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### High Dimensional Learning

- High-dimensional  $x = (x(1), ..., x(d)) \in \mathbb{R}^d$ :
- Classification: estimate a class label f(x)given n sample values  $\{x_i, y_i = f(x_i)\}_{i \le n}$

Image Classification  $d = 10^6$ Huge variability Joshua Tree Anchor Lotus Beaver Water Lily inside classes Find invariants

### High Dimensional Learning

- High-dimensional  $x = (x(1), ..., x(d)) \in \mathbb{R}^d$ :
- Regression: approximate a functional f(x)given n sample values  $\{x_i, y_i = f(x_i) \in \mathbb{R}\}_{i \le n}$

Physics: energy f(x) of a state vector x

#### Astronomy



Quantum Chemistry



Importance of symmetries.

### Curse of Dimensionality

• f(x) can be approximated from examples  $\{x_i, f(x_i)\}_i$  by local interpolation if f is regular and there are close examples:





• Need  $e^{-d}$  points to cover  $[0, 1]^d$  at a Euclidean distance eProblem:  $||x - x_i||$  is always large





- Variables x(u) indexed by a low-dimensional u: time/space... pixels in images, particles in physics, words in text...
  - Mutliscale interactions of d variables:



From  $d^2$  interactions to  $O(\log^2 d)$  multiscale interactions.

• Multiscale analysis: wavelets on groups of symmetries. hierarchical architecture.



- 1 Hidden Layer Network, Approximation theory and Curse
- Kernel learning
- Dimension reduction with change of variables
- Deep Neural networks and symmetry groups
- Wavelet Scattering transforms
- Applications and many open questions

Understanding Deep Convolutional Networks, arXiv 2016.

## Learning as an Approximation

- To estimate f(x) from a sampling  $\{x_i, y_i = f(x_i)\}_{i \leq M}$ we must build an *M*-parameter approximation  $f_M$  of f.
  - Precise sparse approximation requires some "regularity".

• For binary classification 
$$f(x) = \begin{cases} 1 & \text{if } x \in \Omega \\ -1 & \text{if } x \notin \Omega \end{cases}$$
  
$$f(x) = \operatorname{sign}(\tilde{f}(x))$$

where  $\tilde{f}$  is potentially regular.

• What type of regularity ? How to compute  $f_M$  ?

## 1 Hidden Layer Neural Networks

One-hidden layer neural network: ridge functions  $\rho(x.w_n + b_n)$ 

$\rho(w_{n})$	$a \cdot x + b_n)$	$f_M(x) = \sum_{n=1}^M \alpha_n \rho(w_n \cdot x + b_n)$ $\{w_{k,k}\}_{k,n} \text{ and } \{\alpha_n\}_n \text{ are learned}$
	M	non-linear approximation.

Cybenko, Hornik, Stinchcombe, White **Theorem:** For "resonnable" bounded  $\rho(u)$ and appropriate choices of  $w_{n,k}$  and  $\alpha_n$ :  $\forall f \in \mathbb{L}^2[0,1]^d \quad \lim_{M \to \infty} \|f - f_M\| = 0$ .

No big deal: curse of dimensionality still there.

## 1 Hidden Layer Neural Networks

One-hidden layer neural network:

Fourier series: 
$$\rho(u) = e^{iu}$$
  
 $f_M(x) = \sum_{n=1}^M \alpha_n e^{iw_n \cdot x}$ 

For nearly all  $\rho$ : essentially same approximation results.

## Piecewise Linear Approximation



Need  $M = \epsilon^{-1}$  points to cover [0, 1] at a distance  $\epsilon$ 

$$\Rightarrow ||f - f_M|| \le C M^{-1}$$

### Linear Ridge Approximation

• Piecewise linear ridge approximation:  $x \in [0, 1]^d$ 

If f is Lipschitz:  $|f(x) - f(x')| \le C ||x - x'||$ Sampling at a distance  $\epsilon$ :

$$\Rightarrow |f(x) - \tilde{f}(x)| \le C \epsilon.$$

need  $M = \epsilon^{-d}$  points to cover  $[0, 1]^d$  at a distance  $\epsilon$ 

$$\Rightarrow \|f - f_M\| \le C M^{-1/d}$$

Curse of dimensionality!

