Introduction to Deep Learning

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2022-2023



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About this class

- Deep learning
 - Very dynamic field of research
 - * Increased computational power
 - * Increased data availability
 - ▶ Different kinds of neural networks, depending on applications
 - ★ Convolutional networks for image processing
 - * Recursive neural networks for natural language processing
 - ★ Generative adversarial network for physical simulations and image processing
 - ▶ But not many impressive results obtained by using a neural network as a black box, with no knowledge on how they work or on the data
 - * Other ML techniques can outperform neural networks, depending on the problem at hand
- Goal of this class
 - ▶ Present the fundamentals of deep learning by implementing an efficient Multilayer Perceptron (MLP) from scratch
 - ▶ Use this MLP to solve a regression problem (supervised learning)



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Main outline

- Origins of neural networks and deep learning
- Main properties of neural networks
- Learning techniques
 - ▶ Basis (gradient descent, overfitting, ...)
 - ▶ Improvements (gradient optimization, regularization, ...)
- Application to a pricing problem
 - Question: can a neural network be used as a proxy for a costly function?



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Timetable

- Introduction, multilayer perceptrons, forward propagation
 - ► Hands-on: forward propagation
- @ Gradient descents, backpropagation
 - ▶ Hands-on: backpropagation for stochastic gradient descent
- Mini-batch gradient descent, gradient descent optimization
 - ► Hands-on: mini-batch gradient descent
- Mands-on: mini-batch, Momentum
- Regularization
 - ► Hands-on: L2 regularization
- Feature preprocessing, batch normalization
 - Pricing project
- Energy considerations
 - Pricing project
- Pricing project



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Some resources

- Goodfellow, Bengio, Courville. Deep Learning: https://www.deeplearningbook.org/
- Aggarwal. Neural Networks and Deep Learning
- Nielsen. Neural Networks and Deep Learning: http://neuralnetworksanddeeplearning.com
- Lectures by Mallat at Collège de France: https://www.college-de-france.fr/site/stephane-mallat/
- Lectures by Le Cun at Collège de France: https://www.college-de-france.fr/site/yann-lecun/
- Stanford School of Engineering channel: https://www.youtube.com/user/stanfordeng



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Some landmarks

- 1943 W. McCulloch, W. Pitts: A Logical Calculus of the Ideas Immanent in Nervous Activity
 - Formal model of a neuron
 - Weighted inputs, binary outputs
- 1948 N. Wiener: Cybernetics: Or Control and Communication in the Animal and the Machine
 - "Self-regulating mechanisms"
 - Notion of feedback
- 1950 A. Turing: The Turing Test
 - Proposal: build a program simulating a child's mind, then educate
 it
- 1951 M. Minsky and D. Edmonds: Stochastic Neural Analog Reinforcement Calculator (SNARC)
 - First neural network machine



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A classification problem

1958. F. Rosenblatt: The Perceptron: A Probabilistic Model for Information Storage and Organization in the Brain

- Input: $\{(\chi_{(i)}, \rho_{(i)}) \mid i = 1, \dots, N\}$, where $\chi_{(i)} \in \mathbb{R}^d$ and $\rho_{(i)} \in \{+1, -1\}$
- Goal: construct a classifier that correctly labels the training set
- Perceptron: outputs $sign(\omega^T \chi + \beta)$
- Problem: find ω, β such that $\forall i = 1, ..., N$, $\operatorname{sign}(\omega^{\mathrm{T}}\chi_{(i)} + \beta) = \rho_{(i)}$
- Reformulation: find ω, β such that $\forall i = 1, \dots, N, \ \rho_{(i)} \cdot (\omega^{\mathrm{T}} \chi_{(i)} + \beta) > 0$



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Parameter update algorithm

Notations

We define:

$$\bullet \ \theta \stackrel{\text{def}}{=} (\beta, \omega_1, \dots, \omega_d)^{\mathrm{T}} \text{ and } \overline{\chi} \stackrel{\text{def}}{=} (1, \chi_1, \dots, \chi_d)^{\mathrm{T}}$$

