

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Questions

- What are good assumptions on f^* for image problems?
- How does the kernel/norm/architecture exploit this for sample efficiency?

Kernels for Convolutional Models

This talk (B. et al., 2021; B., 2022):

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

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Invariance

Locality
Long-range interactions

Why Kernels?

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Clean and well-developed theory

- Tractable **optimization** algorithms (convex)
- Universal **approximation** guarantees
- Optimal **statistical** rates for many problems
  - *e.g.*, smooth functions (Caponnetto and De Vito, 2007), interaction splines (Wahba, 1990)

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- Approximation benefits of depth: *no algorithms*
  - (Eldan and Shamir, 2016; Mhaskar and Poggio, 2016; Telgarsky, 2016; Cohen and Shashua, 2017; Schmidt-Hieber, 2020)
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A starting point to understand CNNs

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

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A starting point to understand CNNs

- Understand the **features** $\Phi(x)$ provided by architectures ($\approx$ least squares before Lasso)
- Good performance on Cifar10 (Mairal, 2016; Li et al., 2019; Shankar et al., 2020; B., 2022)

Outline

1. Invariance and Stability (B., Venturi, and Bruna, 2021)

2. Locality and Depth (B., 2022)

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Invariance and Geometric Stability

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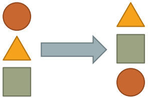
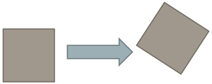
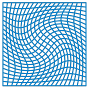
Q: Does invariance improve statistical efficiency?

Invariance and Geometric Stability: Definitions

Functions $f : \mathcal{X} \subset \mathbb{R}^d \to \mathbb{R}$ that are "smooth" along known transformations of input x

- *e.g.*, translations, rotations, permutations, deformations

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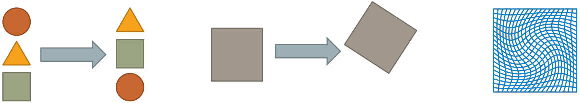

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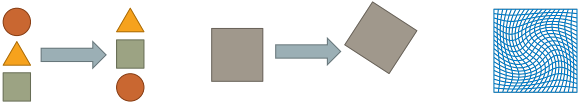

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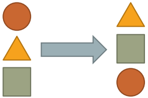

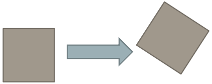

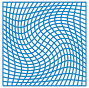

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Geometric stability: For other sets G (*e.g.*, local shifts, deformations), we want

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

Interlude: Kernels for Wide Shallow Networks

$$f(x) = \frac{1}{\sqrt{m}} \sum_{i=1}^{m} v_i \rho(\langle w_i, x \rangle)$$

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$$\begin{aligned} f(x) &= \frac{1}{\sqrt{m}} \sum_{i=1}^m v_i \rho(\langle w_i, x \rangle) \\ &= \langle v, \varphi(x) \rangle, \qquad \text{with } \varphi(x) = \frac{1}{\sqrt{m}} \rho(Wx) \in \mathbb{R}^m \end{aligned}$$

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

$$K_{RF}(x, x') = \lim_{m \to \infty} \langle \varphi(x), \varphi(x') \rangle$$

$$= \mathbb{E}_w[\rho(\langle w, x \rangle)\rho(\langle w, x' \rangle)] = \kappa_\rho(\langle x, x' \rangle) \quad \text{when } x, x' \in \mathbb{S}^{d-1}$$

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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

$$\varphi(x) = \frac{1}{\sqrt{m}} \rho(Wx)$$

Convolutional network with pooling (group averaging)

$$f_G(x) = \langle v, \underbrace{\frac{1}{|G|} \sum_{\sigma \in G} \varphi(\sigma \cdot x)}_{\Phi(x)} \rangle$$

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Invariant kernel (Haasdonk and Burkhardt, 2007; Mroueh et al., 2015)

$$K_G(x, x') = \frac{1}{|G|}\sum_{\sigma \in G} \kappa(\langle \sigma \cdot x, x' \rangle), \quad \text{when } x, x' \in \mathbb{S}^{d-1}$$