## Approximation with Regularity

- What prior condition makes learning possible ?
- Approximation of regular functions in  $\mathbf{C}^{s}[0,1]^{d}$ :
- $\forall x, u \quad |f(x) p_u(x)| \le C |x u|^s \text{ with } p_u(x) \text{ polynomial}$



Need  $M^{-d/s}$  point to cover  $[0,1]^d$  at a distance  $\epsilon^{1/s}$ 

$$\Rightarrow \|f - f_M\| \le C M^{-s/d}$$

• Can not do better in  $\mathbf{C}^{\mathbf{s}}[0,1]^d$ , not good because  $s \ll d$ . Failure of classical approximation theory. **Kernel Learning** 

Change of variable  $\Phi(x) = \{\phi_k(x)\}_{k \le d'}$ 

to nearly linearize f(x), which is approximated by:



- How and when is possible to find such a  $\Phi$  ?
- What "regularity" of f is needed ?

### Increase Dimensionality

**Proposition:** There exists a hyperplane separating any two subsets of N points  $\{\Phi x_i\}_i$  in dimension d' > N + 1if  $\{\Phi x_i\}_i$  are not in an affine subspace of dimension < N.

 $\Rightarrow$  Choose  $\Phi$  increasing dimensionality !

**Problem:** generalisation, overfitting.

**Example:** Gaussian kernel  $\langle \Phi(x), \Phi(x') \rangle = \exp\left(\frac{-\|x - x'\|^2}{2\sigma^2}\right)$ 

 $\Phi(x)$  is of dimension  $d' = \infty$ 

If  $\sigma$  is small, nearest neighbor classifier type:



### **Reduction of Dimensionality**

- Discriminative change of variable  $\Phi(x)$ :  $\Phi(x) \neq \Phi(x')$  if  $f(x) \neq f(x')$   $\Rightarrow \exists \tilde{f} \text{ with } f(x) = \tilde{f}(\Phi(x))$ 
  - If  $\tilde{f}$  is Lipschitz:  $|\tilde{f}(z) \tilde{f}(z')| \le C ||z z'||$   $z = \Phi(x) \iff |f(x) - f(x')| \le C ||\Phi(x) - \Phi(x')||$ Discriminative:  $||\Phi(x) - \Phi(x')|| \ge C^{-1} |f(x) - f(x')|$

• For  $x \in \Omega$ , if  $\Phi(\Omega)$  is bounded and a low dimension d' $\Rightarrow \|f - f_M\| \le C M^{-1/d'}$ 

### **Deep Convolution Neworks**

• The revival of neural networks: Y. LeCun



Optimize  $L_j$  with architecture constraints: over 10<sup>9</sup> parameters Exceptional results for *images, speech, language, bio-data...* Why does it work so well ? A difficult problem

### ImageNet Data Basis

• Data basis with 1 million images and 2000 classes



# Alex Deep Convolution Network

 A. Krizhevsky, Sutsever, Hinton
Imagenet supervised training: 1.2 10<sup>6</sup> examples, 10<sup>3</sup> classes 15.3% testing error in 2012





New networks with 5% errors. Up to 150 layers!

### **Image Classification**



grine	mushivoni	citoriy	madagascar car
convertible	agaric	dalmatian	squirrel monkey
grille	mushroom	grape	spider monkey
pickup	jelly fungus	elderberry	titi
beach wagon	gill fungus	ffordshire bullterrier	indri
fire engine	dead-man's-fingers	currant	howler monkey

### Scene Labeling / Car Driving







Why Understading ?

Szegedy, Zaremba, Sutskever, Bruna, Erhan, Goodfellow, Fergus

with  $\|\epsilon\| < 10^{-2} \|x\|$ 

 $\epsilon = \tilde{x}$  $\mathcal{X}$ correctly classified as classified ostrich

• Trial and error testing can not guarantee reliability.

