## Learning Music, Images and Physics with Deep Neural Networks

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## High Dimensional Learning

- High-dimensional $x=(x(1), \ldots, x(d)) \in \mathbb{R}^{d}$ :
- Classification: estimate a class label $f(x)$
given $n$ sample values $\left\{x_{i}, y_{i}=f\left(x_{i}\right)\right\}_{i \leq n}$
Image Classification $d=10^{6}$


Huge variability inside classes

## High Dimensional Learning

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Audio: instrument recognition
Huge variability inside classes



## High Dimensional Learning

- High-dimensional $x=(x(1), \ldots, x(d)) \in \mathbb{R}^{d}$ :
- Regression: approximate a functional $f(x)$ given $n$ sample values $\left\{x_{i}, y_{i}=f\left(x_{i}\right) \in \mathbb{R}\right\}_{i \leq n}$

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

Astronomy


Quantum Chemistry


## Curse of Dimensionality

- $f(x)$ can be approximated from examples $\left\{x_{i}, f\left(x_{i}\right)\right\}_{i}$ by local interpolation if $f$ is regular and there are close examples:

- Need $\epsilon^{-d}$ points to cover $[0,1]^{d}$ at a Euclidean distance $\epsilon$ $\Rightarrow\left\|x-x_{i}\right\|$ is always large


Huge variability inside classes

## Learning by Euclidean Embedding

## Data: $x \in \mathbb{R}^{d}$

$\left\|x-x^{\prime}\right\|:$ non-informative


Representation
$\Phi x \in \mathcal{H}$
Linear Classifier


$$
\left\|\Phi x-\Phi x^{\prime}\right\|
$$

Equivalent Euclidean metric:

$$
C_{1}\left\|\Phi x-\Phi x^{\prime}\right\| \leq \Delta\left(x, x^{\prime}\right) \leq C_{2}\left\|\Phi x-\Phi x^{\prime}\right\|
$$

How to define $\Phi$ ?

## Deep Convolution Neworks

- The revival of an old (1950) idea: Y. LeCun, G. Hinton


Optimize the $L_{k}$ with support constraints: over $10^{9}$ parameters Exceptional results for images, speech, bio-data classification. Products by FaceBook, IBM, Google, Microsoft, Yahoo... Why does it work so well ?

## Overview

- Deep multiscale networks: invariant and stable metrics on groups
- Image classification
- Models of audio and image textures: information theory
- Learning physics: quantum chemistry energy regression


## Image Metrics

- Low-dimensional "geometric shapes"


Deformation metric: (classic mechanics) Grenander
Diffeomorphism action: $D_{\tau} x(u)=x(u-\tau(u))$

$$
\Delta\left(x, x^{\prime}\right) \sim \min _{\tau}\left\|D_{\tau} x-x^{\prime}\right\|+\|\nabla \tau\|_{\infty}\|x\|
$$

Invariant to translations
diffeomorphism amplitude

## Image Metrics

- High dimensional textures: $X(u)$ ergodic stationary processes


2D Turbulence

## Highly non-Gaussian processes

- A Euclidean metric is a Maximum Likelihood on Gaussian models.
- Can we find $\Phi$ so that $\Phi(X)$ is nearly Gaussian, without loosing information?


## Euclidean Metric Embedding

- Stability to additive perturbations:

$$
\left\|\Phi x-\Phi x^{\prime}\right\| \leq C\left\|x-x^{\prime}\right\|
$$

- Invariance to translations:

$$
x_{c}(u)=x(u-c) \Rightarrow \Phi\left(x_{c}\right)=\Phi(x)
$$

- Stability to deformations:

$$
x_{\tau}(u)=x(u-\tau(u)) \Rightarrow\left\|\Phi x-\Phi x_{\tau}\right\| \leq C\|\nabla \tau\|_{\infty}\|x\|
$$

Failure of Fourier and classic invariants

## Wavelet Transform

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



Q-constant band-pass filters $\hat{\psi}_{\lambda}$

- Wavelet transform: $\quad W x=\binom{x \star \phi_{2^{J}}(t)}{x \star \psi_{\lambda}(t)}_{\lambda \leq 2^{J}} \begin{aligned} & \text { : average } \\ & : \begin{array}{l}\text { higher } \\ \text { frequencies }\end{array}\end{aligned}$

Preserves norm: $\|W x\|^{2}=\|x\|^{2}$.

## $\mathrm{DNS}_{\mathrm{ENS}}$ Scale separation with Wavelets

- Complex wavelet: $\psi(t)=g(t) \exp i \xi t$, $t=\left(t_{1}, t_{2}\right)$
rotated and dilated: $\psi_{\lambda}(t)=2^{-j} \psi\left(2^{-j} r_{\theta} t\right)$ with $\lambda=\left(2^{j}, \theta\right)$
real parts

imaginary parts
- Wavelet transform: $W x=\binom{x \star \phi_{2^{J}}(t)}{x \star \psi_{\lambda}(t)}_{\lambda \leq 2^{J}} \begin{aligned} & \text { : average } \\ & \text { higher } \\ & \text { frequencies }\end{aligned}$ Preserves norm: $\|W x\|^{2}=\|x\|^{2}$.



