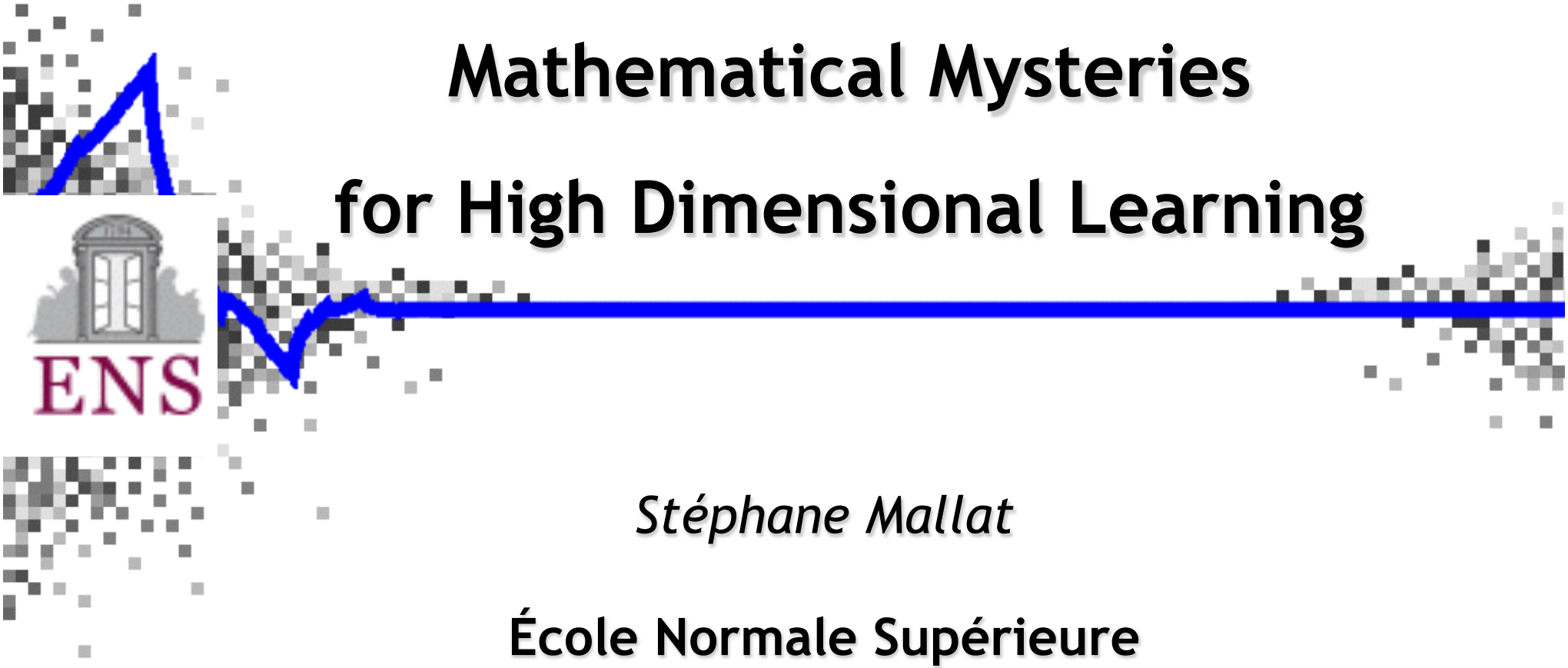
Deep Neural Network Mathematical Mysteries for High Dimensional Learning



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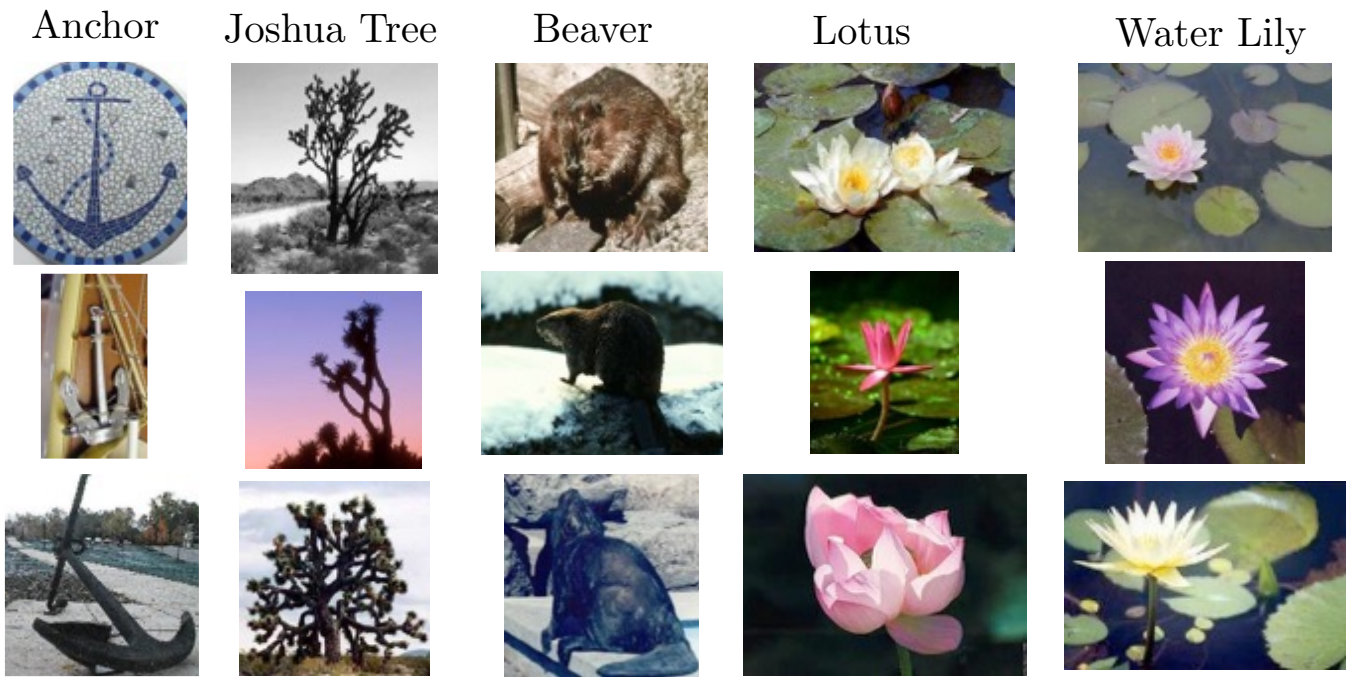
www.di.ens.fr/data

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 $\{x_i\,,\, y_i = f(x_i)\}_{i \leq n}$

Image Classification $d = 10^6$



Huge variability inside classes

Find invariants

High Dimensional Learning

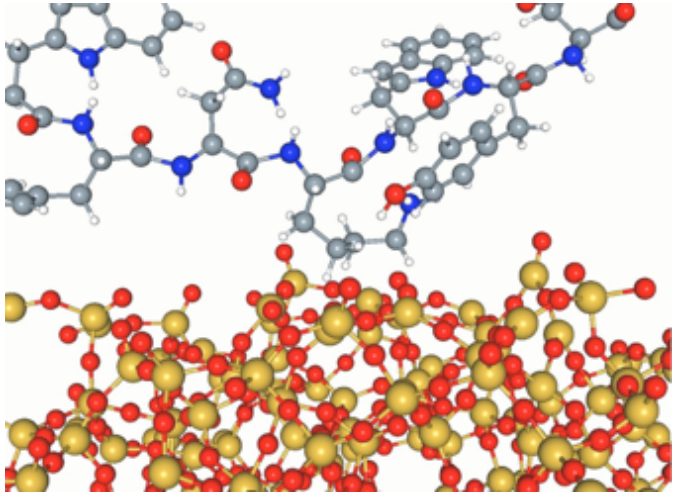
- High-dimensional $x = (x(1), ..., x(d)) \in \mathbb{R}^d$:

- **Regression:** approximate a *functional* $f(x)$
  given n sample values $\{x_i\,,\, y_i = f(x_i) \in \mathbb{R}\}_{i \leq n}$

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

Astronomy

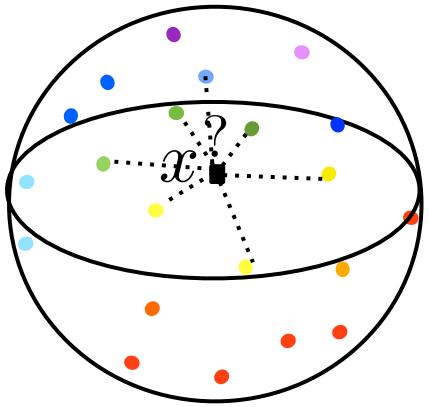
Quantum Chemistry

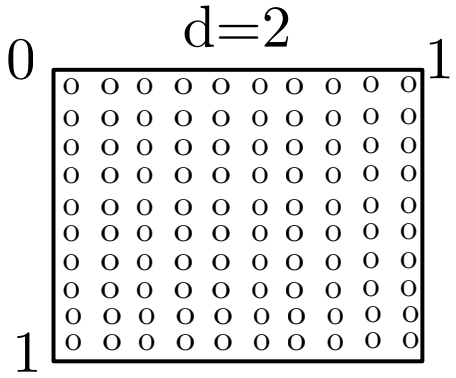


Importance of symmetries.