# Deep Convolutional Networks



•  $L_j$  is a linear combination of convolutions and subsampling:

$$x_{j}(u,k_{j}) = \rho\left(\sum_{\substack{k \\ \text{sum across channels}}} x_{j-1}(\cdot,k) \star h_{k_{j},k}(u)\right)$$

•  $\rho$  is contractive:  $|\rho(u) - \rho(u')| \le |u - u'|$  $\rho(u) = \max(u, 0) \text{ or } \rho(u) = |u|$ 

### Linearisation in Deep Networks

A. Radford, L. Metz, S. Chintala



• On a data basis including bedrooms: interpolaitons





- Why convolutions ? Translation covariance.
- Why no overfitting ? Contractions, dimension reduction
- Why hierarchical cascade ?
- Why introducing non-linearities ?
- How and what to linearise ?
- What are the roles of the multiple channels in each layer ?





If level sets (classes) are parallel to a linear space then variables are eliminated by linear projections: *invariants*.





- If level sets  $\Omega_t$  are not parallel to a linear space
  - Linearise them with a change of variable  $\Phi(x)$
  - Then reduce dimension with linear projections
- Difficult because  $\Omega_t$  are high-dimensional, irregular, known on few samples.

# Level Set Geometry: Symmetries

• Curse of dimensionality  $\Rightarrow$  not local but global geometry Level sets: classes, characterised by their global symmetries.



• A symmetry is an operator g which preserves level sets:

$$\forall x , f(g.x) = f(x) : global$$

If  $g_1$  and  $g_2$  are symmetries then  $g_1.g_2$  is also a symmetry  $f(g_1.g_2.x) = f(g_2.x) = f(x)$ 



• Group of dimension n if it has n generators:

$$g = g_1^{p_1} \, g_2^{p_2} \dots g_n^{p_n}$$

• Lie group: infinitely small generators (Lie Algebra)

### **Translation and Deformations**

• Digit classification:

$$u) \qquad x'(u) = x(u - \tau(u))$$



 $\mathcal{X}($ 

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- Globally invariant to the translation group: small
- Locally invariant to small diffeomorphisms: huge group



Video of Philipp Scott Johnson

### **Frequency Transpositions**



H : Heisenberg group of "time-frequency" translations

**Frequency Transpositions** 

#### Time and frequency translations and deformations:



• Frequency transposition invariance is needed

for speech recognition not for locutor recognition.

## Rotation and Scaling Variability

• Rotation and deformations



### Group: $SO(2) \times \text{Diff}(SO(2))$

#### • Scaling and deformations









Group:  $\mathbb{R} \times \text{Diff}(\mathbb{R})$ 

### Linearize Symmetries

• A change of variable  $\Phi(x)$  must linearize the orbits  $\{g.x\}_{g\in G}$ 



• Linearise symmetries with a change of variable  $\Phi(x)$ 



• Lipschitz:  $\forall x, g$  :  $\|\Phi(x) - \Phi(g.x)\| \le C \|g\|$ 

### **Translation and Deformations**

• Digit classification:









- Globally invariant to the translation group
- Locally invariant to small diffeomorphisms

Linearize small diffeomorphisms:  $\Rightarrow$  Lipschitz regular



Video of Philipp Scott Johnson

**Translations and Deformations** 

• Invariance to translations:

$$g.x(u) = x(u-c) \Rightarrow \Phi(g.x) = \Phi(x)$$
.

• Small diffeomorphisms:  $g.x(u) = x(u - \tau(u))$ Metric:  $||g|| = ||\nabla \tau||_{\infty}$  maximum scaling Linearisation by Lipschitz continuity

$$\|\Phi(x) - \Phi(g.x)\| \le C \|\nabla \tau\|_{\infty}.$$

• Discriminative change of variable:  $\|\Phi(x) - \Phi(x')\| \ge C^{-1} |f(x) - f(x')|$  Fourier Deformation Instability

• Fourier transform  $\hat{x}(\omega) = \int x(t) e^{-i\omega t} dt$ 

$$x_c(t) = x(t-c) \implies \hat{x}_c(\omega) = e^{-ic\omega} \hat{x}(\omega)$$

The modulus is invariant to translations:

 $\Phi(x) = |\hat{x}| = |\hat{x}_c|$ 

• Instabilites to small deformations  $x_{\tau}(t) = x(t - \tau(t))$ :  $||\hat{x}_{\tau}(\omega)| - |\hat{x}(\omega)||$  is big at high frequencies  $\tau(t) = \epsilon t \quad |\hat{x}_{\tau}(\omega)| \quad |\hat{x}(\omega)|$  $\longrightarrow \quad ||\hat{x}| - |\hat{x}_{\tau}|| \gg ||\nabla \tau||_{\infty} ||x||$


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## Deep Convolutional Trees



 $L_j$  is composed of convolutions and subs samplings:

$$x_j(u,k_j) = \rho\Big(x_{j-1}(\cdot,k) \star h_{k_j,k}(u)\Big)$$

No channel communication: how far can we go? Why hierachical cascade? **Translations and Deformations** 

• Invariance to translations:

$$g.x(u) = x(u-c) \Rightarrow \Phi(g.x) = \Phi(x)$$
.

