Dynamical aspects of Deep Learning

Yacine Chitour
Joint work with Z. Liao and R. Couillet
DEUSTO-TECH, Bilbao

L2S, CentraleSupélec
Université Paris-Saclay
Paris, France

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CentraleSupélec

Outline

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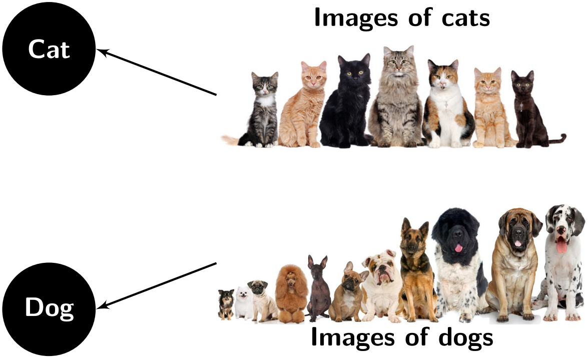
Motivation: "learn" to automatically classify images

Machine Learning:

- given m images of cats $x_1^{cat}, x_2^{cat}, \ldots, x_m^{dog}$ and dogs $x_1^{dog}, x_2^{dog}, \ldots, x_m^{dog}$ of labels y_{cat} and y_{dog} ($y_{cat} \neq y_{dog}$), respectively.



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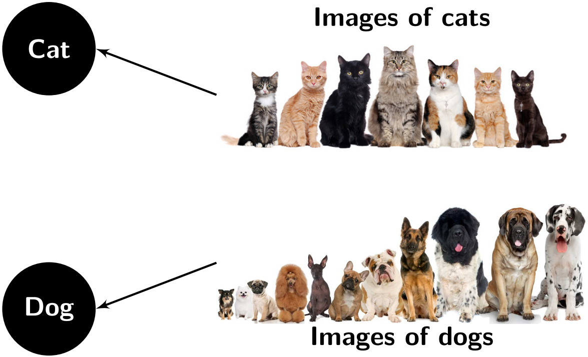

- **Goal**: for a new image $x_{new}^{?}$ with $? \in \{cat, dog\}$, predict ?=cat or ?=dog.

How to "learn" to classify?

Learning phase: find W that minimizes $\sum_{i,j} \|y_{cat} - Wx_i^{cat}\|^2 + \|y_{dog} - Wx_j^{dog}\|^2$, where $x_i^{cat}, x_j^{dog} \in \mathbb{R}^{d_x}$ and $y_{cat}, y_{dog} \in \mathbb{R}^{d_y}$ **chosen by user**.

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- **Input**: (X, Y), images $X = [x_1^{cat}, \dots, x_1^{dog}, \dots] \in \mathbb{R}^{d_x \times 2m}$ with associated labels $Y = [y_{cat}, \dots, y_{dog}, \dots] \in \mathbb{R}^{d_y \times 2m}$.

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- $y_{new}^?$ to be a dog otherwise

From Linear Regression to Deep Neural Networks

Objective: given (X, Y), find W that minimizes the difference $\|Y - WX\|^2$.

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- does not work well for difficult problems (e.g., cat & dogs classification, face recognition, etc.)

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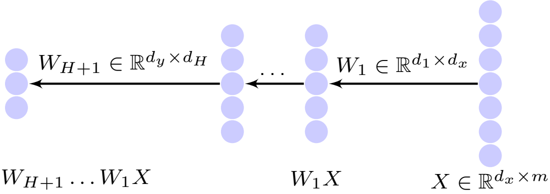

Figure: Illustration of H-hidden-layer linear neural network

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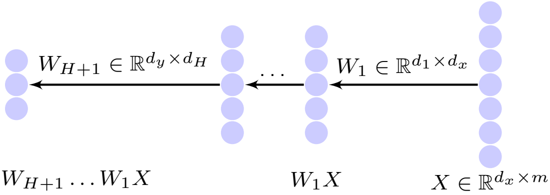