Curse of Dimensionality

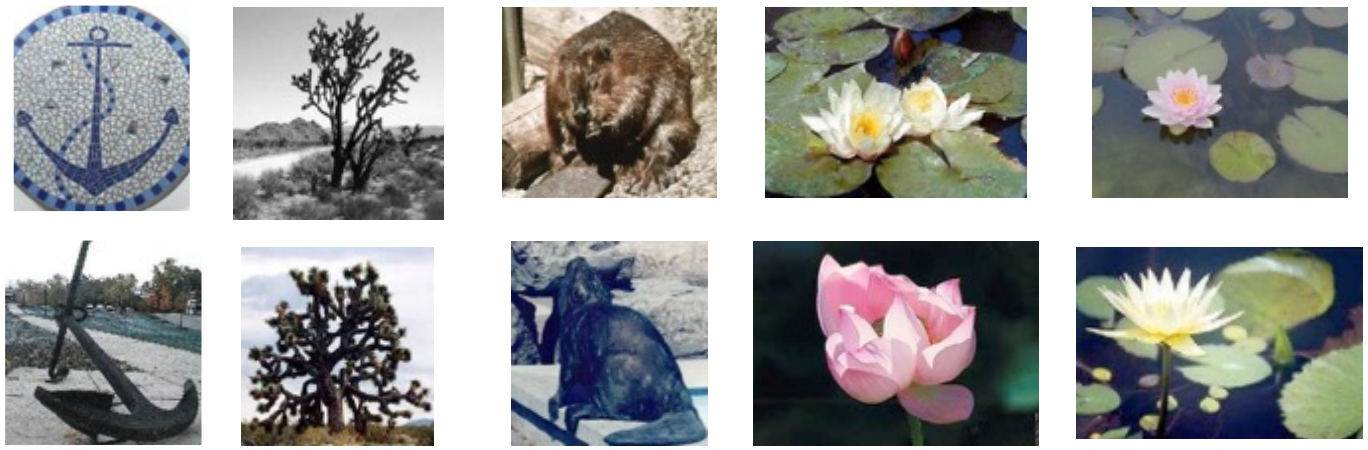
- $f(x)$ can be approximated from examples $\{x_i\ ,\ f(x_i)\}_i$ by local interpolation if f is regular and there are close examples:





- Need ϵ^{-d} points to cover $[0,1]^d$ at a Euclidean distance ϵ

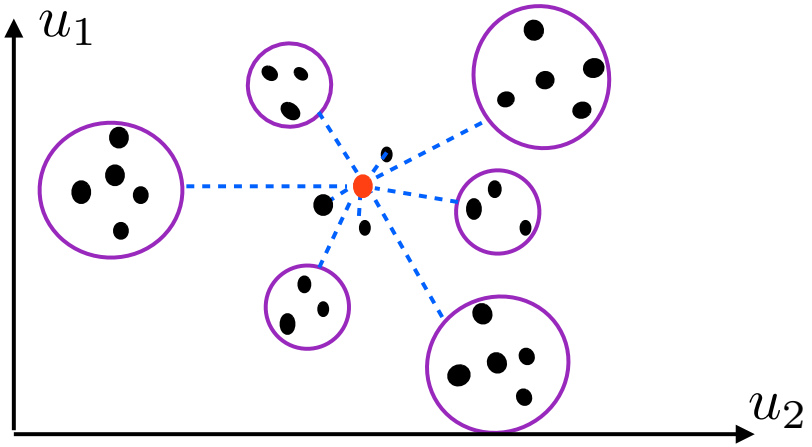
Problem: $\|x - x_i\|$ is always large



Multiscale Separation

- 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.

Overview

- 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 $f(x) = \begin{cases} 1 & \text{if } x \in \Omega \\ -1 & \text{if } x \notin \Omega \end{cases}$

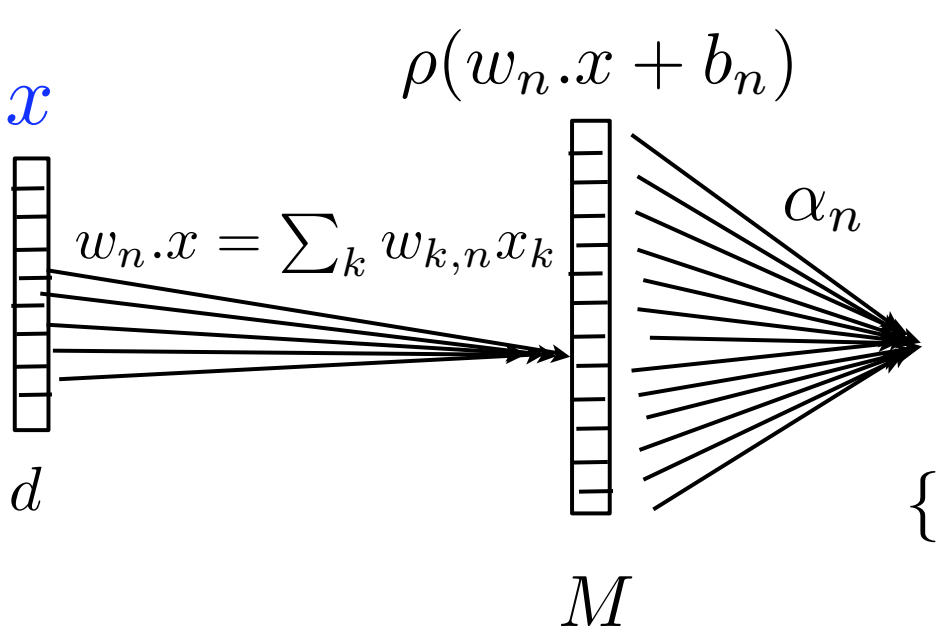
$$f(x) = \text{sign}(\tilde{f}(x))$$

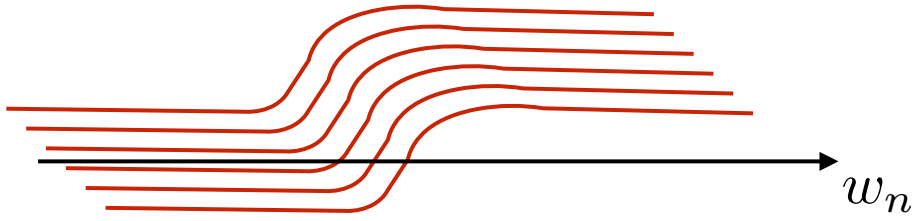
  where $\tilde{f}$ is potentially regular.

- What type of regularity ? How to compute f_M ?

1 Hidden Layer Neural Networks

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





$$f_M(x) = \sum_{n=1}^{M} \alpha_n \, \rho(w_n.x + b_n)$$

$\{w_{k,k}\}_{k,n}$ and $\{\alpha_n\}_n$ are learned non-linear approximation.

Cybenko, Hornik, Stinchcombe, White

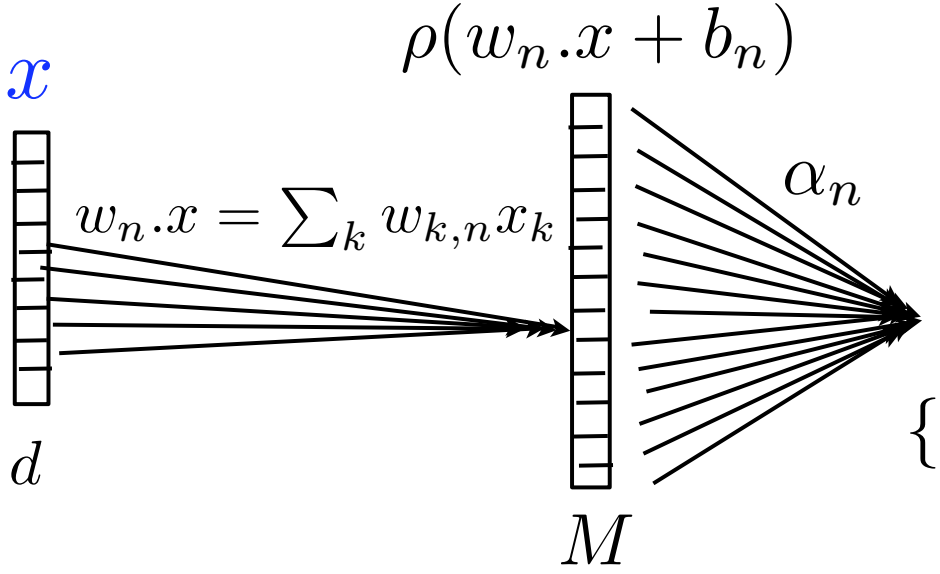
Theorem: For "resonnable" bounded $\rho(u)$ and appropriate choices of $w_{n,k}$ and α_n:

$$\forall f \in \mathbb{L}^2[0,1]^d \qquad \lim_{M \to \infty} \|f - f_M\| = 0 \; .$$

No big deal: curse of dimensionality still there.

1 Hidden Layer Neural Networks

One-hidden layer neural network:



$$f_M(x) = \sum_{n=1}^{M} \alpha_n \, \rho(w_n.x + b_n)$$

$\{w_{k,k}\}_{k,n}$ and $\{\alpha_n\}_n$ are learned non-linear approximation.

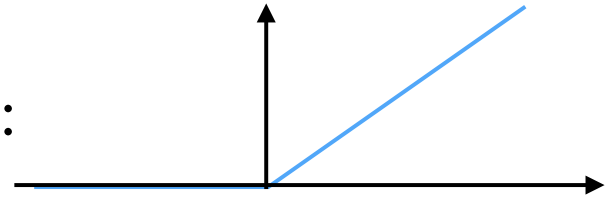
Fourier series: $\rho(u) = e^{iu}$

$$f_M(x) = \sum_{n=1}^{M} \alpha_n \, e^{i w_n.x}$$

For nearly all ρ: essentially same approximation results.

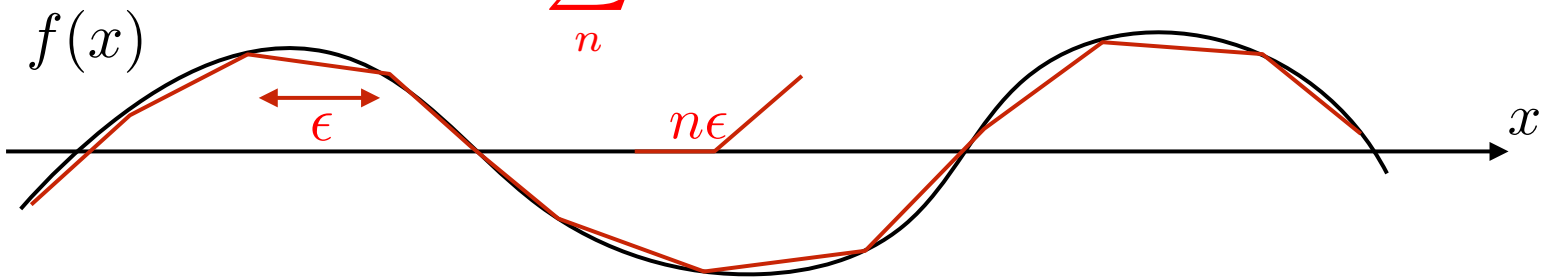
Piecewise Linear Approximation

- Piecewise linear approximation:



$$\rho(u) = \max(u, 0)$$

$$\tilde{f}(x) = \sum_n a_n \, \rho(x - n\epsilon)$$



If f is Lipschitz: $|f(x) - f(x')| \leq C\,|x - x'|$

$$\Rightarrow \quad |f(x) - \tilde{f}(x)| \leq C\,\epsilon.$$

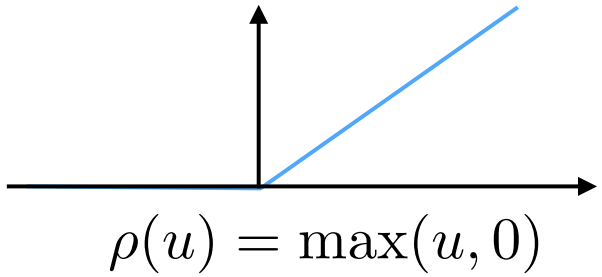
Need $M = \epsilon^{-1}$ points to cover $[0, 1]$ at a distance ϵ