• Small diffeomorphisms:  $g.x(u) = x(u - \tau(u))$ Metric:  $||g|| = ||\nabla \tau||_{\infty}$  maximum scaling Linearisation by Lipschitz continuity

$$\|\Phi(x) - \Phi(g.x)\| \le C \|\nabla \tau\|_{\infty}.$$

• Discriminative change of variable:  $\|\Phi(x) - \Phi(x')\| \ge C^{-1} |f(x) - f(x')|$ 



- Wavelet Scattering transform along translations
- Generation of textures and random processes
- Channel connections for more general groups
- Image and audio classification with small training sets
- Quantum chemistry
- Open problems

Understanding Deep Convolutional Networks, arXiv 2016.

### **Multiscale Wavelet Transform**

• Dilated wavelets:  $\psi_{\lambda}(t) = 2^{-j/Q} \psi(2^{-j/Q}t)$  with  $\lambda = 2^{-j/Q}$ 



$$x \star \psi_{\lambda}(t) = \int x(u) \,\psi_{\lambda}(t-u) \,du \; \Rightarrow \; x \star \psi_{\lambda}(\omega) = \widehat{x}(\omega) \,\psi_{\lambda}(\omega)$$

• Wavelet transform: 
$$Wx = \begin{pmatrix} x \star \phi_{2^J}(t) \\ x \star \psi_{\lambda}(t) \end{pmatrix}_{\lambda \leq 2^J}$$
: average frequencies

Preserves norm:  $||Wx||^2 = ||x||^2$ .



Why Wavelets ?

if 
$$\psi_{\lambda,\tau}(t) = \psi_{\lambda}(t - \tau(t))$$
 then

$$\|\psi_{\lambda} - \psi_{\lambda,\tau}\| \le C \sup_{t} |\nabla \tau(t)|$$

• Wavelets separate multiscale information.

• Wavelets provide sparse representations.

### **Singular Functions**





# Wavelet Translation Invariance



Modulus improves invariance:  $|x \star \psi_{\lambda_1}(x) \star \psi_{\lambda_1}(x) \star \psi_{\lambda_1}(x) \star \psi_{\lambda_1}^a(x) + \psi_{\lambda_1}^a(x) \star \psi_{\lambda_1}^a(x) + \psi_{\lambda_1}^a(x) \star \psi_{\lambda_1}^a(x) + \psi_{\lambda_1$ 



Second wavelet transform modulus

$$|W_2| |x \star \psi_{\lambda_1}| = \left( \begin{array}{c} |x \star \psi_{\lambda_1}| \star \phi_{2J}(t) \\ |x \star \psi_{\lambda_1}| \star \psi_{\lambda_2}(t)| \end{array} \right)_{\lambda_2}$$

### **Singular Functions**



### **Amplitude Modulation**

Harmonic sound:  $x(t) = a(t) e \star h(t)$  with varying a(t)







## **Scale separation with Wavelets**

• Wavelet filter  $\psi(u)$ : = +i =

rotated and dilated:  $\psi_{2^{j},\theta}(u) = 2^{-j} \psi(2^{-j}r_{\theta}u)$ 



• Wavelet transform:  $Wx = \begin{pmatrix} x \star \phi_{2^{J}}(u) \\ x \star \psi_{2^{j},\theta}(u) \end{pmatrix}_{j \leq J,\theta}$ : average index in the integral of the transform.

Preserves norm:  $||Wx||^2 = ||x||^2$ .





 $Hx(u) = x \star h(2u)$  and  $Gx(u) = x \star g(2u)$ 

where h is a low frequency and g is a high frequency filter.







