4AI10 - Machine Learning

Introduction to Neural Networks and Deep Learning

Matthieu Labeau, Enzo Tartaglione

Outline

- Introduction
- The formal neuron and Perceptron
- Probabilistic Learning
- From Perceptron to Multi-Layer Perceptron
- Deep Learning

Machine Learning

Reminder: Tom Mitchell's definition (*Machine Learning,* 1997)

A computer program is said to learn

- from **experience** *E*
- with respect to some class of **tasks** *T*
- and **performance** measure *P*

if its performance at tasks in *T*, as measured by *P*, improves with experience *E.*

Machine Learning

Reminder: Tom Mitchell's definition (*Machine Learning,* 1997)

A computer program is said to learn

- from **experience** *E*
- with respect to some class of **tasks** *T*
- and **performance** measure *P*

if its performance at tasks in *T*, as measured by *P*, improves with experience *E.*

- Tasks: *Classification*, *Regression*... and many others

Machine Learning

Reminder: Tom Mitchell's definition (*Machine Learning,* 1997)

A computer program is said to learn

- from **experience** *E*
- with respect to some class of **tasks** *T*
- and **performance** measure *P*

if its performance at tasks in *T*, as measured by *P*, improves with experience *E.*

- Tasks: *Classification*, *Regression*... and many others
- Performance: For example, *Accuracy* - but can be tricky to choose !

Supervised vs *Unsupervised* Learning

Experience: What kind of *dataset* do you have ?

Supervised vs *Unsupervised* Learning

Dataset X: collection of n *data points* $(\mathbf{x}_i)_{i=1}^n \in \mathbb{R}^d$

Supervised vs *Unsupervised* Learning

Dataset X: collection of n *data points* $(\mathbf{x}_i)_{i=1}^n \in \mathbb{R}^d$

$\rightarrow$ Each consisting of d *features* $(x_i^j)_{j=1}^d \in \mathbb{R}$

Supervised vs *Unsupervised* Learning

Dataset X: collection of n *data points* $(\mathbf{x}_i)_{i=1}^n \in \mathbb{R}^d$

With *Supervised* learning, each data point $\mathbf{x}_i$ is associated with a *label* or *target* y_i.

- We learn a function that can predict y_i from $\mathbf{x}_i$.

Supervised vs *Unsupervised* Learning

Dataset X: collection of n *data points* $(\mathbf{x}_i)_{i=1}^n \in \mathbb{R}^d$

With *Supervised* learning, each data point $\mathbf{x}_i$ is associated with a *label* or *target* y_i.

- We learn a function that can predict y_i from $\mathbf{x}_i$.

With *Unsupervised* learning, we don't have labels.

- We try to make sense of the $\mathbf{x}_i$
- It can be with *clustering*, or by learning the *probability distribution* that generated them

Supervised vs *Unsupervised* Learning

Supervised vs *Unsupervised* Learning

Supervised and *Unsupervised* learning are rough categories, and are **not formal**.

- Other variants are possible: for example, *Semi-supervised* learning
- Datasets are not necessarily fixed: for example, with *Reinforcement* learning

Supervised vs *Unsupervised* Learning

Supervised and *Unsupervised* learning are rough categories, and are **not formal**.

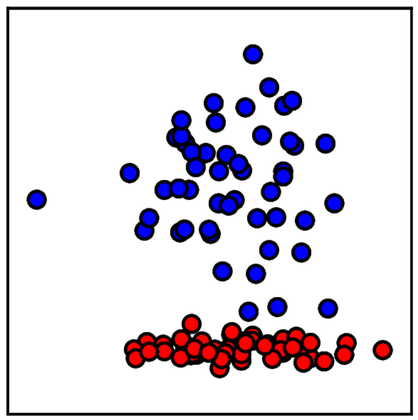
- Other variants are possible: for example, *Semi-supervised* learning
- Datasets are not necessarily fixed: for example, with *Reinforcement* learning

→ Neural networks and Deep learning can be used for all these variants !

Back to (supervised) binary classification

Data points $\mathbf{x}_i \in \mathbb{R}^2$ with labels $y_i \in \{0, 1\}$

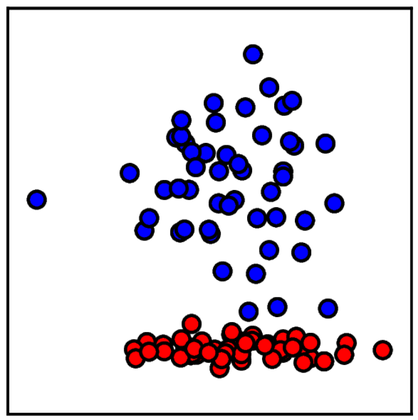
$\rightarrow$ Learn a function $f(\mathbf{x}_i)$ able to predict y_i