$$\Rightarrow \; \|f - f_M\| \leq C\,M^{-1}$$

Linear Ridge Approximation

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

$$\tilde{f}(x) = \sum_n a_n \, \rho(w_n.x - n\epsilon)$$



If f is Lipschitz: $|f(x) - f(x')| \leq C \, \|x - x'\|$

Sampling at a distance ϵ:

$$\Rightarrow \quad |f(x) - \tilde{f}(x)| \leq C \, \epsilon.$$

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

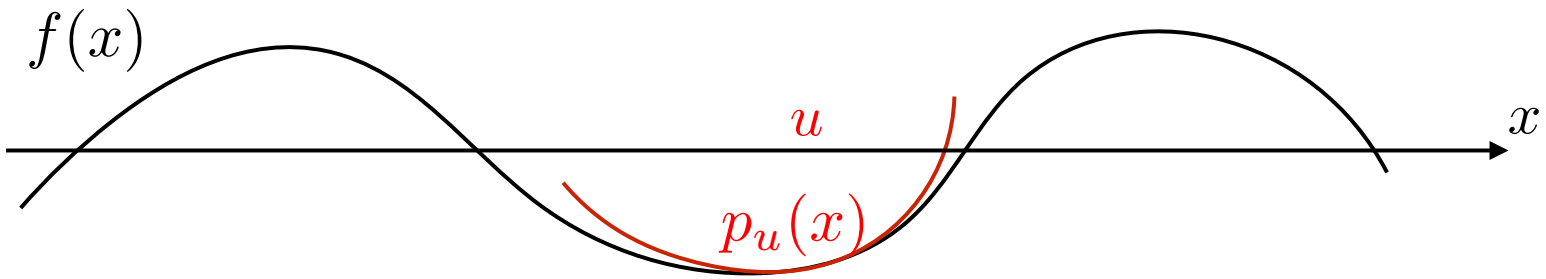
$$\Rightarrow \; \|f - f_M\| \leq C \, M^{-1/d}$$

Curse of dimensionality!

Approximation with Regularity

- What prior condition makes learning possible ?
- Approximation of regular functions in $\mathbf{C}^s[0,1]^d$:

$$\forall x, u \quad |f(x) - p_u(x)| \leq C\,|x-u|^s \quad \text{with} \quad p_u(x) \quad \text{polynomial}$$



$$|x-u| \leq \epsilon^{1/s} \quad \Rightarrow \quad |f(x) - p_u(x)| \leq C\,\epsilon$$

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

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

- Can not do better in $\mathbf{C^s}[0,1]^d$, not good because $s \ll d$.

Failure of classical approximation theory.

Kernel Learning

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

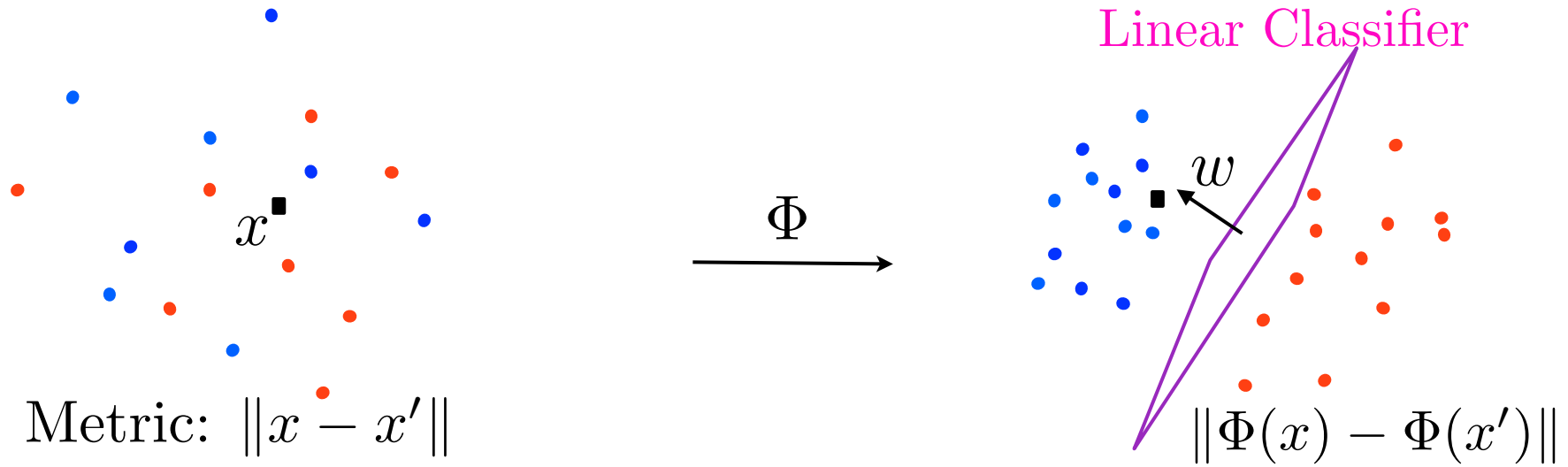
to nearly linearize $f(x)$, which is approximated by:

$$\tilde{f}(x) = \langle \Phi(x)\,,\, w \rangle = \sum_k w_k\, \phi_k(x)\ .$$

1D projection

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

$\Phi(x) \in \mathbb{R}^{d'}$



- How and when is possible to find such a Φ ?
- 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 $d' > N+1$ if $\{\Phi x_i\}_i$ are not in an affine subspace of dimension $< N$.

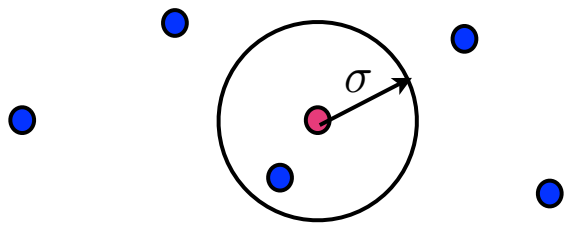
$\Rightarrow$ Choose Φ increasing dimensionality !

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 σ is small, nearest neighbor classifier type:



Reduction of Dimensionality

- Discriminative change of variable $\Phi(x)$:

$$\Phi(x) \neq \Phi(x') \quad \text{if} \quad f(x) \neq f(x')$$

$$\Rightarrow \quad \exists \tilde{f} \quad \text{with} \quad f(x) = \tilde{f}(\Phi(x))$$

- If $\tilde{f}$ is Lipschitz: $|\tilde{f}(z) - \tilde{f}(z')| \leq C \, \|z - z'\|$

$$z = \Phi(x) \quad \Leftrightarrow \quad |f(x) - f(x')| \leq C \, \|\Phi(x) - \Phi(x')\|$$

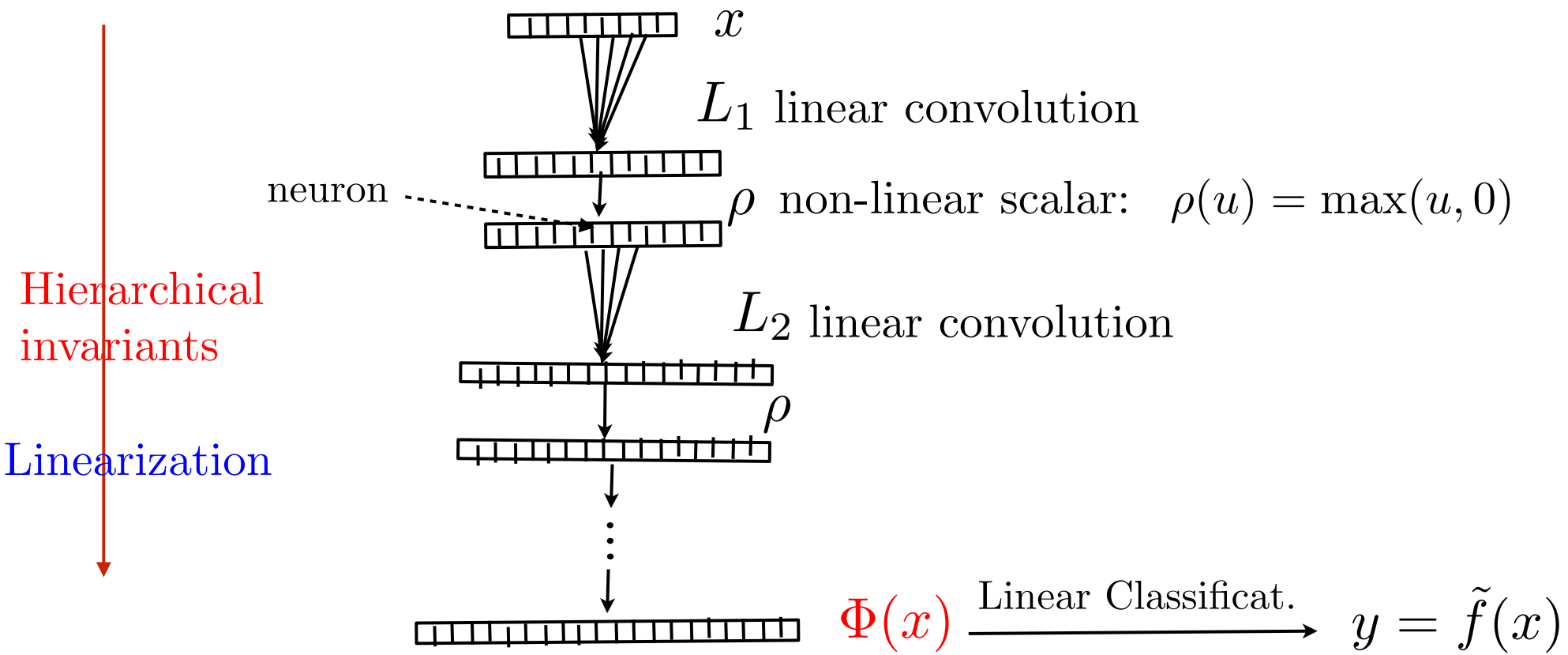
Discriminative: $\|\Phi(x) - \Phi(x')\| \geq C^{-1} \, |f(x) - f(x')|$

