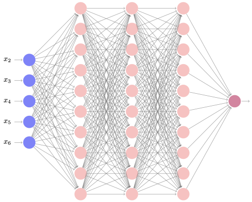

Perceptrons and Multilayer Perceptrons

Vincent Barra
LIMOS, UMR 6158 CNRS, Université Clermont Auvergne

Perceptron

Multilayer perceptrons

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Threshold Logic Unit

Mc Culloch and Pitts, 1943

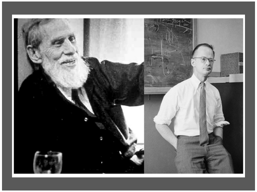
First mathematical model for a neuron
For $\boldsymbol{x}$ boolean vector, $w, b \in \mathbb{R}$:

$$f(x) = \mathbb{1}_{\{w \sum_i x_i + b \geq 0\}}$$

and in particular

- $OR(x, y) = \mathbb{1}_{\{x+y-0.5 \geq 0\}}$
- $AND(x, y) = \mathbb{1}_{\{x+y-1.5 \geq 0\}}$
- $NOT(x) = \mathbb{1}_{\{-x+0.5 \geq 0\}}$

Any Boolean function can be build with such units.



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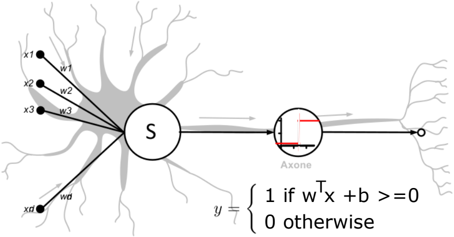
Perceptron

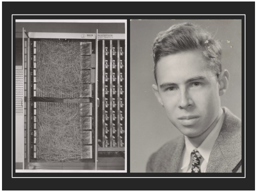
Rosenblatt 1957

Generalization: $\boldsymbol{w}, \boldsymbol{x} \in \mathbb{R}^d,\ b \in \mathbb{R}$

$$f(x) = \mathbb{1}_{\{\boldsymbol{w}^T \boldsymbol{x} + b \geq 0\}}$$

Relation to biology





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Perceptron

A more general view

$$f(\boldsymbol{x}) = \sigma(\boldsymbol{w}^T\boldsymbol{x} + b)$$

where

- $\boldsymbol{w}$: synaptic weights
- b: bias
- $\boldsymbol{w}^T\boldsymbol{x}$: post synaptic potential
- σ: activation function

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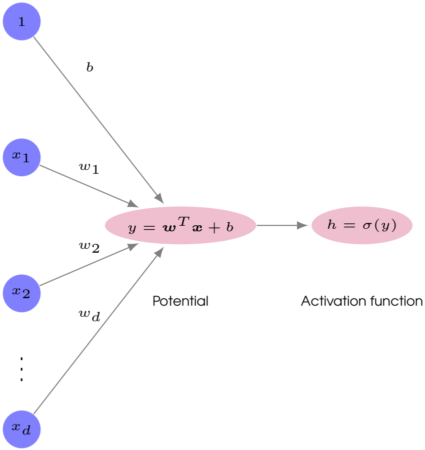
Representing the Perceptron

Graphical representations

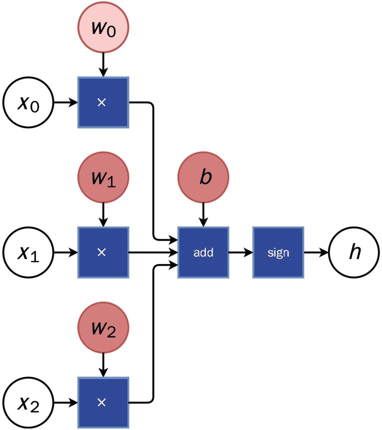
1. "Neural" representation
2.



Representing the Perceptron

Graphical representations

1. "Neural" representation
2. Computational graph
   - white nodes: inputs and outputs
   - red nodes: model parameters
   - blue nodes: operations



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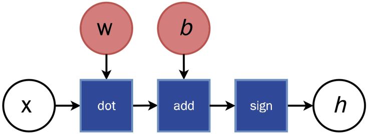

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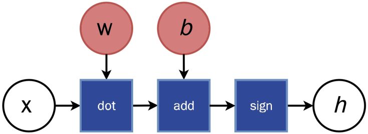
Representing the Perceptron

Basic brick

This unit is the basic brick of all neural networks



LEARNING THE PERCEPTRON

Problem statement

How to build the model ?