Back to (supervised) binary classification

Data points $\mathbf{x}_i \in \mathbb{R}^2$ with labels $y_i \in \{0, 1\}$

$\rightarrow$ Learn a function $f(\mathbf{x}_i)$ able to predict y_i



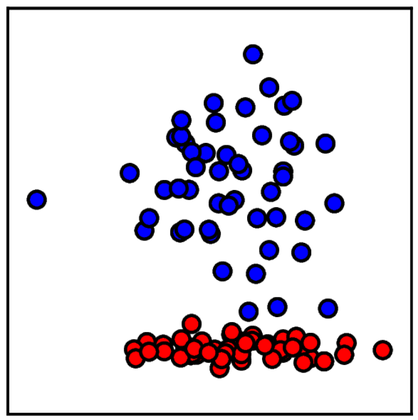
Reminder: **Generative approach**

- How can we model the joint distribution $p(\mathbf{x}_i, y_i)$ of the features and classes ?

Back to (supervised) binary classification

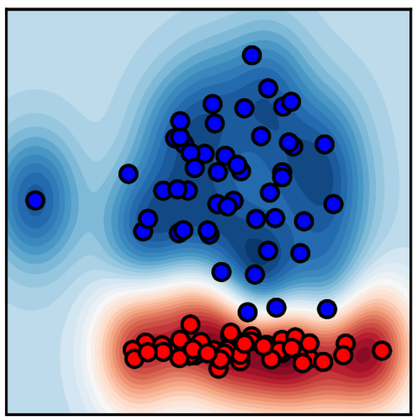
Data points $\mathbf{x}_i \in \mathbb{R}^2$ with labels $y_i \in \{0, 1\}$

$\rightarrow$ Learn a function $f(\mathbf{x}_i)$ able to predict y_i



Reminder: **Generative approach**

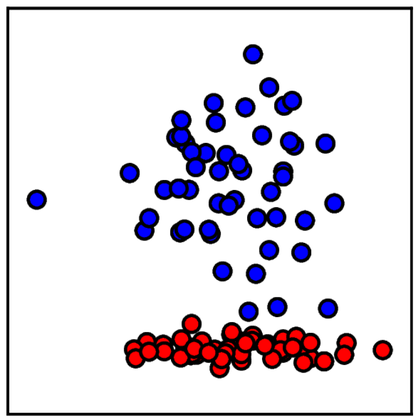
- How can we model the joint distribution $p(\mathbf{x}_i, y_i)$ of the features and classes ?
- Using the estimated $\hat{p}(\mathbf{x}_i | y_i)$ and prior probalities !



Back to (supervised) binary classification

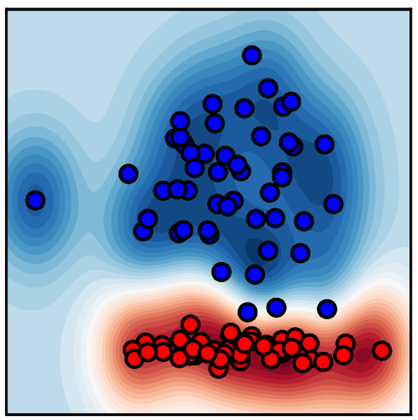
Data points $\mathbf{x}_i \in \mathbb{R}^2$ with labels $y_i \in \{0, 1\}$

$\rightarrow$ Learn a function $f(\mathbf{x}_i)$ able to predict y_i



Reminder: **Generative approach**

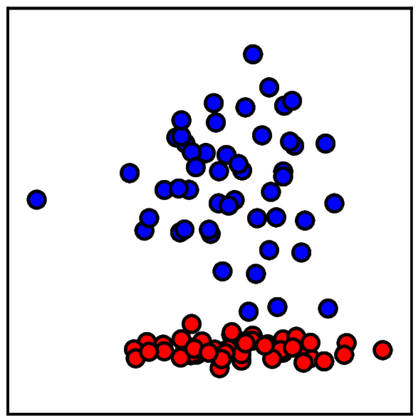
- How can we model the joint distribution $p(\mathbf{x}_i, y_i)$ of the features and classes ?
- Examples: Naïve Bayes, Generative/Hidden Markov Models



Back to (supervised) binary classification

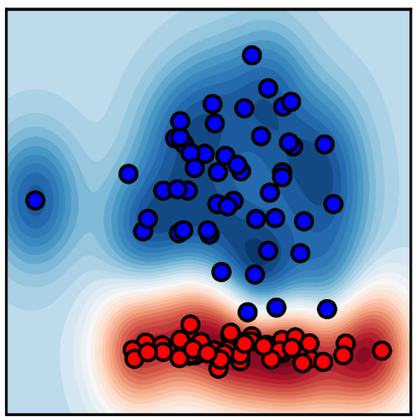
Data points $\mathbf{x}_i \in \mathbb{R}^2$ with labels $y_i \in \{0, 1\}$