- When $\kappa = \kappa_\rho$, this corresponds to Random Features kernel for f_G

Statistical Benefits of Group Invariance

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Theorem (Benefits of invariance (B., Venturi, and Bruna, 2021))

*Assume f^* is G-**invariant** and s-**smooth**. KRR with kernel K_G vs K achieves*

$$\mathbb{E}\, R(\hat{f}_{K_G,n}) - R(f^*) \leq C_d \left(\frac{1 + o(1)}{|G| n} \right)^{\frac{2s}{2s+d-1}} \qquad \text{vs.} \qquad \mathbb{E}\, R(\hat{f}_{K,n}) - R(f^*) \leq C_d \left(\frac{1}{n} \right)^{\frac{2s}{2s+d-1}}$$

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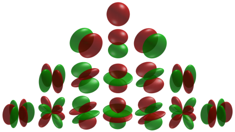
$\Longrightarrow$ **asymptotic gains by a factor $|G|$ in sample complexity.**

- $|G|$ can be exponential in d for some groups (*e.g.*, the full permutation group)
- Rate and dimension-dependence in constant C_d are asymptotically minimax optimal

Key Technical Ingredient: Counting Invariant Harmonics

- Expand in $L^2(\mathbb{S}^{d-1})$ basis of **spherical harmonics** $Y_{k,j}$
- $N(d,k)$ harmonics of degree k, form a basis of $V_{d,k}$
- Pooling projects $V_{d,k}$ to $\overline{N}(d,k)$ **invariant harmonics**



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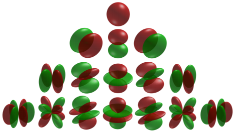

Theorem ((B., Venturi, and Bruna, 2021))

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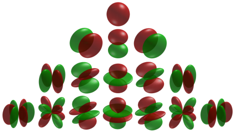

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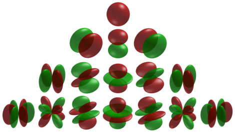

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- Decay rate can be quantified using cycle statistics of $\sigma \in G$
- Uses a characterization of $\gamma_d(k)$ due to Mei et al. (2021), who study a different regime:
  - They study $d \to \infty$ with fixed k ($\gamma_d(k) = \Theta_d(d^{-\alpha})$), gains at most polynomial in d
  - We study $k \to \infty$ with fixed d, gain $|G|$ can be exponential in d.

Extension to Stability and Discussion

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

- Pooling operation is no longer a projection, but leads to natural assumption
- Similar bounds with effective sample size $n|G|$
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Curse of dimensionality

- If the target f^* is non-smooth, *e.g.*, only Lipschitz, the rate is cursed! (and unimprovable)

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Q: How can we break this curse?

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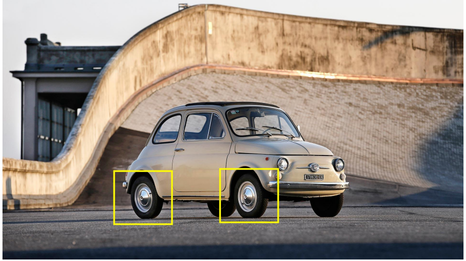
2. Locality and Depth (B., 2022)

Locality



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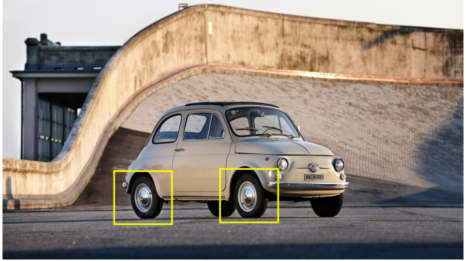
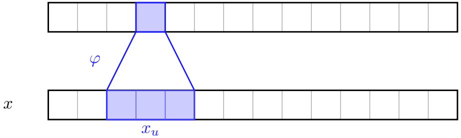


Q: Can locality improve statistical efficiency?