- Input: Learning set $Z = \{(\boldsymbol{x}_i, y_i), i \in [\![1 \cdots n]\!], \boldsymbol{x}_i \in \mathbb{R}^{d+1}, y_i \in \mathbb{R}\}$
- Unknown: $\boldsymbol{w} \in \mathbb{R}^{d+1}$

LEARNING THE PERCEPTRON

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- Unknown: $\boldsymbol{w} \in \mathbb{R}^{d+1}$

Key Idea

For each $\boldsymbol{x}_i \in Z$:

- expected output: y_i
- computed output: $h_i = \sigma(\boldsymbol{w}^T \boldsymbol{x}_i) = f_{\boldsymbol{w}}(\boldsymbol{x})$

If $\mathcal{L} : \mathbb{R}^{d+1} \times \mathbb{R}^{d+1} \to \mathbb{R}$ is a loss function

$$\hat{\boldsymbol{w}} = Arg \min_{\boldsymbol{w}} \sum_{(\boldsymbol{x},y) \in Z} \mathcal{L}\left(f_{\boldsymbol{w}}(\boldsymbol{x}), y\right)$$

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EXAMPLES OF LOSS FUNCTIONS

Binary classification (-1/1)

1. Characteristic function: $\mathcal{L}(f_{\boldsymbol{w}}(x), y) = \mathbb{1}_{y f_{\boldsymbol{w}}(x) \leq 0}$
2. Logistic loss : $\mathcal{L}(f_{\boldsymbol{w}}(x), y) = ln\left(1 + e^{-y f_{\boldsymbol{w}}(x)}\right)$
3. binary cross-entropy: $\mathcal{L}(f_{\boldsymbol{w}}(x), y) = -\left(y log(f_{\boldsymbol{w}}(x)) + (1-y) log(1 - f_{\boldsymbol{w}}(x))\right)$

Regression

1. Hinge loss : $\mathcal{L}(f_{\boldsymbol{w}}(x), y) = (1 - y f_{\boldsymbol{w}}(x))_+ = max\,(0, 1 - y f_{\boldsymbol{w}}(x))$
2. MSE (L_2 loss) : $\mathcal{L}(f_{\boldsymbol{w}}(x), y) = \|f_{\boldsymbol{w}}(x) - y\|^2$
3. Huber loss : $\mathcal{L}(f_{\boldsymbol{w}}(x), y) = \begin{cases} \frac{1}{2\epsilon}(f_{\boldsymbol{w}}(x) - y)^2 & \text{if } |f_{\boldsymbol{w}}(x) - y| \geq \epsilon \\ 0 & \text{otherwise} \end{cases}$
4. Vapnik loss: $\mathcal{L}(f_{\boldsymbol{w}}(x), y) = \begin{cases} 0 & \text{if } |f_{\boldsymbol{w}}(x) - y| \leq \epsilon \\ |f_{\boldsymbol{w}}(x) - y| - \epsilon & \text{otherwise} \end{cases}$

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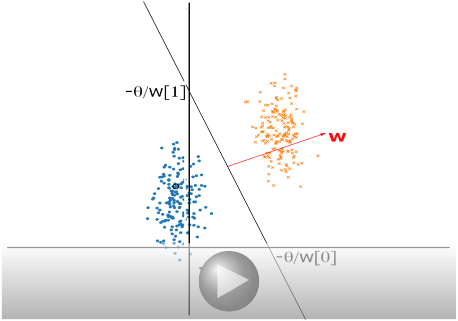
FIRST TRAINING ALGORITHM

Here, $\sigma(x) \in \{-1, 1\}$
Given a training set

$$Z = \{(\boldsymbol{x}_i, y_i), i \in [\![1 \cdots n]\!], \boldsymbol{x}_i \in \mathbb{R}^{d+1}, y_i \in \{-1, 1\}\}$$

this linear operator can be trained for a binary classification problem.