#### Fast Wavelet Filter Bank





## Wavelet Convolution Network Tree



 $S_4 x = |L_4| |L_3| |L_2| |L_1| x = |W_4| |W_3| |W_2| |W_1| x$ 

#### Contraction

 $Wx = \begin{pmatrix} x \star \phi(t) \\ x \star \psi_{\lambda}(t) \end{pmatrix}_{t,\lambda} \text{ is linear and } ||Wx|| = ||x||$  $\rho(u) = |u|$  $|W|x = \begin{pmatrix} x \star \phi(t) \\ |x \star \psi_{\lambda}(t)| \end{pmatrix}_{t,\lambda} \text{ is non-linear}$ 

- it is contractive  $|||W|x |W|y|| \le ||x y||$ because for  $(a, b) \in \mathbb{C}^2$   $||a| - |b|| \le |a - b|$
- it preserves the norm |||W|x|| = ||x||



 $\texttt{Wnanka:} \| \texttt{W}[W_k, \mathcal{D}_{\tau}] \| W_k \texttt{W}_k \mathcal{W}_k \mathcal{D}_k \texttt{W}_k \texttt{$ 

**Theorem:** For appropriate wavelets, a scattering is contractive  $||S_J x - S_J y|| \le ||x - y||$  (L<sup>2</sup> stability) preserves norms  $||S_J x|| = ||x||$ 

translations invariance and deformation stability: if  $D_{\tau}x(u) = x(u - \tau(u))$  then  $\lim_{J \to \infty} \|S_J D_{\tau}x - S_J x\| \le C \|\nabla \tau\|_{\infty} \|x\|$ 

#### **Digit Classification: MNIST**

3681796691

6757863485

2179712845

4819018894

Joan Bruna





 $\rightarrow y = f(x)$ 

Invariants to translations Linearises small deformations No learning Invariants to specific deformations Separates different patterns

#### Classification Errors

Training size	Conv. Net.	Scattering	
50000	0.4%	0.4%	
LeCun et. al.			

### **Classification of Stationary Textures** -

 $\Omega_1$ 





2D Turbulence

- What stochastic models ? Non Gaussian with long-range dependance.
  - Can we "Gaussianize" (linearize) such distributions in a reduced dimensional space ?



#### **Classification of Textures**

J. Bruna

#### CUREt database





Classification Errors

Training	Fourier	Scattering
per class	Spectr.	
46	1%	0.2 %

Scattering Moments of Processes

The scattering transform of a stationary process X(t)

$$S_{J}X = \begin{pmatrix} X \star \phi_{2^{J}}(t) \\ |X \star \psi_{\lambda_{1}}| \star \phi_{2^{J}}(t) \\ ||X \star \psi_{\lambda_{2}}| \star \psi_{\lambda_{2}}| \star \phi_{2^{J}}(t) \\ |||X \star \psi_{\lambda_{2}}| \star \psi_{\lambda_{2}}| \star \psi_{\lambda_{3}}| \star \phi_{2^{J}}(t) \\ \dots \end{pmatrix}^{1} : \text{ stationary vector}$$
$$J \to \infty \begin{vmatrix} \text{Central limit theorem} \\ \text{with "weak" ergodicity conditions} \\ \text{Gaussian distribution: } \mathcal{N}\Big(\mathbb{E}(SX), \Sigma_{J} \to 0\Big) \\ \mathbb{E}(SX) = \begin{pmatrix} \mathbb{E}(X) \\ \mathbb{E}(|X \star \psi_{\lambda_{1}}|) \\ \mathbb{E}(||X \star \psi_{\lambda_{1}}| \star \psi_{\lambda_{2}}|) \\ \mathbb{E}(||X \star \psi_{\lambda_{2}}| \star \psi_{\lambda_{2}}| \star \psi_{\lambda_{3}}|) \\ \dots \end{pmatrix}^{1}_{\lambda_{1},\lambda_{2},\lambda_{3},\dots}$$

Scattering Moments of Processes

The scattering transform of a stationary process X(t)

$$S_{J}X = \begin{pmatrix} X \star \phi_{2^{J}}(t) \\ |X \star \psi_{\lambda_{1}}| \star \phi_{2^{J}}(t) \\ ||X \star \psi_{\lambda_{1}}| \star \psi_{\lambda_{2}}| \star \phi_{2^{J}}(t) \\ ||X \star \psi_{\lambda_{2}}| \star \psi_{\lambda_{2}}| \star \psi_{\lambda_{3}}| \star \phi_{2^{J}}(t) \\ \dots \end{pmatrix} : \text{ statistic}$$