$\rightarrow$ Learn a function $f(\mathbf{x}_i)$ able to predict y_i



Reminder: **Generative approach**

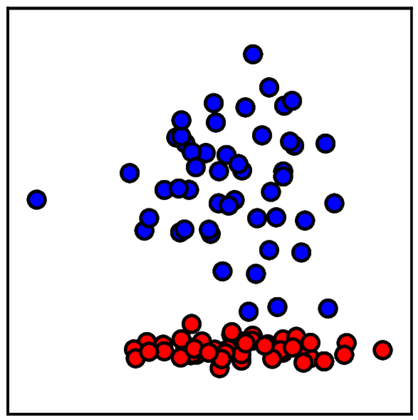
- How can we model the joint distribution $p(\mathbf{x}_i, y_i)$ of the features and classes ?
- Examples: Naïve Bayes, Generative/Hidden Markov Models



Back to (supervised) binary classification

Data points $\mathbf{x}_i \in \mathbb{R}^2$ with labels $y_i \in \{0, 1\}$

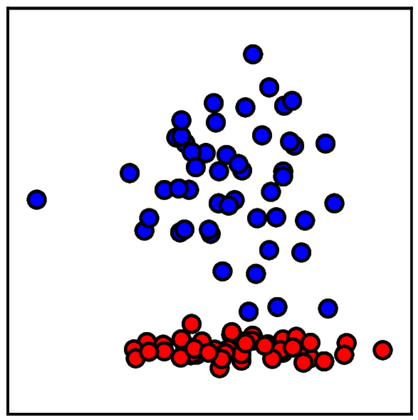
$\rightarrow$ Learn a function $f(\mathbf{x}_i)$ able to predict y_i



Back to (supervised) binary classification

Data points $\mathbf{x}_i \in \mathbb{R}^2$ with labels $y_i \in \{0, 1\}$

$\rightarrow$ Learn a function $f(\mathbf{x}_i)$ able to predict y_i



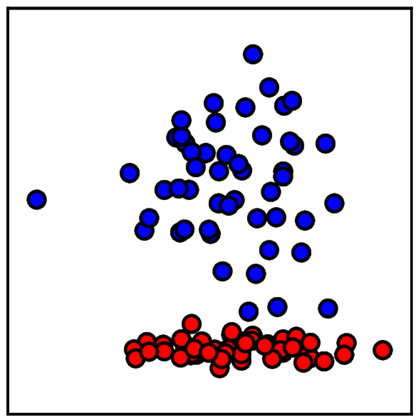
Reminder: **Discriminative approach**

- Which features x_i^j can allow us to distinguish between the classes ?

Back to (supervised) binary classification

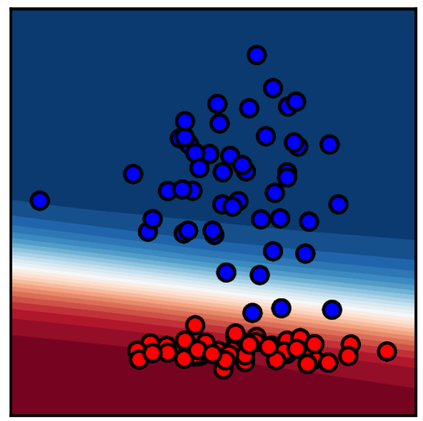
Data points $\mathbf{x}_i \in \mathbb{R}^2$ with labels $y_i \in \{0, 1\}$

$\rightarrow$ Learn a function $f(\mathbf{x}_i)$ able to predict y_i



Reminder: **Discriminative approach**

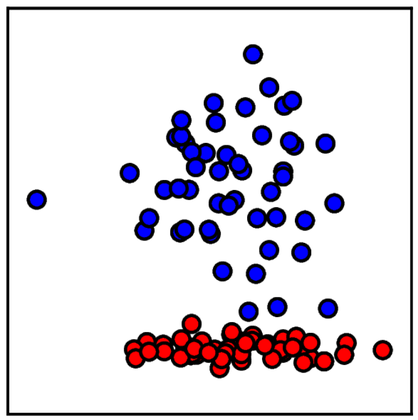
- Which features x_i^j can allow us to distinguish between the classes ?
- It means finding a boundary between the classes - which can be by computing $p(y_i|\mathbf{x}_i)$