$\boldsymbol{w}^0 = \boldsymbol{0}$
$k = 0$
while $\exists i$ *such that* $y_i((\boldsymbol{w}^{\boldsymbol{k}})^T \boldsymbol{x}_i) \leq 0$ **do**
  $\boldsymbol{w}^{k+1} = \boldsymbol{w}^k + y_i \boldsymbol{x}_i$
  $k = k + 1$
end



FIRST TRAINING ALGORITHM

Convergence iff:

- Points lie in a sphere of radius R: $(\forall i \in [\![1 \cdots n]\!]) \ \|\boldsymbol{x}_i\| \leq R$
- The two classes can be separated by a margin:

$$\exists \tilde{\boldsymbol{w}}, \|\tilde{\boldsymbol{w}}\| = 1 \ \exists \gamma > 0, \ (\forall i \in [\![1 \cdots n]\!]) \ \ y_i(\tilde{\boldsymbol{w}}^T \boldsymbol{x}_i) \geq \gamma/2$$

If so, the perceptron stops as soon as it finds a separating hyperplane.

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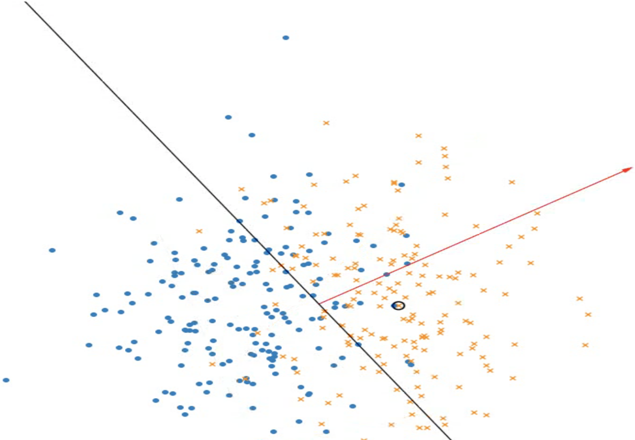
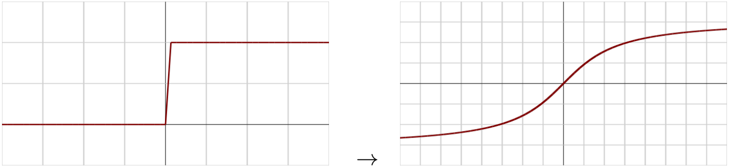
If so, the perceptron stops as soon as it finds a separating hyperplane. But what if the data is non linearly separable ?



Second training algorithm

One possible solution: minimize the amount of errors.

1. Change σ function to make it differentiable



2. Error

$$\ell(\boldsymbol{w}) = \sum_{(\boldsymbol{x},y)\in Z} \mathcal{L}\left(f_{\boldsymbol{w}}(\boldsymbol{x}), y\right)$$

3. Minimize the error w.r.t $\boldsymbol{w}$.

Second training algorithm

Gradient

At a local minimum the gradient is null: $\sum_{(\boldsymbol{x},y)\in Z} \nabla_{\boldsymbol{w}} \mathcal{L}\left(f_{\boldsymbol{w}}(\boldsymbol{x}), y\right) = \boldsymbol{0}$

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SECOND TRAINING ALGORITHM

Gradient

At a local minimum the gradient is null: $\sum_{(\boldsymbol{x},y)\in Z} \nabla_{\boldsymbol{w}} \mathcal{L}\left(f_{\boldsymbol{w}}(\boldsymbol{x}), y\right) = \mathbf{0}$

Gradient Descent Algorithm

1. Initialization: $\boldsymbol{w} = \boldsymbol{w}_0$, $k = 0$
2. While (non stop)

   2.1 $\boldsymbol{g}_k = \frac{1}{|Z|} \sum_{(\boldsymbol{x},y)\in Z} \nabla_{\boldsymbol{w}} \mathcal{L}\left(f_{\boldsymbol{w_k}}(\boldsymbol{x}), y\right)$

   2.2 $\boldsymbol{w}_{k+1} = \boldsymbol{w}_k - \eta \boldsymbol{g}_k$

   2.3 $k = k + 1$

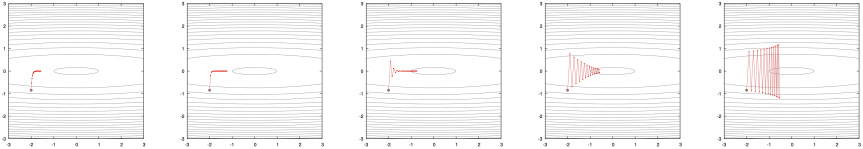
Additional ressource

See Slides “toy example” and “Optimization for deep Learning”.