: stationary vector

 $J \to \infty$  Central limit theorem with "weak" ergodicity conditions

Gaussian distribution: 
$$\mathcal{N}\Big(\mathbb{E}(SX), \Sigma_J \to 0\Big)$$

• Reconstruction: compute  $\tilde{X}$  which minimises  $\|S_J \tilde{X} - S_J X\|^2$ 

• Gradient descent

### **Representation of Audio Textures**



Cocktail Party

## Ergodic Texture Reconstructions

#### Joan Bruna

#### Textures of N pixels

2D Turbulence











Gaussian process model with N second order moments











Second order Gaussian Scattering:  $O(\log N^2)$  moments  $\mathbb{E}(|x \star \psi_{\lambda_1}|)$ ,  $\mathbb{E}(||x \star \psi_{\lambda_1}| \star \psi_{\lambda_2}|)$ 











### Ising Model and Inverse Problem

	Bruna, Dokmanic, Maarten de Hoo					
		$p(x) = Z_{\beta}^{-1} \exp \left[ -\frac{1}{2} \exp \left[ -\frac{1}$	$\left(-\beta \sum J_{i,j} x(t)\right)$	i(x(j)) with	$x(i) = \pm 1$	
	Ising	Gaussian <u>scattering</u>	$\underline{i,j}$ low-resolution	<u>TV optim.</u>	Scat pred.	
$eta_c$						
β						

## Deep Convolutional Trees



 $L_j$  is composed of convolutions and subs samplings:

$$x_j(u,k_j) = \rho\Big(x_{j-1}(\cdot,k) \star h_{k_j,k}(u)\Big)$$

No channel communication: what limitations ?

## Rotation and Scaling Invariance

20

#### UIUC database: 25 classes

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20 %

Laurent Sifre

## Deep Convolutional Networks



•  $L_j$  is a linear combination of convolutions and subsampling:

$$x_{j}(u, k_{j}) = \rho \left( \sum_{\substack{k \\ \text{sum across channels}}} x_{j-1}(\cdot, k) \star h_{k_{j}, k}(u) \right)$$

What is the role of channel connections ? Linearize other symmetries beyond translations.

## **Rotation Invariance**

• Channel connections linearize other symmetries.

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 Invariance to rotations are computed by convolutions along the rotation variable θ with wavelet filters.
 ⇒ invariance to rigid mouvements.

### **Extension to Rigid Mouvements**

Laurent Sifre

Need to capture the variability of spatial directions.

- Group of rigid displacements: translations and rotations
- Action on wavelet coefficients:

rotation & translation rotation & translation , angle translation 
$$x(r_{\alpha}(u \, x(u)) \longrightarrow |W_1| \longrightarrow x_j(u_{\alpha}(\theta) = c_{\beta}, \theta \, \psi_2 \rho_{\theta})(u)|$$

### **Extension to Rigid Mouvements**

Laurent Sifre

• To build invariants: second wavelet transform on  $L^{2}(G)$ : convolutions of  $x_j(u,\theta)$  with wavelets  $\psi_{\lambda_2}(u,\theta)$ 

$$x \circledast \psi_{\lambda}(u,\theta) = \int_{0}^{2\pi} \left( \int_{\mathbb{R}^{2}} x(u',\theta') \psi_{\theta,2^{j}}(r_{-\theta'}(u-u')) \right) \psi_{2^{k}}(\theta-\theta') d\theta' dt'$$

Wavelets

• Scattering on rigid mod  
Wavelets on Translations 
$$\langle W \rangle$$
  
 $x(u) \rightarrow |W_1| \rightarrow x_j(u, \theta)$   
 $\int x(u) du$   
 $\int x_j(u, \theta) du d\theta^{u_1} \int |x_j \otimes \psi_{\lambda_2}(v, \theta)| du d\theta$ 

#### **Rotation and Scaling Invariance** ENS

#### UIUC database: 25 classes



Laurent Sifre

Scattering classification errors


# Learning Physics: N-Body Problem

• Energy of d interacting bodies:

N. Poilvert Matthew Hirn

### Can we learn the interaction energy f(x) of a system with $x = \{ \text{positions, values} \}$ ?

#### Astronomy



#### Quantum Chemistry



Density Functional Theory

Kohn-Sham model:

At equilibrium:

$$f(x) = E(\rho_x) = \min_{\rho} E(\rho)$$

Quantum Chemistry Invariants

#### Quantum chemistry: f(x) is invariant to rigid mouvements, stable to deformations.

### Depends on the true electronic density (Kohn-Sham)

Ground state electronic density computed with Schroedinger





• Can we estimate f(x) from a naive electronic density ?

Density  $\tilde{\rho}_x$  computed as a sum of blobs





• Linear regressions computed with invariant change of variables:

 $\Phi x = \{\phi_n(\tilde{\rho}_x)\}_n : \left| \begin{array}{c} \text{Fourier modulus coefficients and squared} \\ \text{scattering coefficients and squared} \end{array} \right.$ 

$$f_M(x) = \sum_{k=1}^M w_k \, \phi_{n_k}(\tilde{\rho}_x)$$

Regression coefficients  $w_k$ : equivalent potential.

### **Scattering Dictionary**



 $\rho(u)$ 

2nd Order Interferences

Recover translation variability:  $|\rho * \psi_{j_1,\theta_1}| * \psi_{j_2,\theta_2}(u)$ 

• Recover rotation variability:  $|\rho * \psi_{j_1,\cdot}(u)| \circledast \overline{\psi}_{l_2}(\theta_1)$ 

Combine to recover roto-translation variabiltiy:

 $\left\|\rho * \psi_{j_1,\cdot}\right\| * \psi_{j_2,\theta_2}(u) \circledast \overline{\psi}_{l_2}(\theta_1)\right\|$ 

Scattering Regression

Data basis  $\{x_i, f(x_i)\}_{i \leq N}$  of 4357 planar molecules M

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### Time-Frequency Translation Group

J. Anden and V. Lostanlen



### Joint Time-Frequency Scattering

#### J. Anden and V. Lostanl

#### Original

Time Scattering

### Time/Freq Scattering













### **Musical Instrument Classificaiton**

clarinet



female singer



piano



trumpet







tenor saxophone

violin

J. Anden and V. Lostanlen

MedleyDB: 8 classes 10k training examples

class-wise average error 0,39 MFCC audio descriptors 0,31 time scattering ConvNet 0,31 0,18 time-frequency scattering

## Environmental Sound Classification -

#### air conditioner



children playing



drilling



gunshot



siren





### J. Anden and V. Lostanlen

#### UrbanSound8k: 10 classes 8k training examples

class-wise average error

MFCC audio descriptors	0,39
time scattering	0,27
ConvNet (Piczak, MLSP 2015)	0,26
time-frequency scattering	0,2

### **Complex Image Classification**

Arbre de Joshua

ΕN







Ancre







Metronome







Castore







Nénuphare

Edouard Oyallon















Data Basis	Deep-Net	Scat/Unsupervised
CIFAR-10	7%	20%

### Linearisation in Deep Networks

A. Radford, L. Metz, S. Chintala



• On a data basis including bedrooms: interpolaitons





- The convolution network operators  $L_j$  have many roles:
  - Linearize non-linear transformations (symmetries)
  - Reduce dimension with projections
  - Memory storage of « characteristic » structures
- Difficult to separate these roles when analyzing learned networks



- Can we recover symmetry groups from the matrices *Lj*?
- What kind of groups ?
- Can we characterise the regularity of f(x) from these groups ?
- Can we define classes of high-dimensional « regular » functions that are well approximated by deep neural networks ?
- Can we get approximation theorems giving errors depending on number of training exemples, with a fast decay ?



### Conclusions

- Deep convolutional networks have spectacular high-dimensional approximation capabilities.
- Seem to compute hierarchical invariants of complex symmetries
- Used as models in physiological vision and audition
- Close link with particle and statistical physics
- Outstanding mathematical problem to understand them: notions of complexity, regularity, approximation theorems...

Understanding Deep Convolutional Networks, arXiv 2016.