Back to (supervised) binary classification

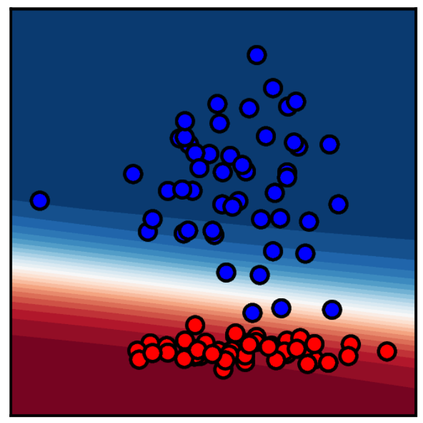
Data points $\mathbf{x}_i \in \mathbb{R}^2$ with labels $y_i \in \{0, 1\}$

$\rightarrow$ Learn a function $f(\mathbf{x}_i)$ able to predict y_i



Reminder: **Discriminative approach**

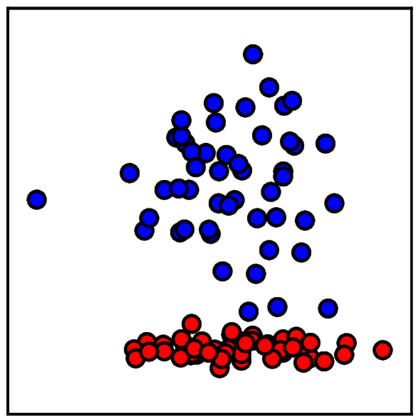
- Which features x_i^j can allow us to distinguish between the classes ?
- Examples: Decision trees, SVM



Back to (supervised) binary classification

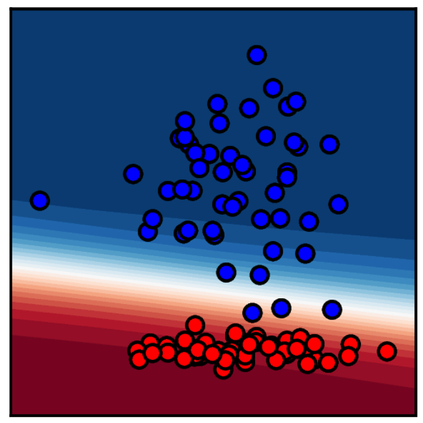
Data points $\mathbf{x}_i \in \mathbb{R}^2$ with labels $y_i \in \{0, 1\}$

$\rightarrow$ Learn a function $f(\mathbf{x}_i)$ able to predict y_i



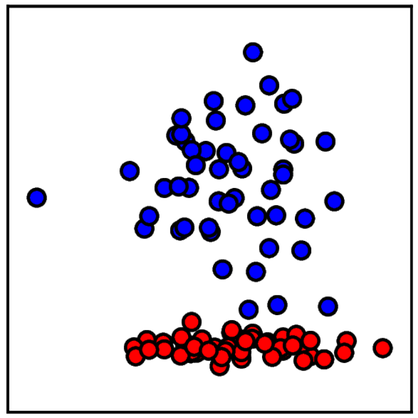
Reminder: **Discriminative approach**

- Which features x_i^j can allow us to distinguish between the classes ?
- Examples: Decision trees, SVM



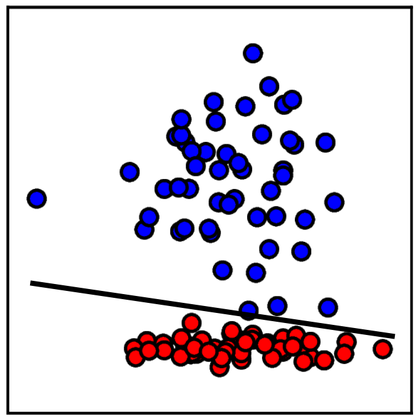
Simple Discriminative classification : Perceptron

Reminder: When the classes are linearly separable, we are looking for a **separating hyperplane** !



Simple Discriminative classification : Perceptron

Reminder: When the classes are linearly separable, we are looking for a **separating hyperplane** !

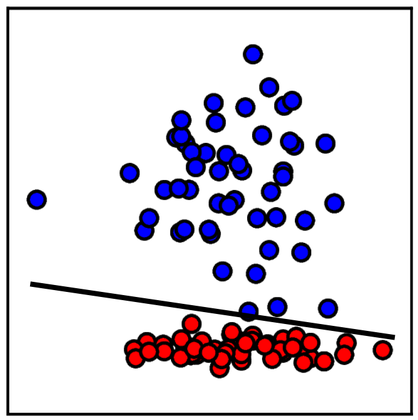


Such an hyperplane is defined by the equation:

$$\mathbf{w}^T\mathbf{x} + b = 0$$

Simple Discriminative classification : Perceptron

Reminder: When the classes are linearly separable, we are looking for a **separating hyperplane** !