SECOND TRAINING ALGORITHM

Algorithm parameters:

- stopping criterion
- η: learning rate
- Weight initialization



$\eta = 10^{-2}$ $\quad$ $\eta = 2.10^{-2}$ $\quad$ $\eta = 4.10^{-2}$ $\quad$ $\eta = 5.10^{-2}$ $\quad$ $\eta = 5.310^{-2}$

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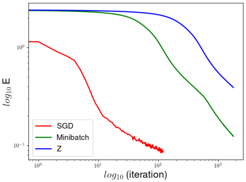
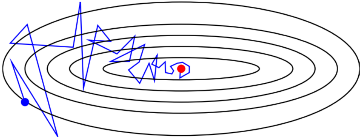
Second training algorithm

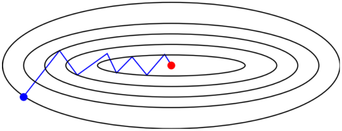
Different learning strategies

- Compute the error over all Z: real gradient descent
- Compute the error on one example only: stochastic gradient descent (SGD)
- Compute the error on a batch of example: batch learning (minibatch)





SGD



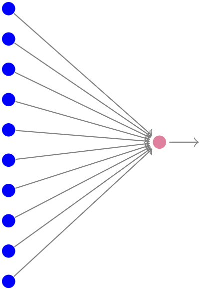
minibatch

But...
If we want to accurately classify the data (and allow a good generalization property), we need to find something else...

Stacking linear classifiers

A linear classifier of the form

$$\begin{aligned} f : \mathbb{R}^{d+1} &\rightarrow \mathbb{R} \\ \boldsymbol{x} &\mapsto \sigma(\boldsymbol{w}^T\boldsymbol{x} + b) \end{aligned}$$



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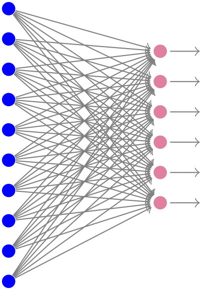
Stacking linear classifiers

A linear classifier of the form

$$\begin{aligned} f : \mathbb{R}^{d+1} &\rightarrow \mathbb{R} \\ \boldsymbol{x} &\mapsto \sigma(\boldsymbol{w}^T \boldsymbol{x} + b) \end{aligned}$$

can naturally be component-wise extended to any function $f : \mathbb{R}^{d+1} \rightarrow \mathbb{R}^c$



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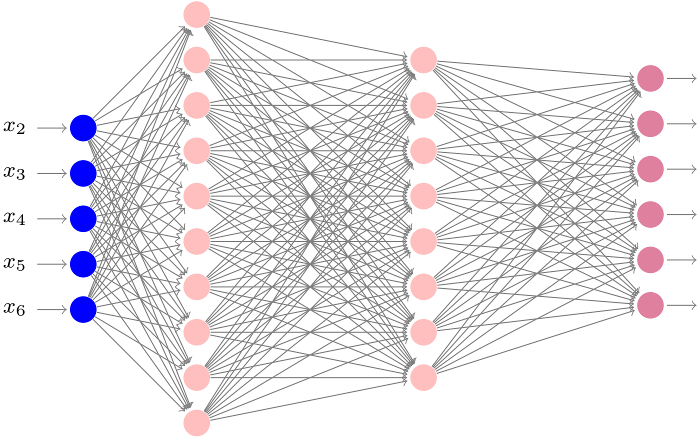
And even...



The general structure can be defined using $\boldsymbol{x}^{(0)} = \boldsymbol{x}$ and

$$(\forall l \in [\![1 \cdots L]\!]) \quad \boldsymbol{x}^{(l)} = \sigma({\boldsymbol{w}^{(l)}}^T \boldsymbol{x}^{(l-1)} + b^{(l)})$$

This is a *Multilayer Perceptron (MLP)*.