One-Layer Convolutional Kernels on Patches



- 1D signal: $x[u]$, $u \in \Omega$
- **Patches**: $x_u = (x[u], \dots, x[u + p - 1]) \in \mathbb{R}^{p}$, features $\varphi(x_u) = \frac{1}{\sqrt{m}} \rho(W x_u)$, $m \to \infty$

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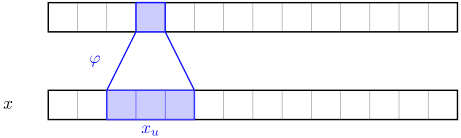

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- **Convolutional network**:

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

- **Convolutional kernel** (with $k(z, z') = \langle \varphi(z), \varphi(z') \rangle$ the RF **patch kernel**)

$$K(x, x') = \sum_{u \in \Omega} k(x_u, x'_u)$$

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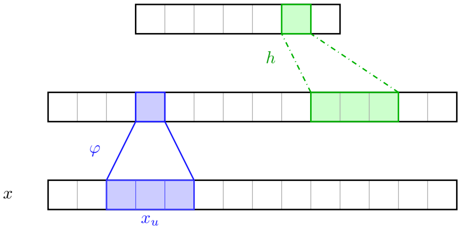

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- **Convolutional network**: with pooling filter h

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

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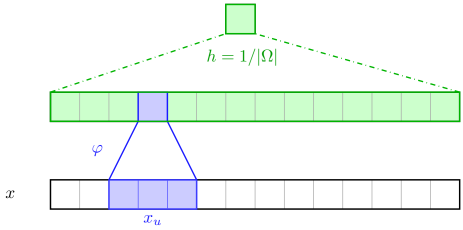

- 1D signal: $x[u]$, $u \in \Omega$
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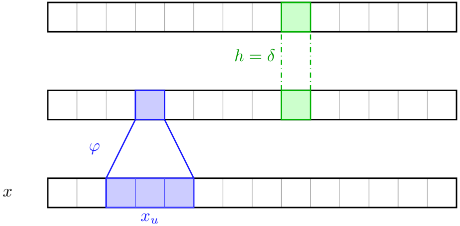

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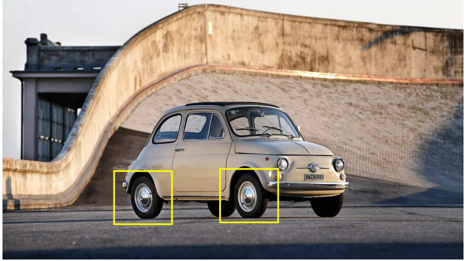
- For overlapping patches, see (Favero et al., 2021; Misiakiewicz and Mei, 2021)

Long-Range Interactions



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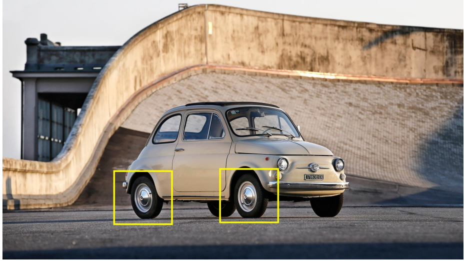

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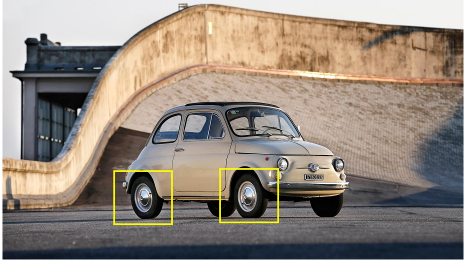

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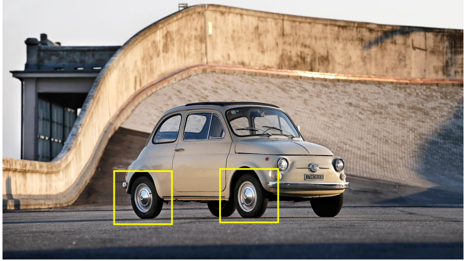

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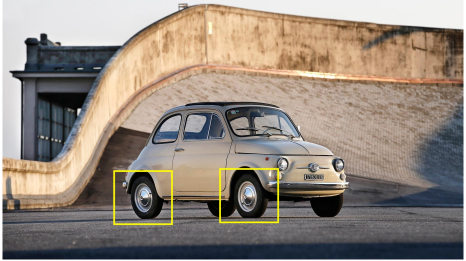