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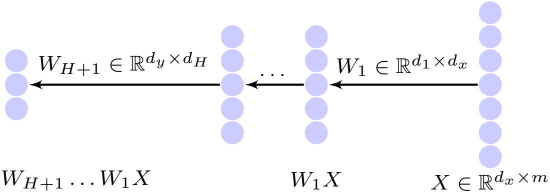

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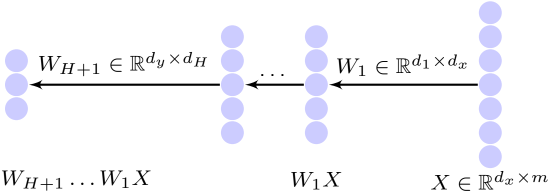

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[Lecun 1998] 5-layer of $60K$ parameters to [He, 2015] 152-layer of $60M$ parameters

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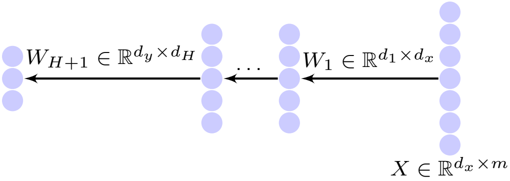

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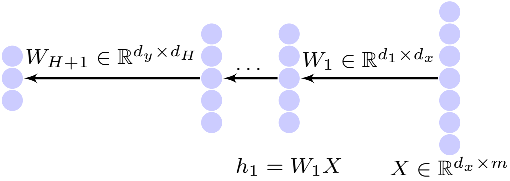

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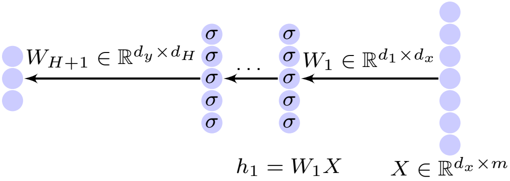

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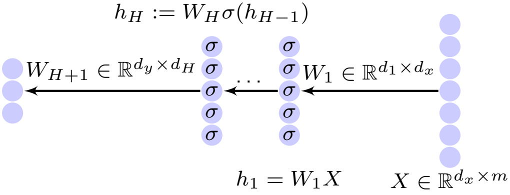

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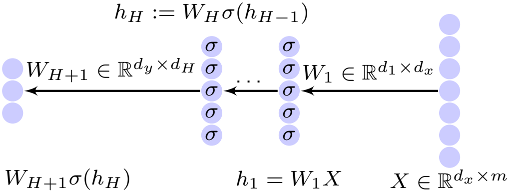

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with (nonlinear) *activation function* $\sigma(z)$: $\mathrm{ReLU}(z) = \max(z, 0)$, Leaky ReLU $\max(z, az)$ (a¿0) or sigmoid $\sigma(z) = \frac{1}{1+e^{-z}}$.

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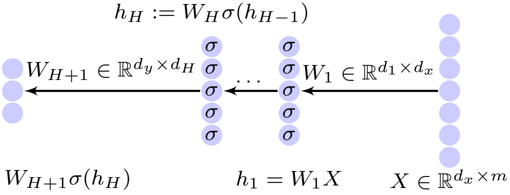

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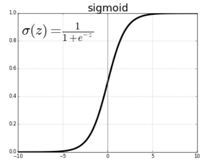

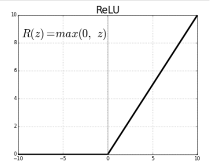

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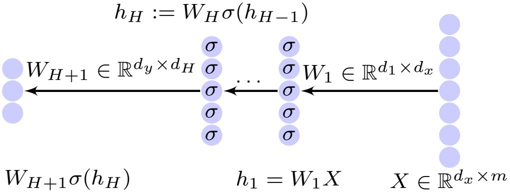

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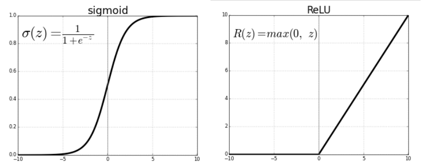

- Or more elaborate structures: convolution, recurrent, residual, etc.