Such an hyperplane is defined by the equation:

$$\mathbf{w}^T\mathbf{x} + b = 0$$

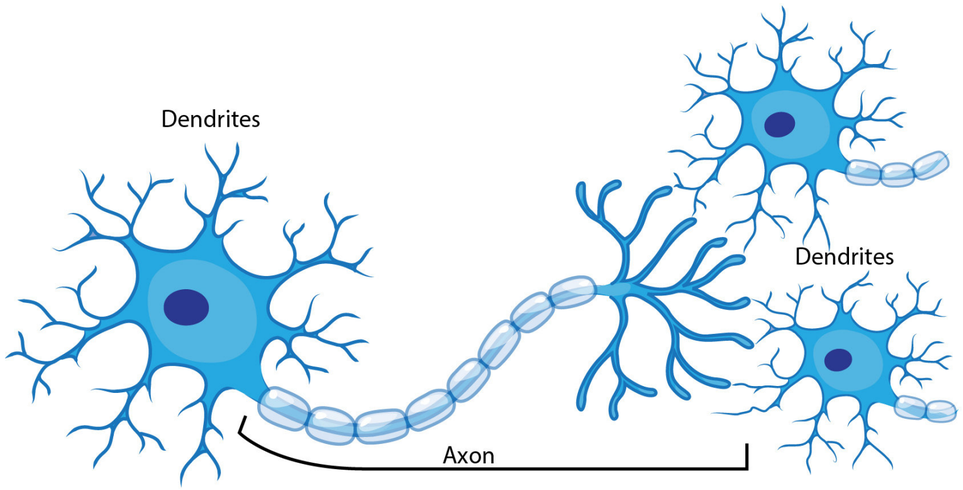
We then have a simple model, called the **Perceptron**, giving the class *y*:

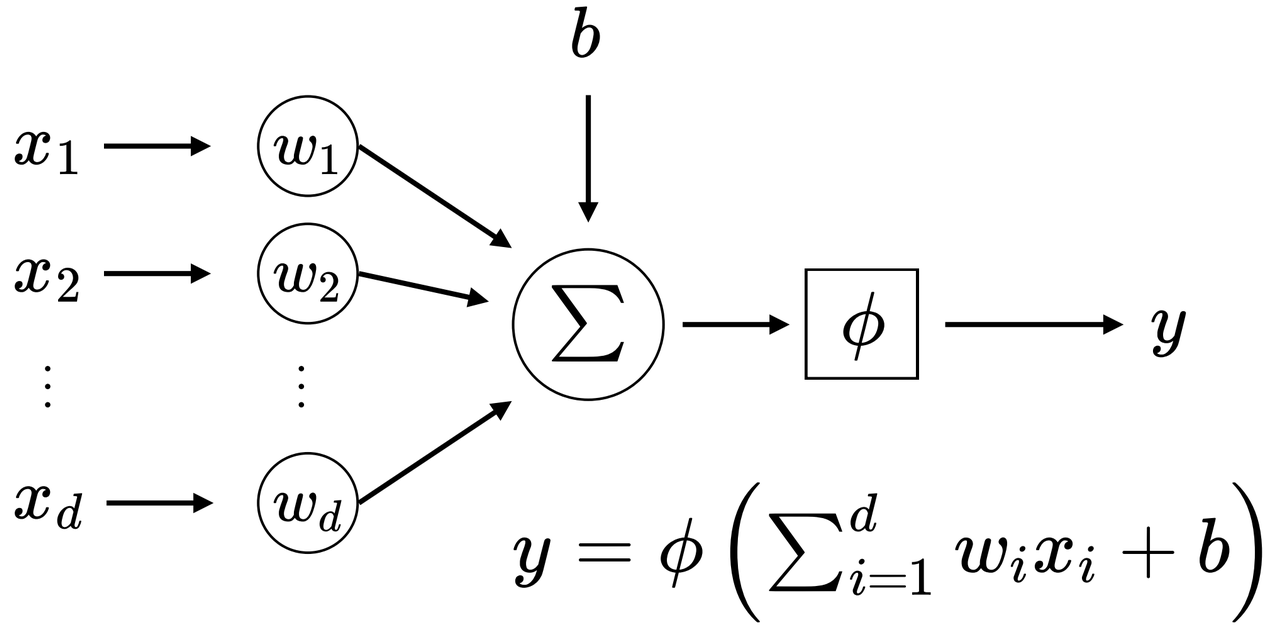
$$\hat{y}_i = f(\mathbf{x}_i, \theta) = sign(\mathbf{w}^T\mathbf{x}_i + b)$$

where $\theta = \{\mathbf{w}, b\}$ are the parameters of the model.

Note: here, $y_i \in -1, 1$ by convienence - for as long as we use the $sign$ function.