Goal: find θ such that $\forall i = 1, ..., N$, $\rho_{(i)} \cdot (\theta^T \overline{\chi_{(i)}}) > 0$

Input:
$$\left\{ \left(\chi_{(i)}, \rho_{(i)} \right) \mid i = 1, \ldots, N \right\}$$

1 $\theta \leftarrow (0, \ldots, 0)^{\mathrm{T}}$;

2 while $\exists j \in \{1, \ldots, N\}$ such that $\rho_{(j)} \cdot \mathrm{sign}(\theta^{\mathrm{T}} \overline{\chi_{(j)}}) < 0$ do

3 $\mid \theta \leftarrow \theta + \rho_{(j)} \overline{\chi_{(j)}}$

4 end

5 return θ



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Convergence

Theorem

If there exists a separating hyperplane for the samples, then the algorithm terminates and the resulting perceptron correctly classifies all samples

- Separating hyperplane: $\exists \overline{\omega^*}$ such that for all i = 1, ..., N, $\rho_{(i)} \cdot (\overline{\omega^*}^T \overline{\chi_{(i)}}) > 0$
 - Note that $\overline{\omega^*} \neq \mathbf{0}$
- Proof principle: determine an upper-bound on the number *k* of iterations in the
- We let:

 - $Arr R \stackrel{\text{def}}{=} \max_i ||\overline{\chi_{(i)}}||$; note that R > 0
- We have (See, e.g., http://www.cs.columbia.edu/~mcollins/courses/6998-2012/ notes/perc.converge.pdf):

$$k \leq \frac{R^2 \|\overline{\omega^*}\|^2}{\delta^2}$$



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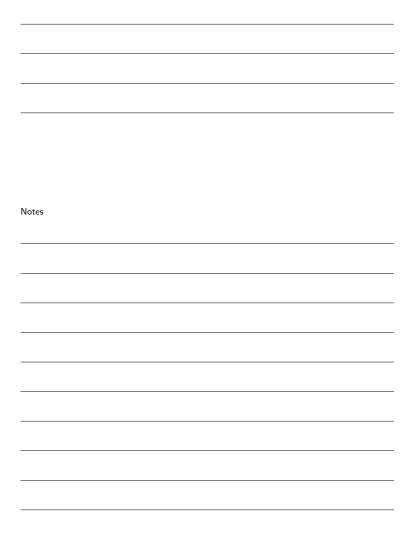
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What if the samples admit no separating hyperplane?

Minsky & Papert (1969): Perceptrons: an introduction to computational geometry

- The XOR function does not admit a separating hyperplane
- The perceptron is incapable of learning this function



Summary on the perceptron

- Simple learning scheme
- Convergence result when there exists a separating hyperplane
 - ▶ It is possible to evaluate the convergence speed
- Minsky & Papert: there are simple functions that cannot be learned
 - ► This negative result slowed research on neural networks for a long time
- Question: what happens if we generalize the perceptron by
 - Interconnecting several neurons together
 - Allowing activation functions other than the sign function?



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Definitions

Definition

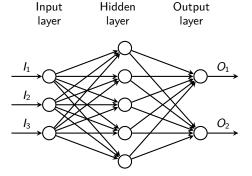
A multilayer perceptron (MLP, or feedforward neural network) is a set of interconnected neurons that forms a Directed Acyclic Graph (DAG)

- The connections between neurons are weighted
- Neurons with no incoming connection from another neuron are **input neurons**. The set of input neurons forms the input layer
- Neurons with no outgoing connection to another neuron are **output neurons**. The set of output neurons forms the output layer
- All other neurons are hidden neurons. Hidden neurons are organized in hidden layers
- Computations are performed in the hidden and output layers.