## Wavelet Transform

## ENS



How to make everything invariant to translation?

## Wavelet Translation Invariance

ENS Wavele
First wavelet transform

 but covariant

$$
\left|x \star \psi_{\lambda_{1}}\right| \star \phi_{2^{J}}(t)
$$

## Scattering Transform




## Scattering Neural Network

 <br> \title{
Scattering Properties <br> \title{

Scattering Properties <br> $$
S_{J} x=\left(\begin{array}{c}
x \star \phi_{2^{J}} \\
\left|x \star \psi_{\lambda_{1}}\right| \star \phi_{2^{J}} \\
\left|\left|x \star \psi_{\lambda_{1}}\right| \star \psi_{\lambda_{2}}\right| \star \phi_{2^{J}} \\
\left|\left|x \star \psi_{\lambda_{2}}\right| \star \psi_{\lambda_{2}}\right| \star \psi_{\lambda_{3}} \mid \star \phi_{2^{J}} \\
\cdots
\end{array}\right)_{\lambda_{1}, \lambda_{2}, \lambda_{3}, \ldots}=\ldots\left|W_{3}\right|\left|W_{2}\right|\left|W_{1}\right| x
$$

}
$W_{k}$ is unitary $\Rightarrow\left|W_{k}\right|$ is contractive
Theorem: For appropriate wavelets, a scattering is
contractive $\left\|S_{J} x-S_{J} y\right\| \leq\|x-y\| \quad\left(\mathbf{L}^{2}\right.$ stability $)$
preserves norms $\left\|S_{J} x\right\|=\|x\|$
translations invariance and deformation stability:

$$
\text { if } x_{\tau}(u)=x(u-\tau(u)) \text { then } \quad \begin{aligned}
& \lim _{J \rightarrow \infty}\left\|S_{J} x_{\tau}-S_{J} x\right\| \leq C\|\nabla \tau\|_{\infty}\|x\|
\end{aligned}
$$

## Digit Classification: MNIST

$368 / 796691$ Joan Bruna
6757863485
2179712845
4819018894


Classification Errors

| Training size | Conv. Net. | Scattering |
| :---: | :---: | :---: |
| 50000 | $0.5 \%$ | $\mathbf{0 . 4} \%$ |

LeCun et. al.

## Classification of Textures

J. Bruna

CUREt database
61 classes


Scat. Moments


Linear Classifier $\longrightarrow y=f(x)$

Classification Errors $\quad 2^{J}=$ image size

| Training <br> per class | Fourier <br> Spectr. | Histogr. <br> Features | Scattering |
| :---: | :---: | :---: | :---: |
| 46 | $1 \%$ | $1 \%$ | $\mathbf{0 . 2} \%$ |

## Representation of Random Processes

$$
\mathbb{E}(S X)=\left(\begin{array}{rcc}
\mathbb{E}(X) & =\mathbb{E}\left(U_{0} X\right) \\
\mathbb{E}\left(\left|X \star \psi_{\lambda_{1}}\right|\right) & =\mathbb{E}\left(U_{1} X\right) \\
\mathbb{E}\left(| | X \star \psi_{\lambda_{1}}\left|\star \psi_{\lambda_{2}}\right|\right) & =\mathbb{E}\left(U_{2} X\right) \\
\mathbb{E}\left(| |\left|X \star \psi_{\lambda_{2}}\right| \star \psi_{\lambda_{2}}\left|\star \psi_{\lambda_{3}}\right|\right) & =\mathbb{E}\left(U_{3} X\right) \\
\cdots &
\end{array}\right)_{\lambda_{1}, \lambda_{2}, \lambda_{3}, \ldots}
$$

Theorem (Boltzmann) The distribution $p(x)$ which satisfies

$$
\int_{\mathbb{R}^{N}} U_{m} x p(x) d x=E\left(U_{m} X\right)
$$

with a maximum entropy $H_{\max }=-\int p(x) \log p(x) d x$ is

$$
\begin{aligned}
p(x)=\frac{1}{Z} \exp & \left(\sum_{m=1}^{\infty} \lambda_{m} \cdot U_{m} x\right) \\
& H_{\max } \geq H(X)(\text { entropie of } \mathrm{X})
\end{aligned}
$$

Little loss of information: $H_{\max } \approx H(X)$


Cocktail Party

Need to express frequency channel interactions: time-frequency image
Bird

Speech


Cello


## Harmonic Spiral

Need to capture frequency variability and structures.
 octave


- Alignment of harmonics in two main groups.

More regular variations along $(\theta, j)$ than $\lambda$


3D separable Spiral wavelet transform $W_{2}$


## Shepard-Risset Glissando <br> ENS

$$
\hat{\uparrow}^{j} \quad x(t)=a(t) e \star h(t)
$$




Scattering classification errors

| Training | Scat. Translation |
| :---: | :---: |
| 20 | $20 \%$ |

## Extension to Rigid Mouvements

Need to capture the variability of spatial directions.