Artificial and biological Neurons





- First proposed to model the **activity of a neuron** by physiologists McCullogh and Pitts (*A logical calculus of the ideas immanent in nervous activity*, 1943)
- The inputs signal is processed by **weighted** synapses, firing if the weighted sum of the components is above a **threshold**

Perceptron: Learning Rule

Proposed by Rosenblatt (*The Perceptron—a perceiving and recognizing automaton*, 1958), with a **learning rule**

$\rightarrow$ Allows to **update** the boundary when new examples are introduced

Perceptron learning procedure:

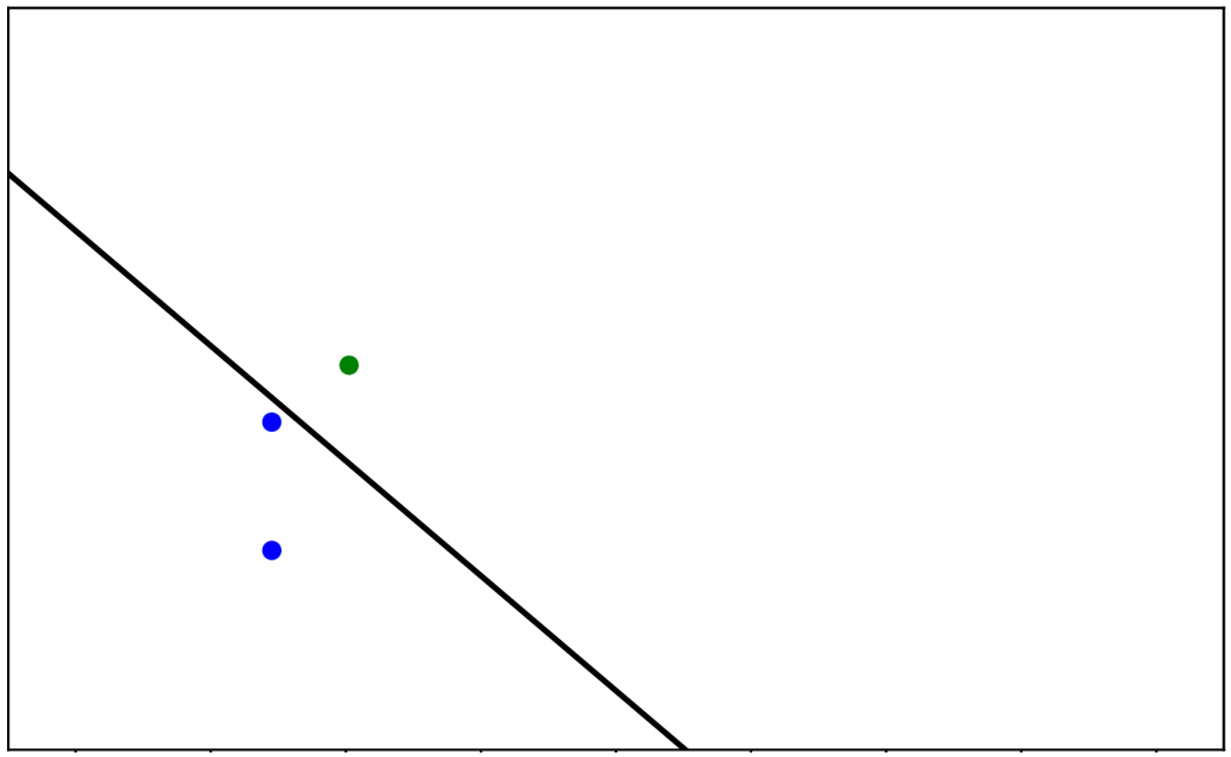
- Start with $t = 1$, $\mathbf{w}_t = 0$, and examples $(\mathbf{x}_i, y_i)_{i=1}^n$ such as $||\mathbf{x}_i|| = 1$
- While the model makes mistakes:
  - For $i \in [1, n]$:
    - Predict $\hat{y}_i = sign(\mathbf{w}^T \mathbf{x}_i)$
    - If $y_i \neq \hat{y}_i$ do $\mathbf{w}_{t+1} = \mathbf{w}_t + sign(y_i)\mathbf{x}$