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Fully connected multilayer perceptron (3 layers)



Definition

A fully connected MLP is an MLP such that all non-input neurons are connected to all the neurons of the previous layer

In what follows, all the MLPs we consider will be fully connected



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Notations and assumptions

Given a fully connected MLP with \boldsymbol{L} layers:

- ullet The neurons of layer i are denoted by $u_1^i,\dots,
 u_{n_i}^i$ (layer 0 denotes the input layer)
- \bullet The weight connecting ν_j^{i-1} to ν_k^i is denoted by $\omega_{j,k}^i$
- The bias of ν_k^i is denoted by β_k^i
- The sample transmitted to the input layer is denoted by $\alpha^0 = (\alpha^0_1, \dots, \alpha^0_{n_0})^T$
- $\bullet \ \ \text{The net input of} \ \nu_k^i \ \text{is} \ \zeta_k^i \stackrel{\text{\tiny def}}{=} \left(\sum_{j=1}^{n_{i-1}} \omega_{j,k}^i \alpha_j^{i-1} \right) + \beta_k^i$
- The **activation** of ν_k^i is denoted by α_k^i
- The activation function of ν_k^i is Φ , so that $\alpha_k^i = \Phi(\zeta_k^i)$
 - ▶ Unless stated otherwise (e.g., **Dropout**), we assume it is the same for all neurons

Assumption

In what follows, unless specified otherwise, we will assume that the MLPs we consider have a single output node



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Matrix representation

- ullet The weights at layer i are stored in a matrix $\Omega^i \in \mathbb{R}^{n_{i-1} \times n_i}$, where $(\Omega^i)_{j,k} = \omega^i_{j,k}$
- The biases at layer i are stored in a vector $\beta^i \stackrel{\text{def}}{=} (\beta^i_1, \dots, \beta^i_{n_i})^{\mathrm{T}}$
- The net inputs at layer i are stored in a vector $\zeta^i \stackrel{\text{def}}{=} (\zeta^i_1, \dots, \zeta^i_{n_i})^{\mathrm{T}}$
- The activation function is extended to vectors: if $u = (u_1, \dots, u_n)^T$, then $\Phi(u) = (\Phi(u_1), \dots, \Phi(u_n))^T$
- The activations of layer i are stored in a vector $\alpha^i \stackrel{\text{def}}{=} (\alpha^i_1, \dots, \alpha^i_{n_i})^{\mathrm{T}}$



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Forward propagation algorithms

```
Input: A network with L layers
Input: \alpha^0 \stackrel{\text{def}}{=} (\alpha_1^0, \dots, \alpha_{n_0}^0)^{\mathrm{T}}
1 for i \leftarrow 1 to L do
2 | for k \leftarrow 1 to n_i do
3 | \zeta_k^i \leftarrow \left(\sum_{j=1}^{n_{i-1}} \omega_{j,k}^i \alpha_j^{i-1}\right) + \beta_k^i;
4 | \alpha_k^i \leftarrow \Phi(\zeta_k^i);
5 | end
6 end
Algorithm 2: Forward propagation, basic version
```



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Identity activation function

What happens if the activation function is the identity?

$$\bullet \ \alpha^{i} = \zeta^{i} = \left[\Omega^{i}\right]^{\mathrm{T}} \alpha^{i-1} + \beta^{i}$$



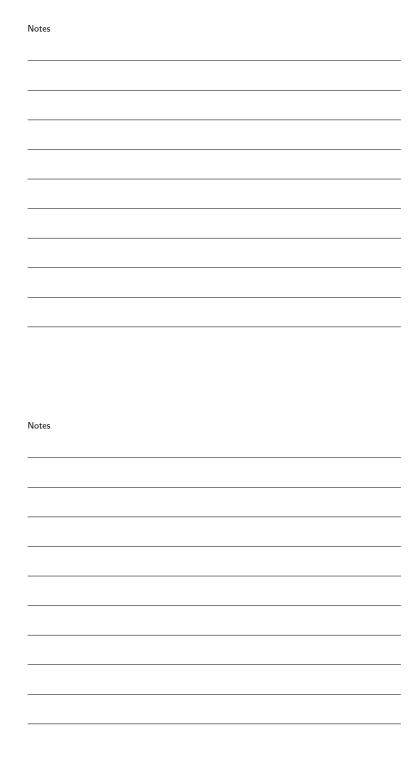
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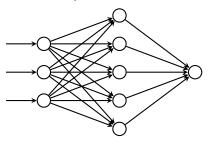
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Linear activation function

What happens if the activation function is linear: $\Phi: z \mapsto \mu z + \lambda$?