- For $x \in \Omega$, if $\Phi(\Omega)$ is bounded and a low dimension d'

$$\Rightarrow \|f - f_M\| \leq C \, M^{-1/d'}$$

Deep Convolution Neworks

- The revival of neural networks: *Y. LeCun*



Optimize L_j with architecture constraints: over 10^9 parameters

Exceptional results for *images, speech, language, bio-data...*

Why does it work so well ? **A difficult problem**

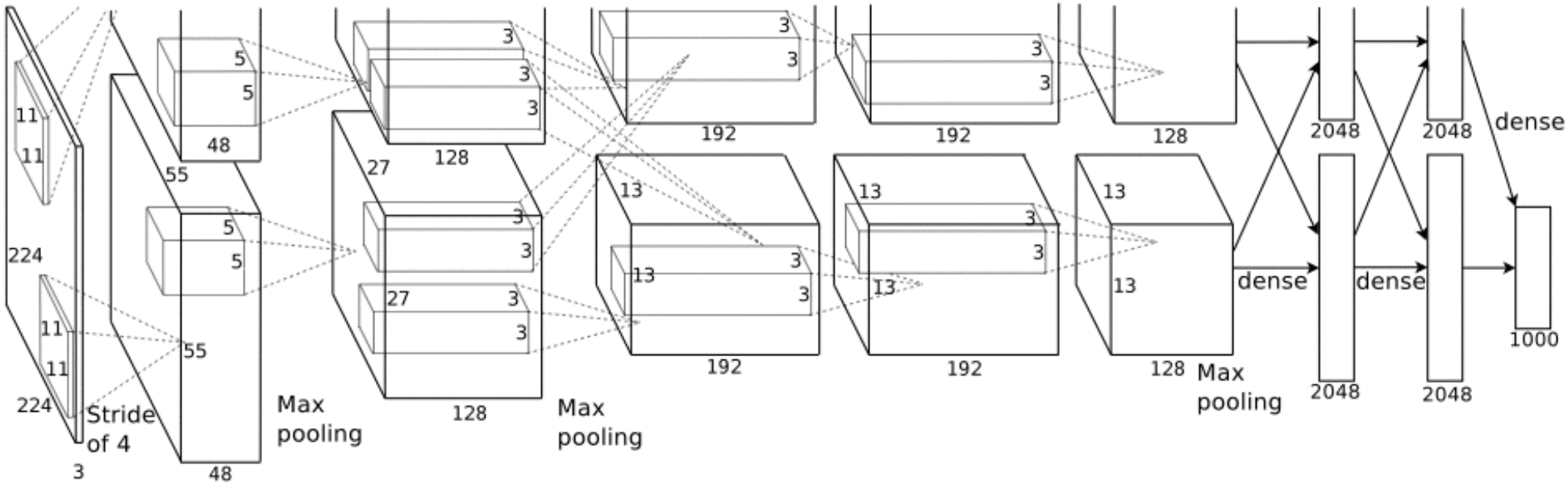
ImageNet Data Basis

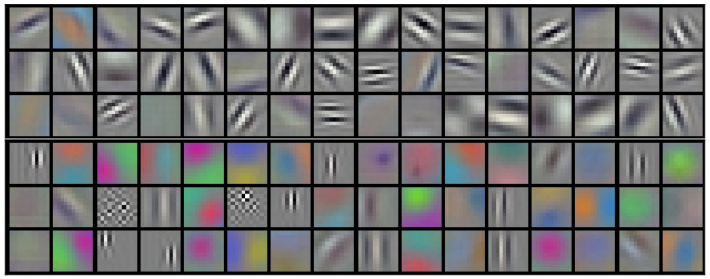
- Data basis with 1 million images and 2000 classes

Alex Deep Convolution Network

A. Krizhevsky, Sutsever, Hinton

- Imagenet supervised training: 1.2 10^6 examples, 10^3 classes
  15.3% testing error in 2012

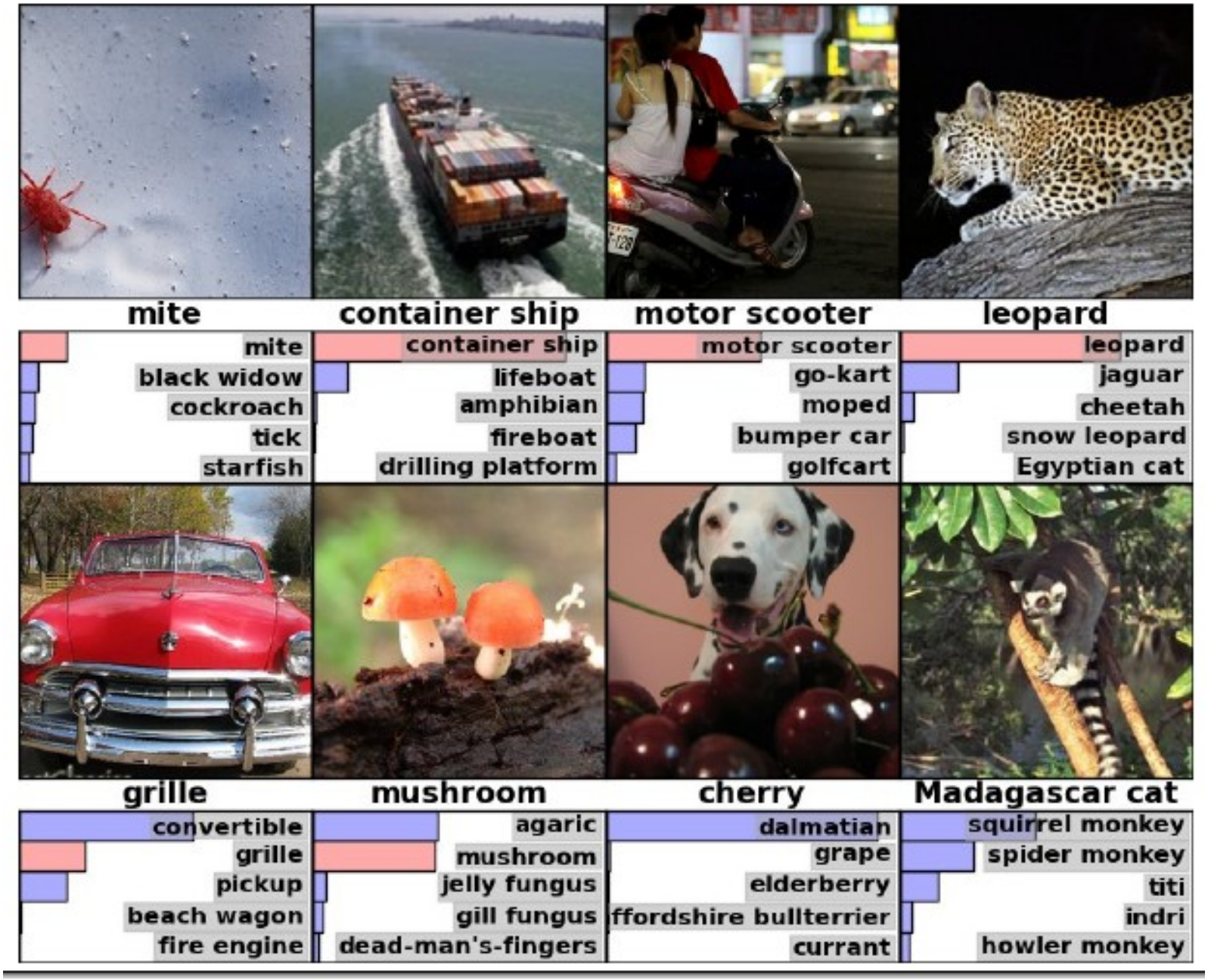




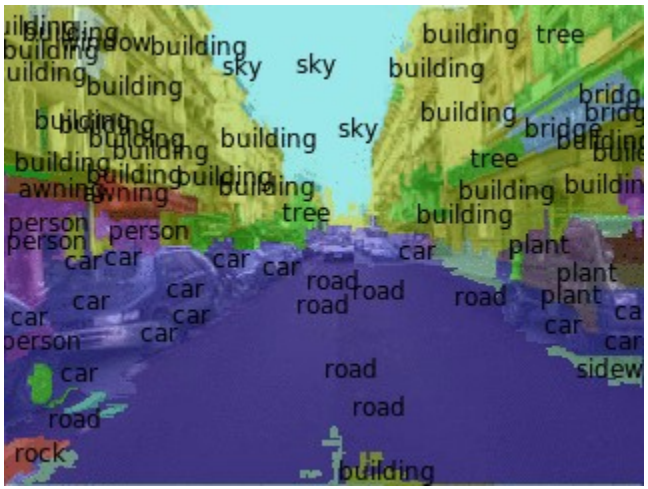
Wavelets

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

Image Classification



Scene Labeling / Car Driving



Why Understading ?

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

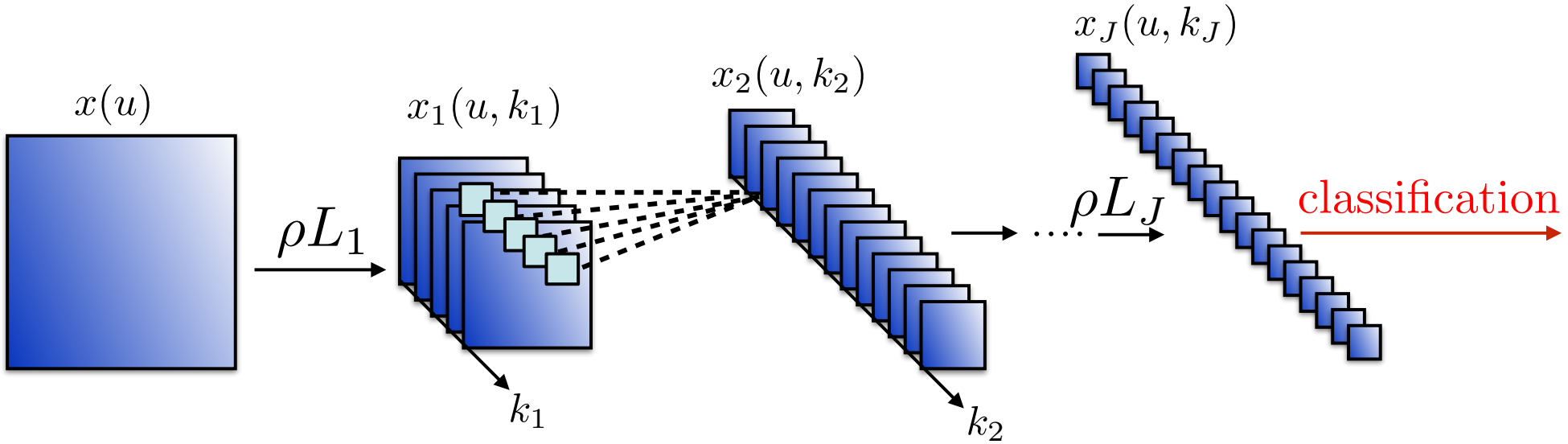
$$x + \epsilon = \tilde{x} \quad \text{with} \quad \|\epsilon\| < 10^{-2}\|x\|$$

correctly classified

classified as ostrich

- Trial and error testing can not guarantee reliability.