Note: we include the bias b in $\mathbf{w}$

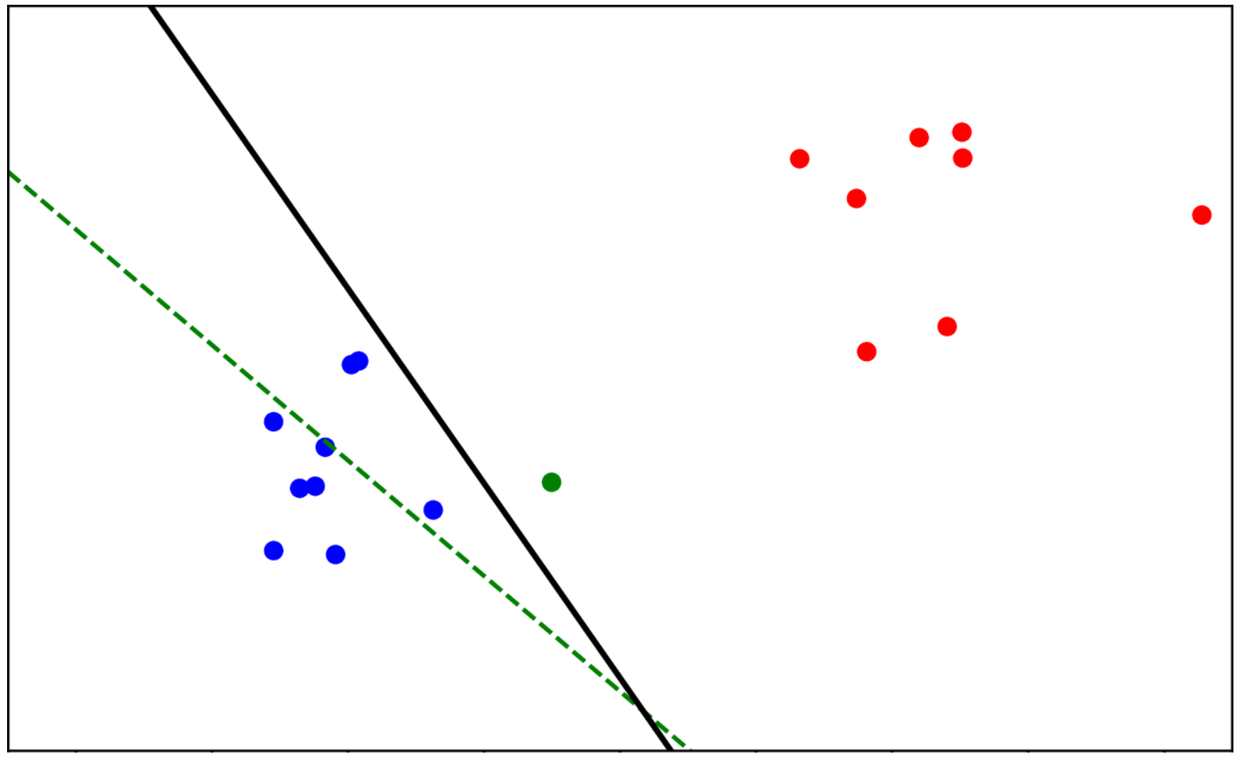
Perceptron: Learning Rule

Perceptron: Learning Rule

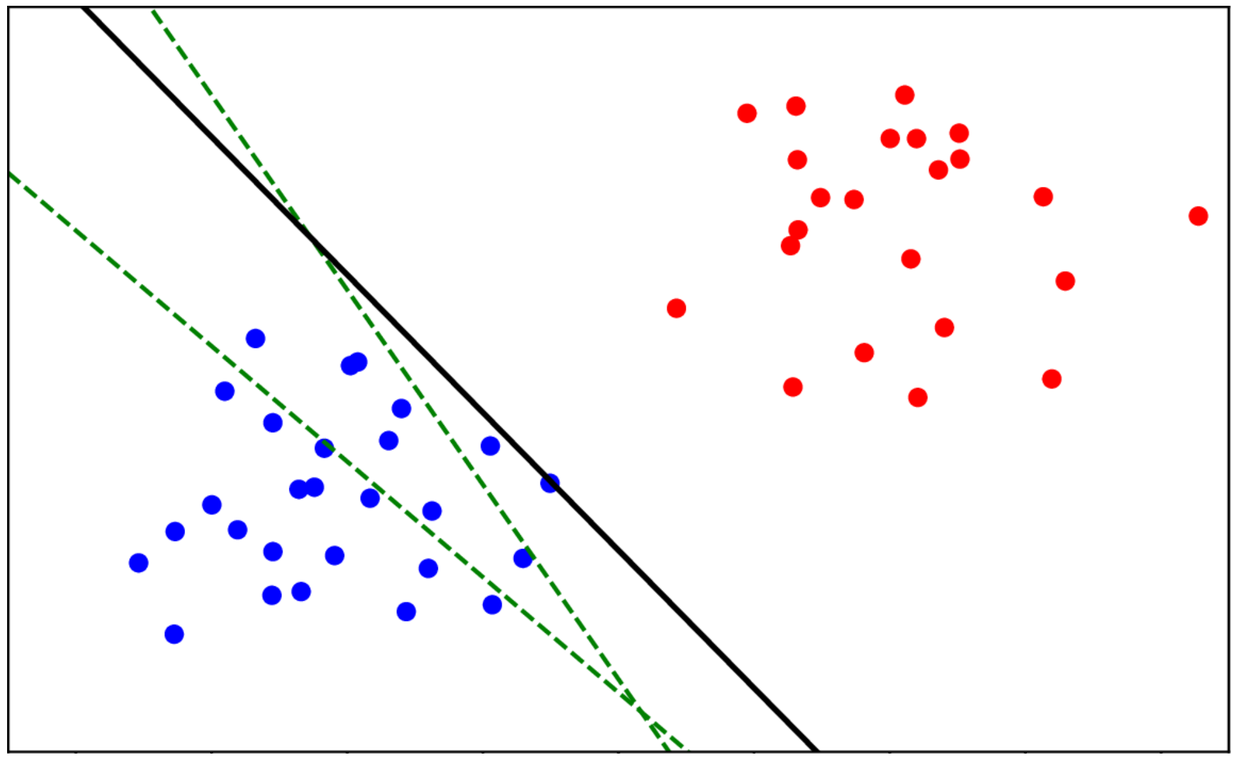
Perceptron: Learning Rule



Perceptron: Learning Rule



Perceptron: Learning Rule



Perceptron: Convergence

The algorithm converges if the classes are exactly **linearly separable**. More formally:

Convergence theorem:

Let us assume that there exists a parameter $\mathbf{w}^*$ such that $||\mathbf{w}^*|| = 1$ and note $\gamma > 0$ such that:

$$\forall i \in [1, n], \qquad y_i \times (\mathbf{x}_i^T \mathbf{w}^*) \geq \gamma$$

and $\exists R > 0$ such that:

$$||\mathbf{x}_i|| \leq R$$

Then the perceptron algorithm converges in at most $\frac{R^2}{\gamma^2}$ iterations

Perceptron: Proof of convergence

Main ideas:

- Linear separability implies the existence of $\mathbf{w}^*$
- γ represents the margin
- R is the maximum norm of an input vector