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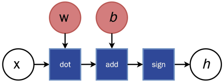
Building complex neural networks

$$h = \sigma(\boldsymbol{w}^T x + b)$$

$h \in \mathbb{R}$,
$\boldsymbol{w}, x \in \mathbb{R}^{d+1}$
$b \in \mathbb{R}$



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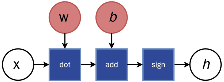
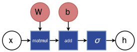


$$\xrightarrow{\text{Parallel composition}}$$

$$\boldsymbol{h} = \sigma(\boldsymbol{W}^T x + \boldsymbol{b})$$

$\boldsymbol{h} \in \mathbb{R}^q$
$\boldsymbol{W} \in \mathcal{M}_{d+1,q}(\mathbb{R})$
$\boldsymbol{b} \in \mathbb{R}^q$,
σ element-wise function



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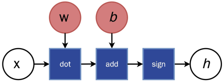

$\xrightarrow{\text{Parallel composition}}$

100× speed up

$$\boldsymbol{h} = \sigma(\boldsymbol{W}^T x + \boldsymbol{b})$$

$\boldsymbol{h} \in \mathbb{R}^q$
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$\boldsymbol{b} \in \mathbb{R}^q$,
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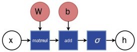
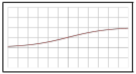
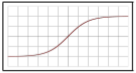
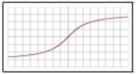
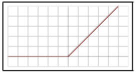
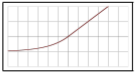


$\boldsymbol{h}$ is the output of a layer.

σ has to be non linear (otherwise equivalent to a perceptron).

Name	**Graph**	f	f'
Logistic / sigmoïd		$f(x) = \frac{1}{1+e^{-x}}$	$f'(x) = f(x)\left(1 - f(x)\right)$
tanh		$f(x) = \frac{2}{1+e^{-2x}} - 1$	$f'(x) = 1 - f^2(x)$
atan		$f(x) = \tan^{-1}(x)$	$f'(x) = \frac{1}{x^2+1}$
ReLU		$f(x) = \begin{cases} 0 & \text{if } x < 0 \\ x & \text{if } x \geq 0 \end{cases}$	$f'(x) = \begin{cases} 0 & \text{if } x \neq 0 \\ 1 & \text{if } x = 0 \end{cases}$
Linear exponential		$f(x) = \begin{cases} \alpha(e^x - 1) & \text{if } x < 0 \\ x & \text{if } x \geq 0 \end{cases}$	$f'(x) = \begin{cases} f(x) + \alpha & \text{if } x < 0 \\ 1 & \text{if } x \geq 0 \end{cases}$

Learning the MLP

Expanding the gradient descent

- At step k of the gradient descent, need to evaluate

$$\nabla_\theta \mathcal{L}\left(f_\theta(\boldsymbol{x}), y\right)$$

- Evaluation of the total derivatives $\frac{\partial \mathcal{L}}{\partial \boldsymbol{W}_j}$ and $\frac{\partial \mathcal{L}}{\partial \boldsymbol{b}_j}$, $j \in [\![1 \ldots L]\!]$

$\Rightarrow$ Automatic differentiation on the computational graph

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$\Rightarrow$ Automatic differentiation on the computational graph

Chain Rule

Let $g : \mathbb{R} \to \mathbb{R}^m$ and $f : \mathbb{R}^m \to \mathbb{R}$

$$f \circ g(x) = f(\boldsymbol{u}) = y \text{ where } \boldsymbol{u} = g(x) = (g_1(x) \dots g_m(x))^T = (u_1 \dots u_m)$$

Chain rule:

$$\frac{dy}{dx} = \sum_{j=1}^{m} \frac{\partial y}{\partial u_j} \underbrace{\frac{du_j}{dx}}_{\text{recursive}}$$

Learning the MLP

Automatic differentiation

- MLP = composition of differentiable functions
- The total derivatives of the loss can be evaluated backward, by applying the chain rule recursively over its computational graph.

LEARNING THE MLP

Automatic differentiation

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Automatic differentiation

1. Forward pass: values are all computed from inputs to outputs
2. Backward pass: the total derivatives are computed by walking through all paths from outputs to parameters in the computational graph and accumulating the terms.

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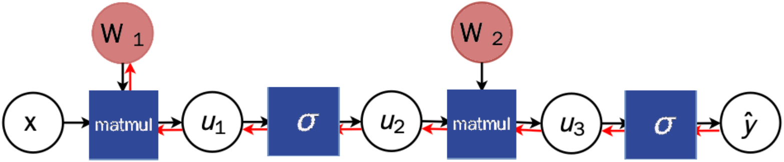
Additional ressource

See Slides “backpropagation” and “Vanishing gradient”.