Deep Convolutional Networks



$$x_j = \rho\, L_j\, x_{j-1}$$

- L_j is a linear combination of convolutions and subsampling:

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

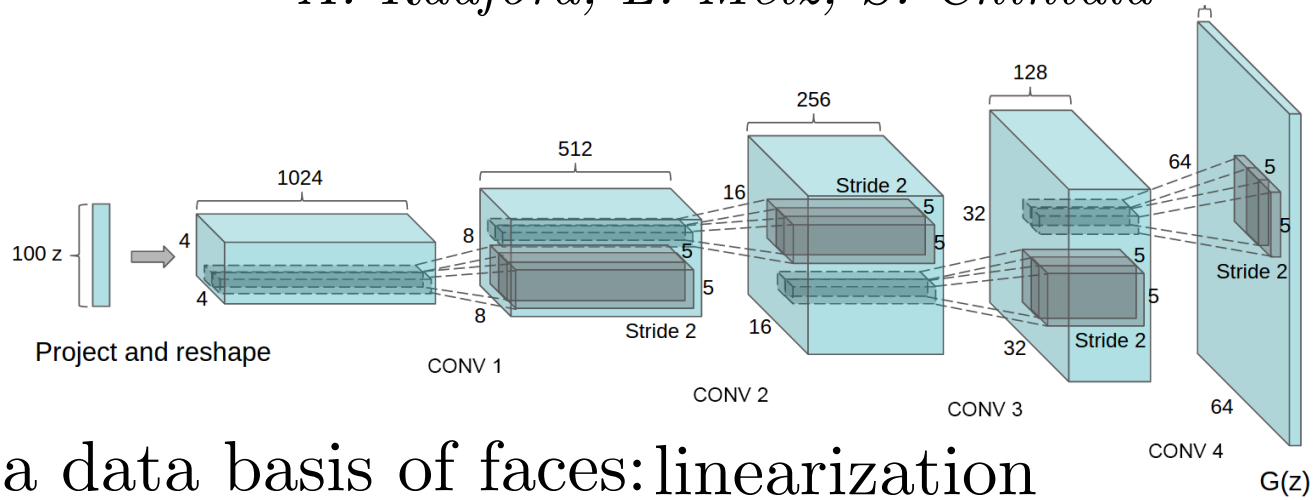
sum across channels

- ρ is contractive: $|\rho(u) - \rho(u')| \leq |u - u'|$

$$\rho(u) = \max(u, 0) \text{ or } \rho(u) = |u|$$

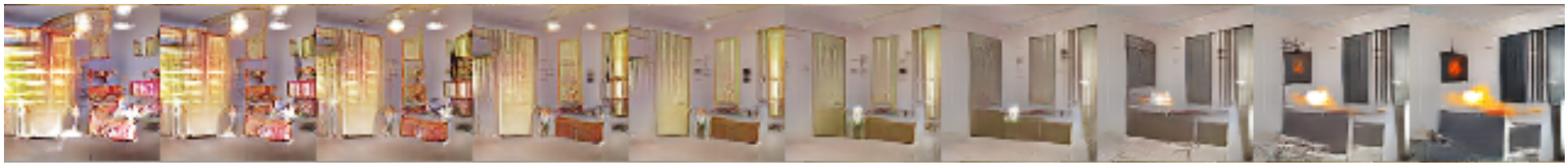
Linearisation in Deep Networks

A. Radford, L. Metz, S. Chintala

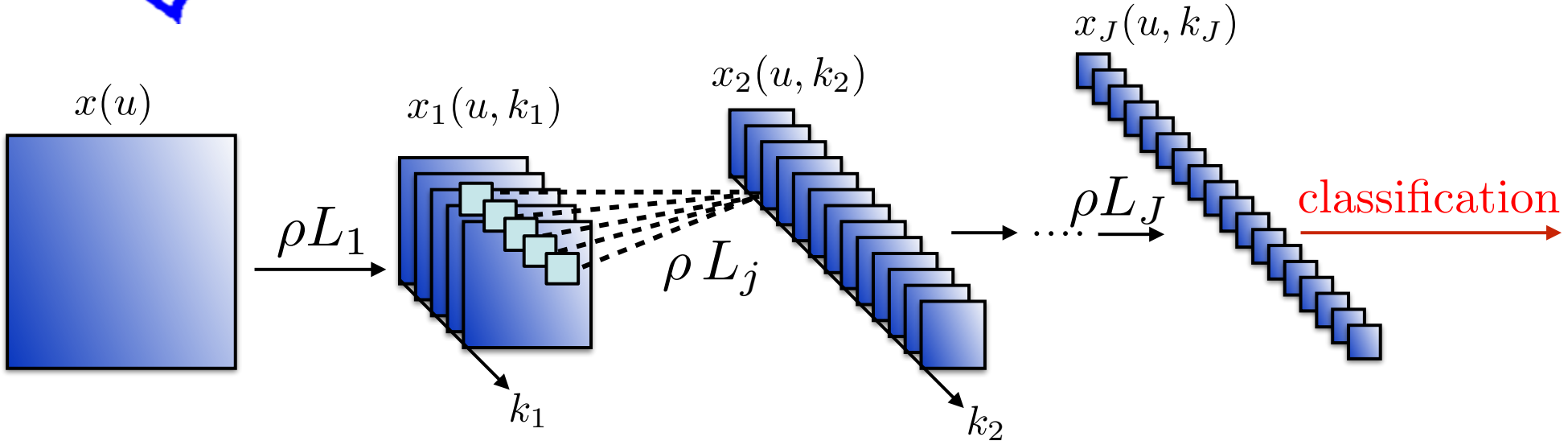


- Trained on a data basis of faces: linearization

- On a data basis including bedrooms: interpolaitons



Many Questions



- Why convolutions ? Translation covariance.
- Why no overfitting ? Contractions, dimension reduction

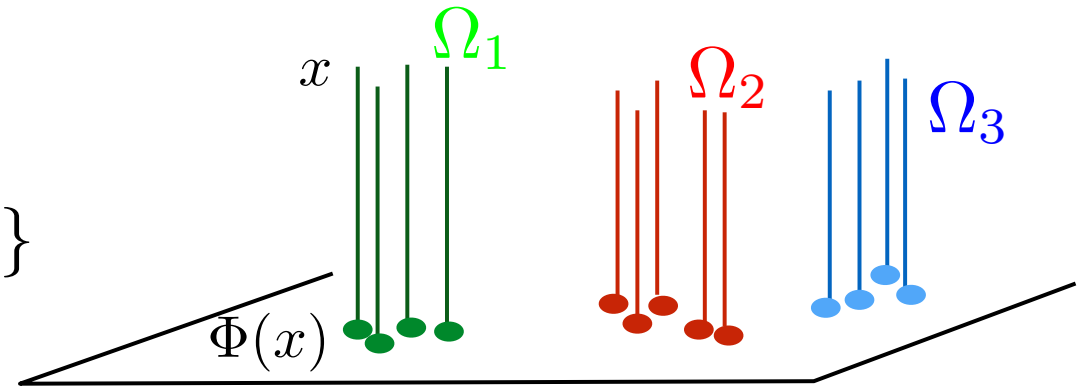
- Why hierarchical cascade ?
- Why introducing non-linearities ?
- How and what to linearise ?
- What are the roles of the multiple channels in each layer ?

Linear Dimension Reduction

Classes

Level sets of $f(x)$

$$\Omega_t = \{x \ : \ f(x) = t\}$$



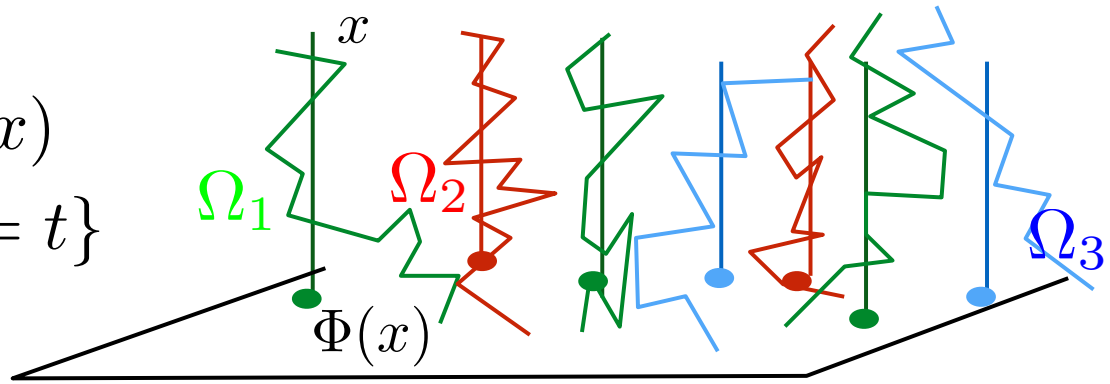
If level sets (classes) are parallel to a linear space then variables are eliminated by linear projections: *invariants*.