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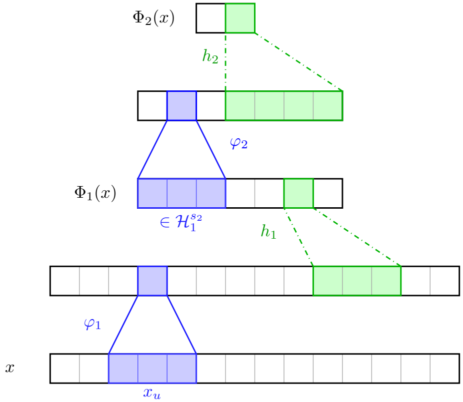

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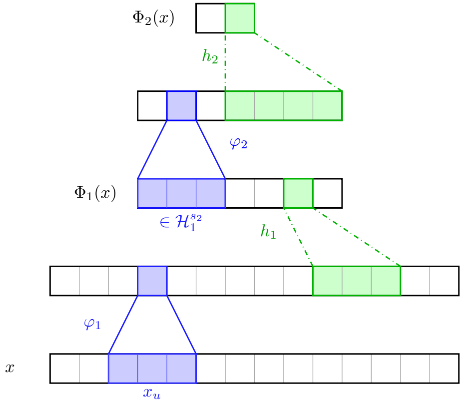

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- Take $\kappa_2(u) = u^2$. RKHS contains

$$f(x) = \sum_{|u-v|\leq r} g_{u,v}(x_u, x_v)$$

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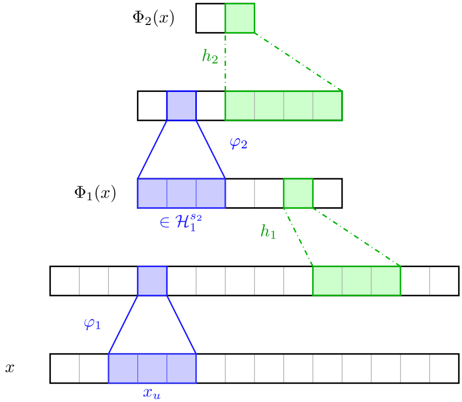

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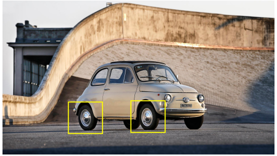

- Effect of RKHS norm:
  - Pooling h_1: invariance to **relative** position
  - Pooling h_2: invariance to **global** position

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- **Polynomial kernels at second layer suffice!**
- **State-of-the-art for kernels on Cifar10** (at a large computational cost...)
    - Shankar et al. (2020): 88.2% with 10 layers (90% with data augmentation)

Statistical Benefits with Two Layers (B., 2022)

- Consider invariant $f^*(x) = \sum_{u,v \in \Omega} g^*(x_u, x_v)$
- Assume $\mathbb{E}_x[k(x_u, x_{u'})k(x_v, x_{v'})] \leq \epsilon$ if $u \neq u'$ or $v \neq v'$
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Excess risk bounds when $g^* \in \mathcal{H}_k \otimes \mathcal{H}_k$ (slow rates)

h_1	h_2	s_2	$R(\hat{f}_n) - R(f^*)$ (for $\epsilon \to 0$)
δ	δ	$\|\Omega\|$	$\|g^*\| \|\Omega\|^{2.5}/\sqrt{n}$
δ	global	$\|\Omega\|$	$\|g^*\| \|\Omega\|^{2}/\sqrt{n}$
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Polynomial gains in $|\Omega|$ when using the right architecture![1]

[1] Best $\approx$ deep sets (Zaheer et al., 2017)

Concluding Remarks

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What's missing?

- Sparsity/adaptivity
  - First layer: adaptive convolutional filters (Gabors)
  - Following layers: structured interactions/symmetries
- Beyond CNNs
  - GNNs, Transformers

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