Learning the MLP

Example: derivatives with respect to $\boldsymbol{W}_1$



1. Forward pass: $\boldsymbol{u}_1, \boldsymbol{u}_2, \boldsymbol{u}_3$ and $\hat{y}$ computed by traversing the graph, given $\boldsymbol{x}$,$\boldsymbol{W}_1$ and $\boldsymbol{W}_2$
2. Backward pass :

$$\begin{aligned}
\frac{d\hat{y}}{d\boldsymbol{W}_1} &= \frac{\partial \hat{y}}{\partial \boldsymbol{u}_3}\frac{\partial \boldsymbol{u}_3}{\partial \boldsymbol{u}_2}\frac{\partial \boldsymbol{u}_2}{\partial \boldsymbol{u}_1}\frac{\partial \boldsymbol{u}_1}{\partial \boldsymbol{W}_1} \\
&= \frac{\partial \sigma(\boldsymbol{u}_3)}{\partial \boldsymbol{u}_3}\frac{\partial \boldsymbol{W}_2^T u_2}{\partial \boldsymbol{u}_2}\frac{\partial \sigma(\boldsymbol{u}_1)}{\partial \boldsymbol{u}_1}\frac{\partial \boldsymbol{W}_1^T u_1}{\partial \boldsymbol{W}_1}
\end{aligned}$$

Evaluating the partial derivatives requires the intermediate values computed forward

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Universal approximation

Theorem (Cybenko 1989; Hornik et al, 1991)

Let σ be a bounded, non-constant continuous function.
Let I_d denote the d-dimensional hypercube, and $C(I_d)$ denote the space of continuous functions on I_d.

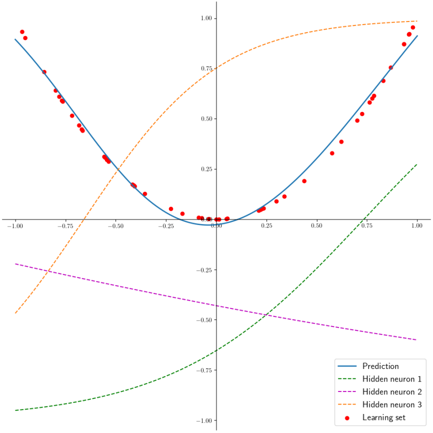
$(\forall f \in C(I_d))(\forall \epsilon > 0)(\exists q > 0, v_i, \mathbf{w_i}, b_i, i \in [\![1 \ldots q]\!])$ such that

$$F(\mathbf{x}) = \sum_{i=1}^{q} v_i \sigma(\mathbf{w}^{\mathbf{T}}\mathbf{x} + b)$$

satisfies

$$\sup_{\mathbf{x} \in I_d} \mid f(\mathbf{x}) - F(\mathbf{x}) \mid < \epsilon$$

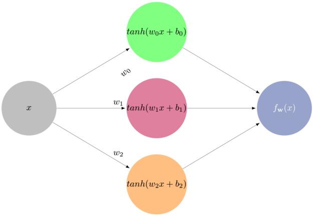
Universal approximation



$f(x) = x^2, |Z| = 50$

A simple example

- $|Z|$ points uniformly sampled (red) over the definition set
- 1 hidden layer MLP, 3 neurons.
- $tanh$ activation function, and linear output neurons
- network output : blue curve
- hidden neurons outputs: dashed curves



Universal approximation

Properties

- Guarantees that a single hidden layer network can represent any classification problem in which the boundary is locally linear (smooth)
- Does not inform about good/bad architectures, nor how they relate to the optimization procedure
- Generalizes to any non-polynomial (possibly unbounded) activation function, including the ReLU

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Universal approximation

Theorem (Barron, 1992)

Let a one-hidden layer MLP with q hidden neurons , p inputs and $|Z| = n$. The mean integrated square error between the estimated network $\hat{F}$ and the target function f is bounded by

$$O\left(\frac{C_f^2}{q} + \frac{qp}{n} log(n)\right)$$

where C_f measures the global smoothness of f.

Properties

- Combines approximation and estimation errors.
- Provided enough data, guarantees that adding more neurons will result in a better approximation

Effect of depth

Theorem (Montúfar et al, 2014)

A MLP with ReLU as activation functions, p inputs, L hidden layers with $q \geq p$ neurons can compute functions having $\Omega\left(\left(\frac{q}{p}\right)^{(L-1)p} q^p\right)$ linear regions (asymptotic lower bound).

Properties

- The number of linear regions of deep models grows exponentially in L and polynomially in q.
- Even for small values of L and q, deep rectifier models are able to produce substantially more linear regions than shallow rectifier models.

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