Linearise for Dimensionality Reduction

Classes

Level sets of $f(x)$

$$\Omega_t = \{x \ : \ f(x) = t\}$$



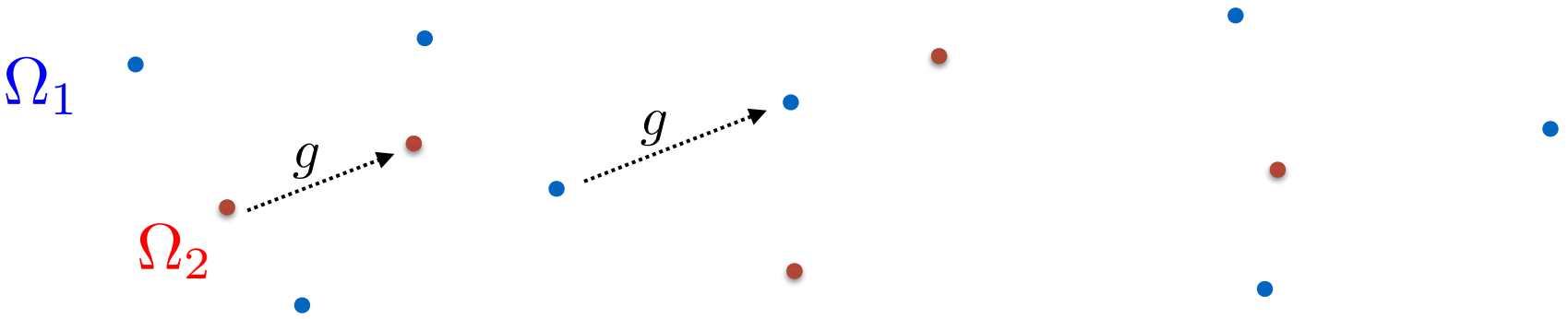
- If level sets Ω_t are not parallel to a linear space
  - Linearise them with a change of variable $\Phi(x)$
  - Then reduce dimension with linear projections

- Difficult because Ω_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:

$$\forall x \quad , \quad f(g.x) = f(x) \; : \; \text{global}$$

If g_1 and g_2 are symmetries then $g_1.g_2$ is also a symmetry

$$f(g_1.g_2.x) = f(g_2.x) = f(x)$$

Groups of symmetries

- $G = \{$ all symmetries $\}$ is a group: unknown

$$\forall (g, g') \in G^2 \quad \Rightarrow g.g' \in G$$

Inverse: $\forall g \in G \quad , \quad g^{-1} \in G$

Associative: $(g.g').g'' = g.(g'.g'')$

If commutative $g.g' = g'.g$: Abelian group.

- Group of dimension n if it has n generators:

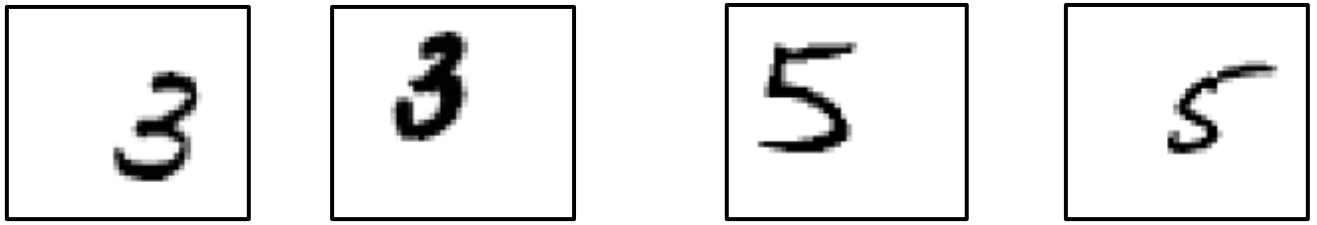
$$g = g_1^{p_1} \, g_2^{p_2} \, ... \, g_n^{p_n}$$

- Lie group: infinitely small generators (Lie Algebra)

Translation and Deformations

- Digit classification:

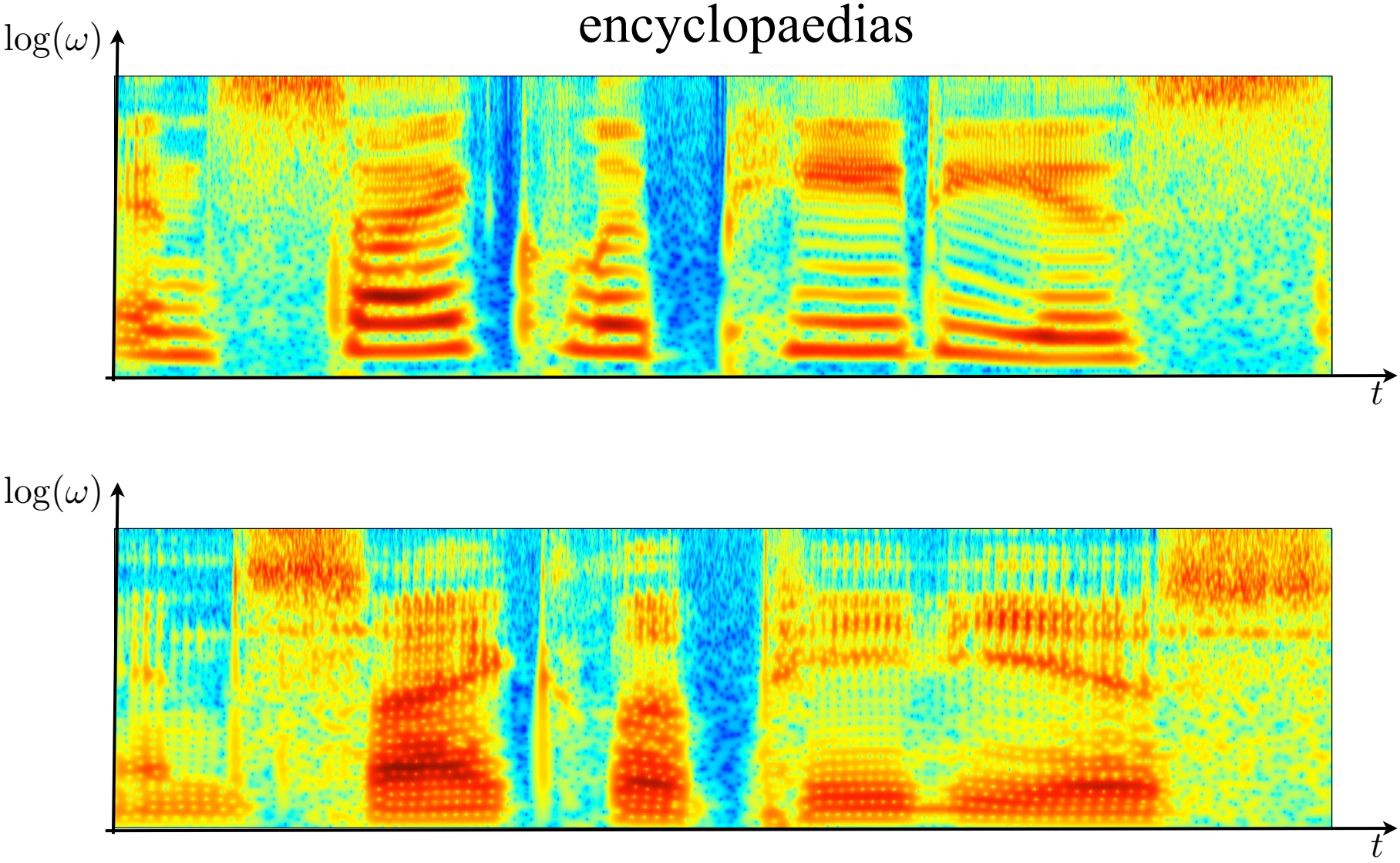
$x(u)$ $\quad$ $x'(u) = x(u - \tau(u))$

Ω_3  Ω_5

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

Video of Philipp Scott Johnson

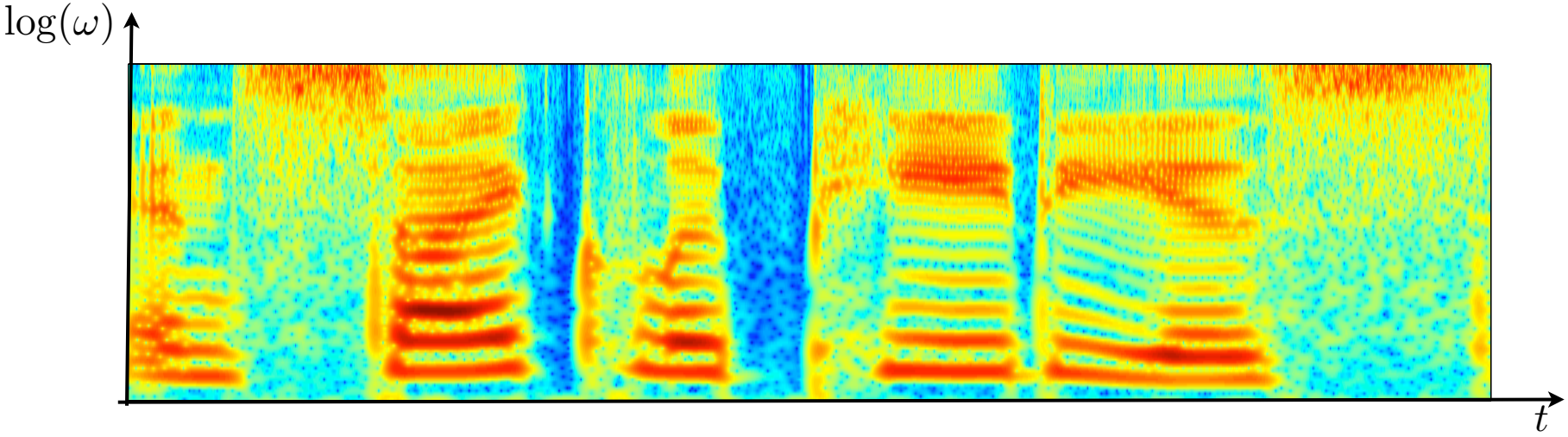
Frequency Transpositions



H : Heisenberg group of "time-frequency" translations

Frequency Transpositions

Time and frequency translations and deformations:

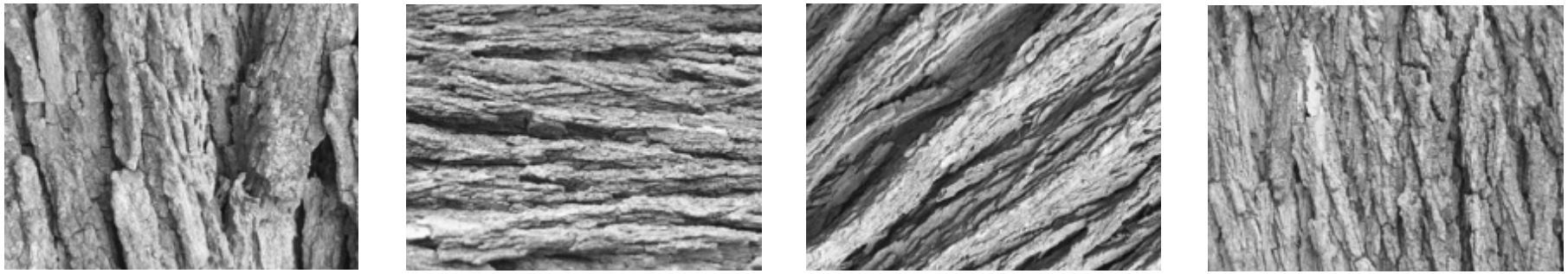


- Frequency transposition invariance is needed

  for speech recognition not for locutor recognition.