- Group of rigid displacements: translations and rotations
- Action on wavelet coefficients:
rotation \& translation

$$
\begin{aligned}
& x\left(r _ { \alpha } ( u x ( u ) ) \longrightarrow \underset { \downarrow } { | W _ { 1 } | } \longrightarrow x _ { j } \left(x_{\alpha \theta}(\theta)=\phi \dot{x}, \theta \not \psi_{2} \alpha_{,},(u) \mid\right.\right. \\
& \int x(u) d u
\end{aligned}
$$

## Extension to Rigid Mouvements

Laurent Sifre

- To build invariants: second wavelet transform on $\mathbf{L}^{2}(G)$ : convolutions of $x_{j}(u, \theta)$ with wavelets $\psi_{\lambda_{2}}(u, \theta)$

$$
x_{j} \circledast \psi_{\lambda_{2}}(u, \theta)=\int_{\mathbb{R}^{2}} \int_{0}^{2 \pi} x_{j}(v, \alpha) \psi_{\lambda_{2}}(u-v, \theta-\alpha) d v d \alpha
$$

- Scattering on rigid mouvements:

Wavelets on Translations Wavelets on Rigid Mvt. Wavelets on Rigid Mvt.

$\int x(u) d u$
$\int x_{j}(u, \theta) d u d \theta$
$\int\left|x_{j} \circledast \psi_{\lambda_{2}}(v, \theta)\right| d u d \theta$


Scattering classification errors

| Training | Scat. Translation | Scat. Rigid Mouvt. |
| :---: | :---: | :---: |
| 20 | $20 \%$ | $\mathbf{0 . 6} \%$ |

# Complex Image Classification 

CalTech 101 data-basis:

Arbre de Joshua


Ancre


Castore


Edouard Oyallon


Bateau


Classification Accuracy

| Data Basis | Deep-Net | Scat.-2 |
| :---: | :---: | :---: |
| CalTech-101 | $\mathbf{8 5 \%}$ | $80 \%$ |
| CIFAR-10 | $\mathbf{9 0 \%}$ | $80 \%$ |

State of the art Unsupervised

# As Learning Physics: N-Body Problem- <br> - Energy of $d$ interacting bodies: 

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

Astronomy


Quantum Chemistry


## 同

- A system of $d$ particles involves $d^{2}$ interactions
- Multiscale separation into $O\left(\log ^{2} d\right)$ interactions



## Quantum Chemistry

Electronic density $\rho_{x}(u)$ : computed by solving Schrodinger

Organic molecules with
Hydrogne, Carbon Nitrogen, Oxygen Sulfur, Chlorine


## $\frac{\sqrt{1 / i}}{\mathrm{ENS}}$ <br> Density Functional Theory

Kohn-Sham model:

$$
E(\rho)=T(\rho)+\int \rho(u) V(u)+\frac{1}{2} \int \frac{\rho(u) \rho(v)}{|u-v|} d u d v+E_{x c}(\rho)
$$

Molecular Kinetic electron-nuclei electron-electron Exchange energy energy attraction Coulomb repulsion correlat. energy

At equilibrium:

$$
f(x)=E\left(\rho_{x}\right)=\min _{\rho} E(\rho)
$$

- $f(x)$ is invariant to isometries and is deformation stable


## Atomization Density

- We do not know the electronic density $\rho_{x}$ at equilibrium.
approximated by the sum of the densities of all atoms:

$$
\tilde{\rho}_{x}(u)=\sum_{k=1}^{d} \rho_{z_{k}}\left(u-r_{k}\right)
$$

Electronic density $\rho_{x}(u)$
Approximate density $\tilde{\rho}_{x}(u)$


- Sparse regression computed over a representation invariant to action of isometries in $\mathbb{R}^{3}$ :
$\Phi x=\left\{\phi_{n}\left(\tilde{\rho}_{x}\right)\right\}_{n}:$
Fourier modulus coefficients and squared scattering coefficients and squared

Partial Least Square regression on the training set:

$$
f_{M}(x)=\sum_{k=1}^{M} w_{k} \phi_{n_{k}}\left(\tilde{\rho}_{x}\right)
$$

M: number of variables

## Scattering Regression

Data basis $\left\{x_{i}, f\left(x_{i}\right)=E\left(\rho_{x_{i}}\right)\right\}_{i \leq N}$ of 4357 planar molecules

$$
\text { Regression: } \quad f_{M}(x)=\sum_{m=1}^{M} w_{m} \phi_{k_{m}}\left(\tilde{\rho}_{x}\right)
$$

Testing error
$2^{-1} \log _{2} \mathbb{E}\left|f_{M}(x)-y(x)\right|^{2}$


## Conclusion

- A major challenge of data analysis is to find

Euclidean embeddings of metrics $\Leftrightarrow$ build Gaussian models

- Continuity to action of diffeomorphisms $\Rightarrow$ wavelets
- Known geometry $\Rightarrow$ no need to learn.

Unknown geometry: learn wavelets on appropriate groups.

- Can learn physics from prior on geometry and invariants.
- Applications to images, audio and natural languages
www.di.ens.fr/data/scattering