A specific MLP



- Input layer of size d
- Single hidden layer of size K
- Single output neuron
- Activation function Φ only on hidden layer (identity on output)
- No bias on output layer



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A class of functions

- $\bullet \ \ \text{We define } \Lambda \stackrel{\scriptscriptstyle\mathsf{def}}{=} \left\{ \left\langle \mathsf{K}, \Phi, \Omega, \omega', \beta \right\rangle \, \middle| \ \mathsf{K} \in \mathbb{N}, \ \Phi : \mathbb{R} \to \mathbb{R}, \ \Omega \in \mathbb{R}^{d \times \mathsf{K}}, \ \beta, \omega' \in \mathbb{R}^{\mathsf{K}} \right\}$
- For $\lambda \in \Lambda$, we define

$$\begin{array}{ccc} f_{\lambda}: \ \mathbb{R}^{d} & \rightarrow & \mathbb{R} \\ x & \mapsto & \left[\omega'\right]^{\mathrm{T}} \cdot \Phi\left(\Omega^{\mathrm{T}}x + \beta\right) = \sum_{k=1}^{K} \omega_{k}' \Phi(\left[\Omega_{k}\right]^{\mathrm{T}}x + \beta_{k}) \end{array}$$

• We consider the set of functions $\mathcal{F}(\Lambda) \stackrel{\text{def}}{=} \{ f_{\lambda} \mid \lambda \in \Lambda \}$

Question

What functions can be approximated by an element from $\mathcal{F}(\Lambda)$?



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The Universal Approximation Theorem

Theorem (see, e.g., Allan Pinkus, 1999)

Let $\mathcal{C}\left(\mathbb{R}^d\right)$ denote the set of continuous functions on \mathbb{R}^d and consider the set $\mathcal{M}(\Phi) \stackrel{\text{\tiny def}}{=} \operatorname{span}\left(\left\{x \mapsto \Phi(\omega^{\mathrm{T}}x + \beta) \mid \omega \in \mathbb{R}^d, \beta \in \mathbb{R}\right\}\right)$. This set is dense in $\mathcal{C}\left(\mathbb{R}^d\right)$, in the topology of uniform convergence on compact sets if and only if Φ is nonpolynomial

In other words: if $f \in \mathcal{C}\left(\mathbb{R}^d\right)$ and $\mathcal{D} \subseteq \mathbb{R}^d$ is a compact set, then for all $\varepsilon > 0$, there exists $\widetilde{f} \in \mathcal{M}(\Phi)$ such that for all $x \in \mathcal{D}$, $|f(x) - \widetilde{f}(x)| \leq \varepsilon$

- For a given $\varepsilon > 0$, there exists $K_{\varepsilon} \in \mathbb{N}$ such that an MLP with a single hidden layer of size K_{ε} can approximate f with a precision of ε
- What is wrong with polynomials?



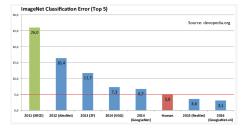
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Issues with the Universal Approximation Theorem

- The size of the hidden layer can be extremely large
 - In practice, this result does not seem very useful
- What happens if we increase the number of hidden layers and bound their sizes?
 - For a long time, not so clear there was anything to gain
 - ▶ Empirically yes: impressive results using deep networks



- More recent theoretical results (Eldan, Shamir. The power of Depth for Feedforward Neural Networks, 2016)
- For the time being, it is still not possible to formally explain why things work so well



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