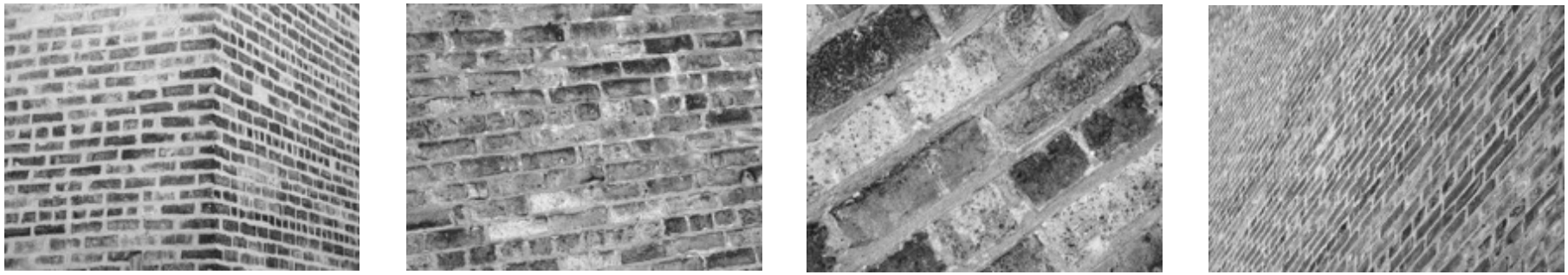
Rotation and Scaling Variability

- Rotation and deformations



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

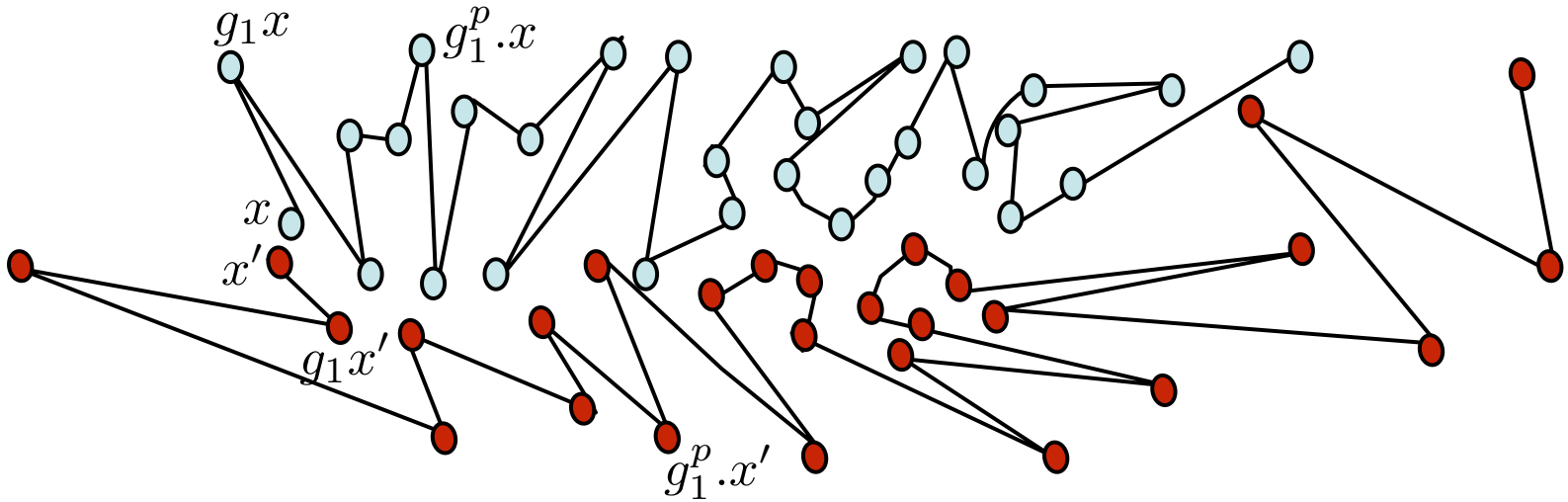
- Scaling and deformations



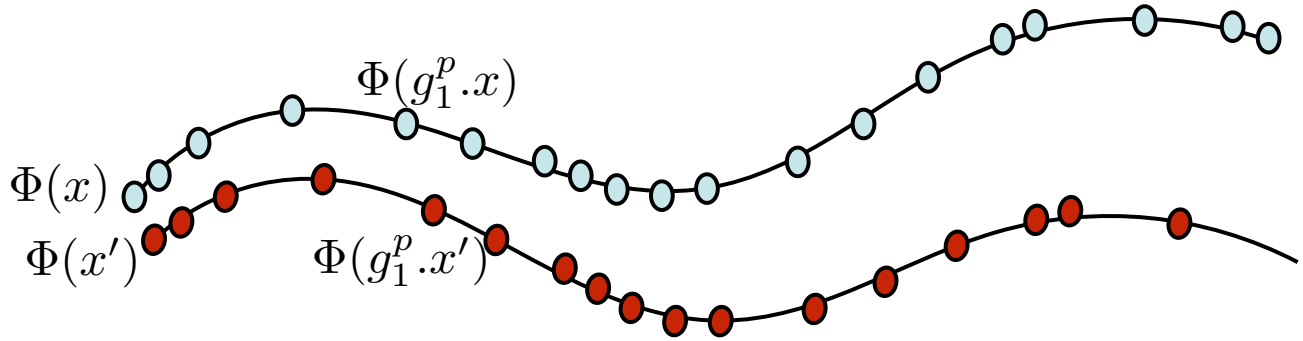
Group: $\mathbb{R} \times \mathrm{Diff}(\mathbb{R})$

Linearize Symmetries

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



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

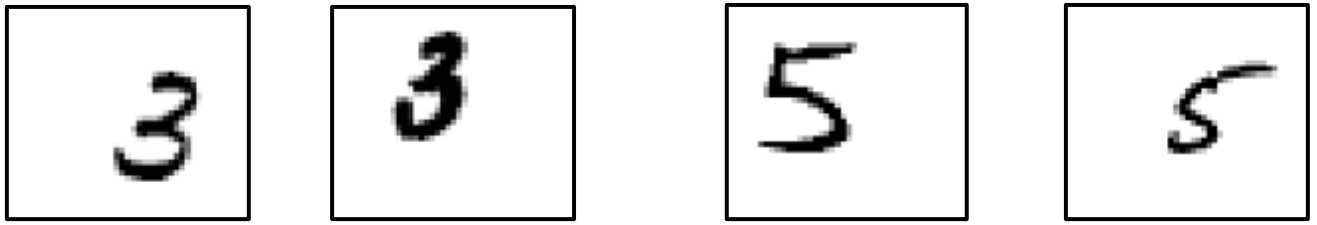


- Lipschitz: $\forall x, g \ : \ \|\Phi(x) - \Phi(g.x)\| \leq C \|g\|$

Translation and Deformations

- Digit classification:

$x(u)$ $x'(u)$



- 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:

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

- Small diffeomorphisms: $g.x(u) = x(u - \tau(u))$

  Metric: $\|g\| = \|\nabla\tau\|_\infty$ maximum scaling

  Linearisation by Lipschitz continuity

$$\|\Phi(x) - \Phi(g.x)\| \leq C \, \|\nabla\tau\|_\infty \ .$$

- Discriminative change of variable:

$$\|\Phi(x) - \Phi(x')\| \geq C^{-1} \, |f(x) - f(x')|$$

Fourier Deformation Instability

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

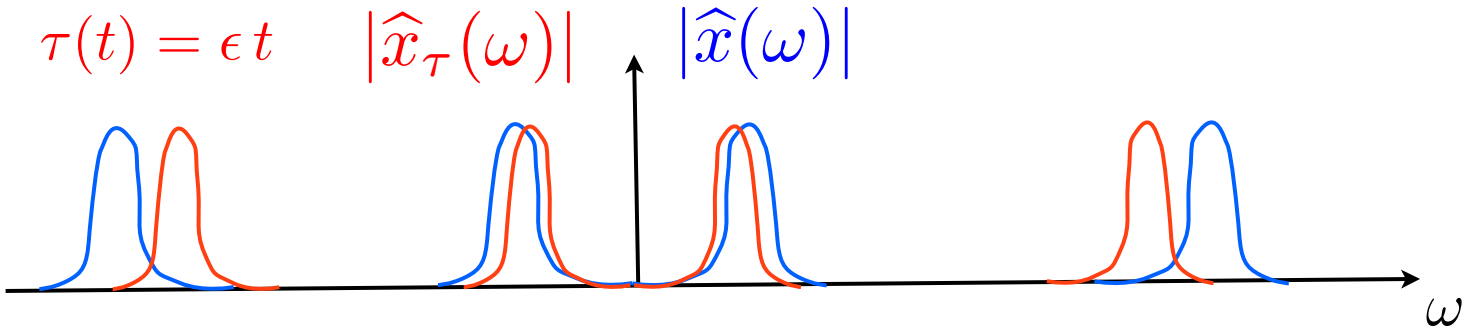
$$x_c(t) = x(t-c) \quad \Rightarrow \quad \hat{x}_c(\omega) = e^{-ic\omega}\, \hat{x}(\omega)$$

The modulus is invariant to translations:

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

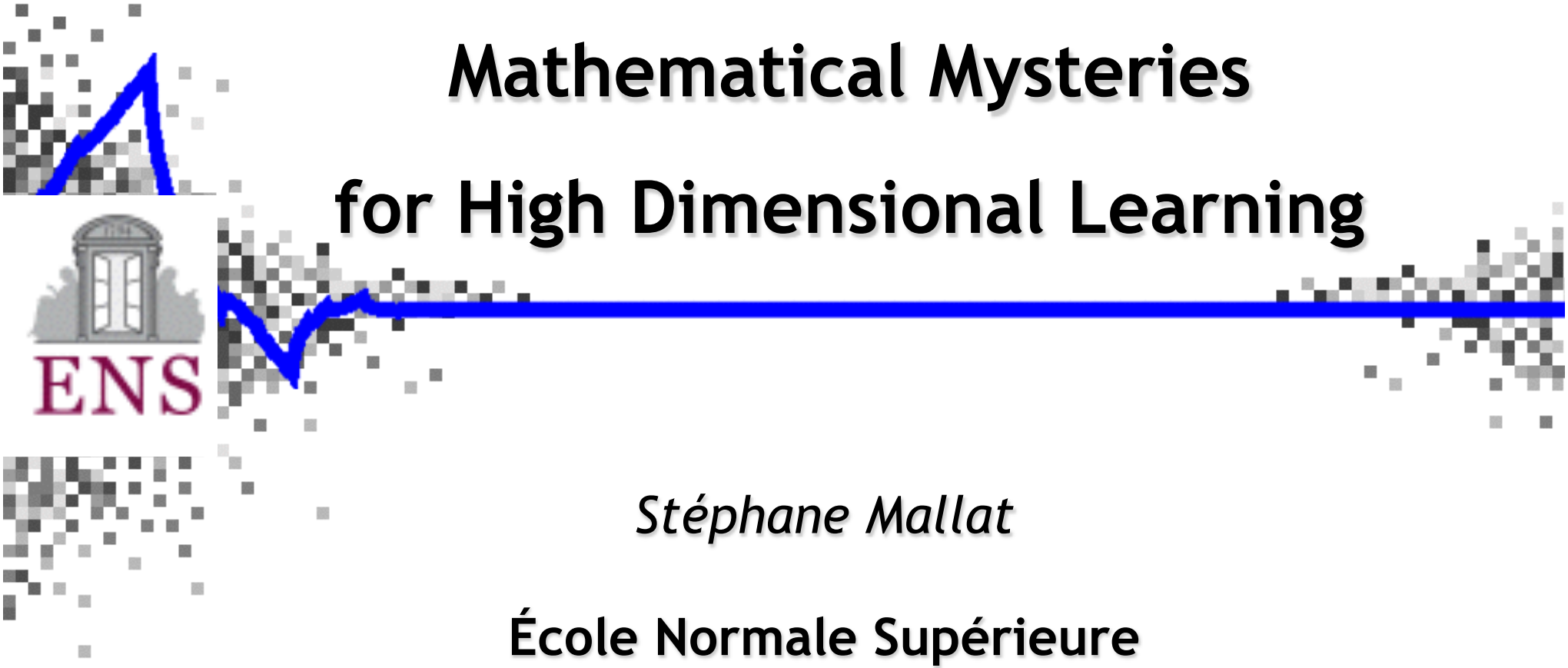
- Instabilites to small deformations $x_\tau(t) = x(t - \tau(t))$:

$\big|\, |\hat{x}_\tau(\omega)| - |\hat{x}(\omega)| \,\big|$ is big at high frequencies



$$\Rightarrow \quad \big\| |\hat{x}| - |\hat{x}_\tau| \big\| \gg \|\nabla \tau\|_\infty \, \|x\|$$

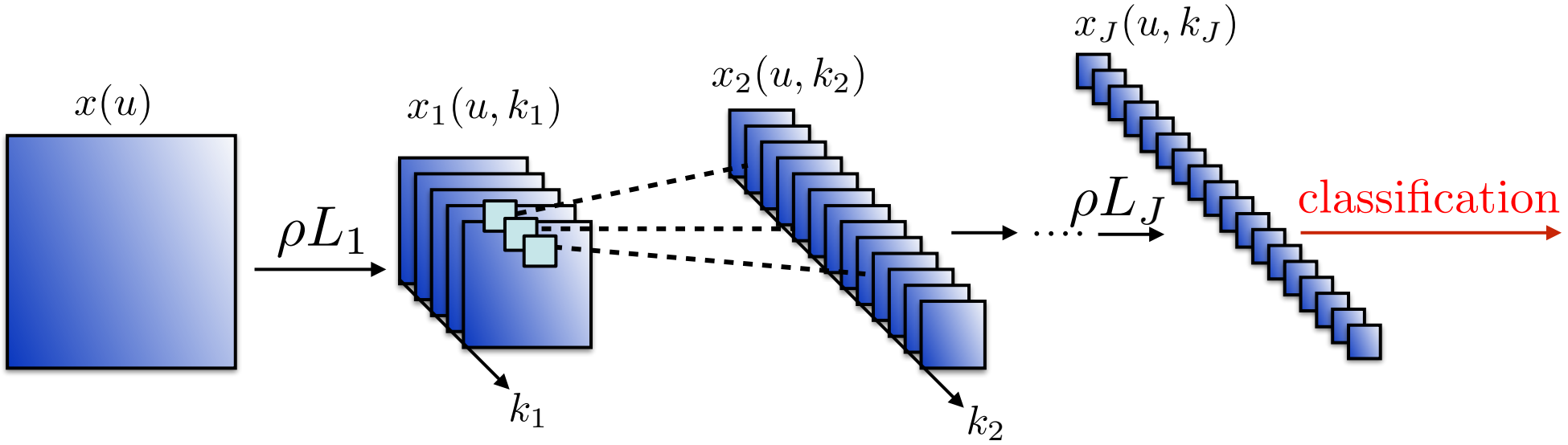
Deep Neural Network Mathematical Mysteries for High Dimensional Learning



Stéphane Mallat

École Normale Supérieure
www.di.ens.fr/data

Deep Convolutional Trees



$$x_j = \rho\, L_j\, x_{j-1}$$

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:

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

- Small diffeomorphisms: $g.x(u) = x(u - \tau(u))$

  Metric: $\|g\| = \|\nabla\tau\|_\infty$ maximum scaling

  Linearisation by Lipschitz continuity

$$\|\Phi(x) - \Phi(g.x)\| \leq C \, \|\nabla\tau\|_\infty \ .$$

- Discriminative change of variable:

$$\|\Phi(x) - \Phi(x')\| \geq C^{-1} \, |f(x) - f(x')|$$

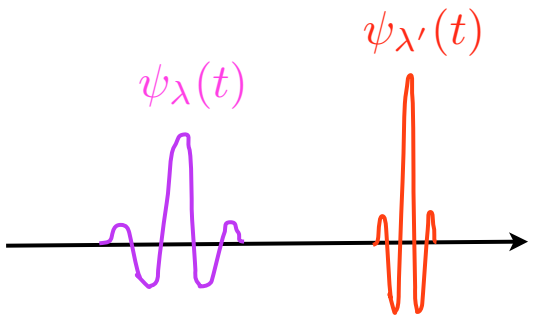
Overview Part II

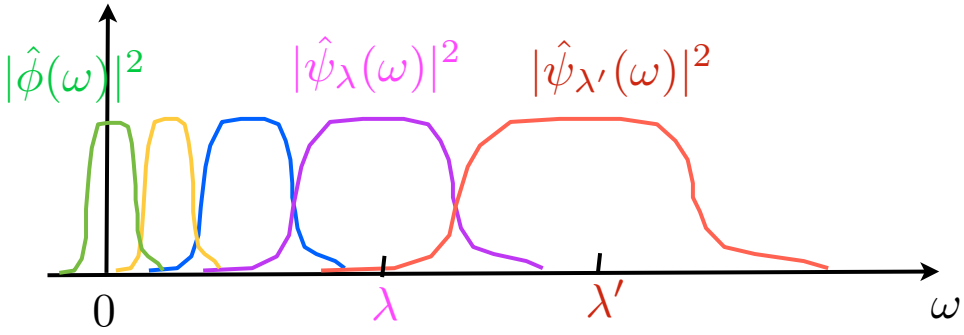
- Wavelet Scattering transform along translations
- Generation of textures and random processes
- Channel connections for more general groups
- Image and audio classification with small training sets
- Quantum chemistry
- Open problems

Understanding Deep Convolutional Networks, arXiv 2016.

Multiscale Wavelet Transform

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



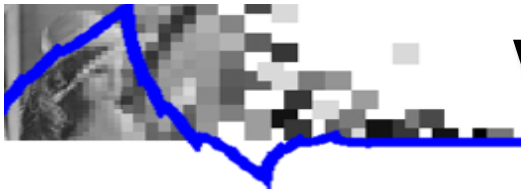


Q-constant band-pass filters $\hat\psi_\lambda$

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

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

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



Why Wavelets ?

- Wavelets are uniformly stable to deformations:

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

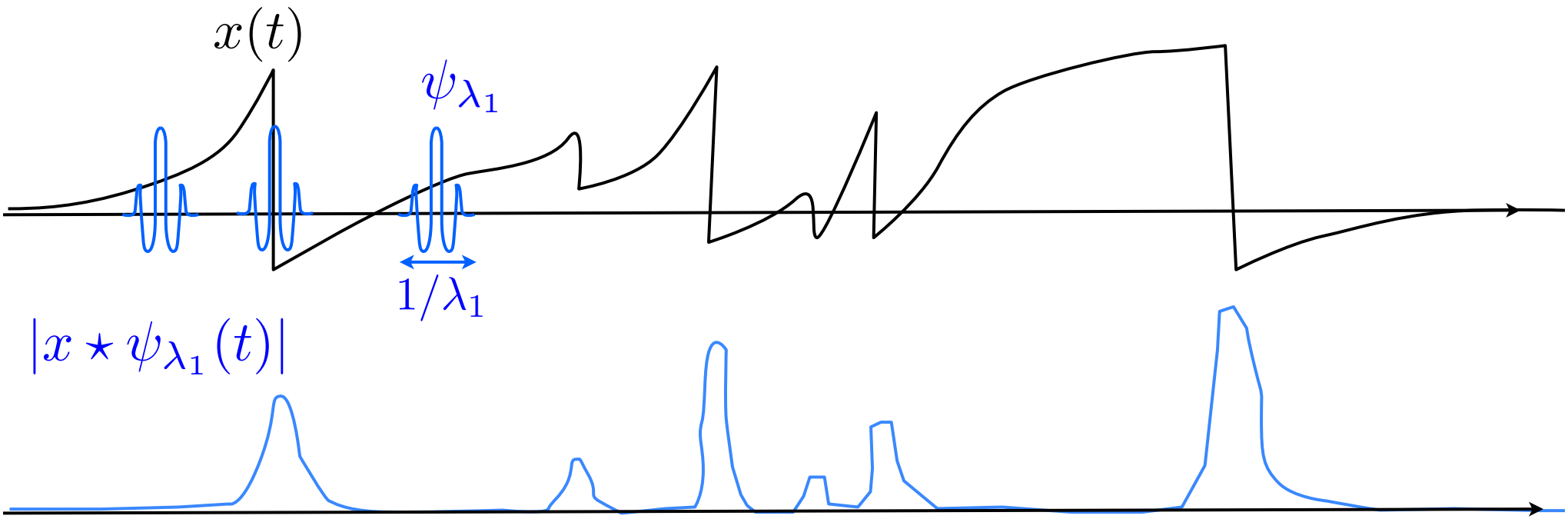
$$\|\psi_\lambda - \psi_{\lambda,\tau}\| \leq C \sup_t |\nabla\tau(t)| \ .$$

- Wavelets separate multiscale information.

- Wavelets provide sparse representations.

Singular Functions

$$|x \star \psi_{\lambda_1}(t)| = \left| \int x(u)\psi_{\lambda_1}(t-u)\,du \right|$$



Time-Frequency Fibers

Wavelet transform modulus: $|W|$