On LINEAR Deep Nonlinear Neural Networks

Set $d_{H+1} := d_y$, $d_0 := d_x$ and consider

$$X \in \mathbb{R}^{d_0 \times m} \quad Y \in \mathbb{R}^{d_{H+1}}.$$

Goal: find $\mathbf{W} = (W_{H+1}, \cdots, W_1)$ that minimizes the function (depending on (X, Y) !!)

$$F(\mathbf{W}) := \|Y - WX\|^2, \quad W = W_{H+1} W_H \cdots W_1,$$

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Define state space $\mathcal{W}$ (recall $d_y = d_{H+1}$ and $d_0 = d_x$)

$$\mathcal{W} = \mathbb{R}^{d_{H+1} \times d_H} \times \cdots \mathbb{R}^{d_1 \times d_0}.$$

and **Gradient Descent associated with** F

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Conjecture ($\Longleftrightarrow$ Overfitting Problem)

(OP): For a.e. (X, Y) and $\mathbf{W}_0 \in \mathcal{W}$, traj. of $(GD)_{(X,Y)}$ starting at $\mathbf{W}_0$ CV to a glob. minimum of F.

Gradient Descent for Linear Neural Networks - First reductions

(Usual) working assumptions

$$X, Y \text{ full rank }, m \geq \max(d_i) \leq \min(d_i) = d_y.$$

Up to SVD and computations, can assume

$$X = Id_{d_x} \text{ (i.e. } m = d_x), \quad Y = \begin{pmatrix} D_Y & 0 \end{pmatrix}, \quad D_Y \in \mathbb{R}^{d_y \times d_y} \text{ diagonal } > 0.$$

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Definition. Critical points $\nabla F(\mathbf{W}) = 0$

$$\mathrm{Crit}(F) = \{\mathbf{W} = (W_{H+1}, \cdots, W_1) \in \mathcal{W}, \; (\Pi W)_{j+1}^{H+1} M (\Pi W)_1^{j-1} = 0\}.$$

Candidates for limit points of trajectories.

Gradient Descent for Linear Neural Networks - Convergence

Theorem (C., Liao, Couillet '18)

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Proof reduces to show that trajectories are bounded.

Proposition (Invariants)

For $1 \leq j \leq H$, *following quantities are conserved along traj. of* $(GD)_{D_Y}$

$$W_{j+1}^{\mathsf{T}} W_{j+1} - W_j W_j^{\mathsf{T}} = \left(W_{j+1}^{\mathsf{T}} W_{j+1} - W_j W_j^{\mathsf{T}}\right)\Big|_{t=0}.$$

$\Longrightarrow \|W_j(t)\|_F^2 = \|W_{H+1}\|_F^2 + C_j \quad t \geq 0,\ 1 \leq j \leq H.$

Set $g(t) = \|W_{H+1}\|_F^2$. Given a traj. of $(GD)_{D_Y}$, one proves that there exists $C_0, C_1 > 0$

$$\frac{dg}{dt} \leq -C_0 g^{H+1}(t) + C_1\left(1 + g^H(t)\right), \quad \forall t \geq 0.$$

Definition

For $\mathbf{W} \in Crit(F)$ define

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Proposition (Landscape of Deep Linear Networks)

Assume $Y = \begin{pmatrix} D_Y & 0 \end{pmatrix}$ *has* **two by two distinct eigenvalues**.

i) $CrV(F) =$ *(finite) set of half sums of squares of any subset of singular values of* Y.

ii) $\mathrm{Crit}_{d_y}(L)$ = *set of local (and global) minima with* $F = 0$ *and* $M = 0$.

iii) *For* $0 \leq r \leq d_y - 1$, $\mathrm{Crit}_r(F)$ *algebraic variety of dim.* > 0 *made of saddle points.*
If $r_Z > r \geq 0$, $Hessian(F)(\mathbf{W})$ *has at least one negative eigenvalue.*

Gradient Descent for Linear Neural Networks - Case $H = 1$

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Proposition (C., Liao, Couillet '18)

Conjecture (OP) true if $H = 1$.

Argument relies on concept of **Normal Hyperbolicity** (due to Fenichel 1972).