$\rightarrow$ With both these quantities, we can bound the amount of change $\mathbf{w}^t$ undergoes after t updates, and therefore obtain a maximum number of iterations after which it separates the classes.

$\rightarrow$ The proof is made by reccurence.

Perceptron: Limitations

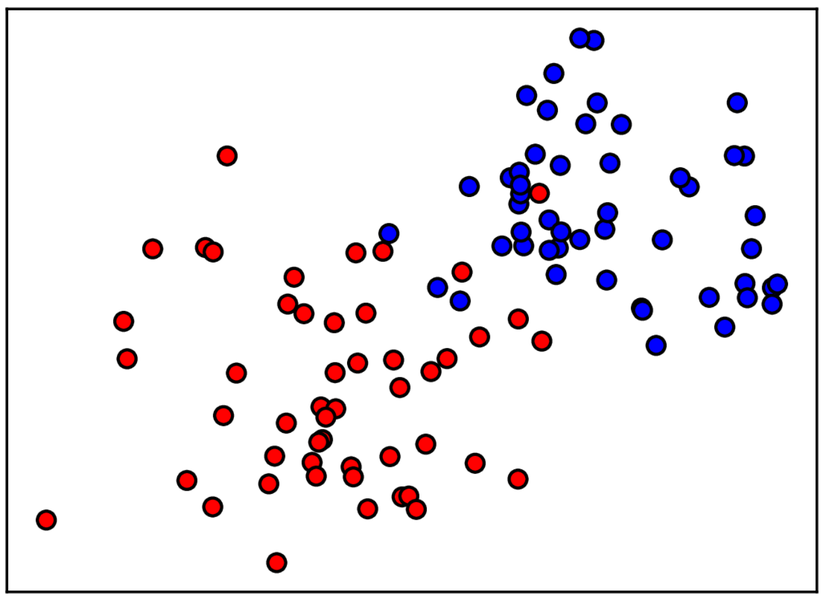
- **Quality of the boundary:** That's what SVM are made for (designed around maximizing a *margin* !)
- **Case of Non-linear separability:**
  - The data is *almost* linearly separable: for example, because of noise.

  $\rightarrow$ The *Bayes classifier* (*classifier minimizing the probability of misclassification*) is still an hyperplane

Perceptron: Limitations

- **Quality of the boundary:** That's what SVM are made for (designed around maximizing a *margin* !)
- **Case of Non-linear separability:**
  - The data is *almost* linearly separable: for example, because of noise.

  $\rightarrow$ The *Bayes classifier* (*classifier minimizing the probability of misclassification*) is still an hyperplane

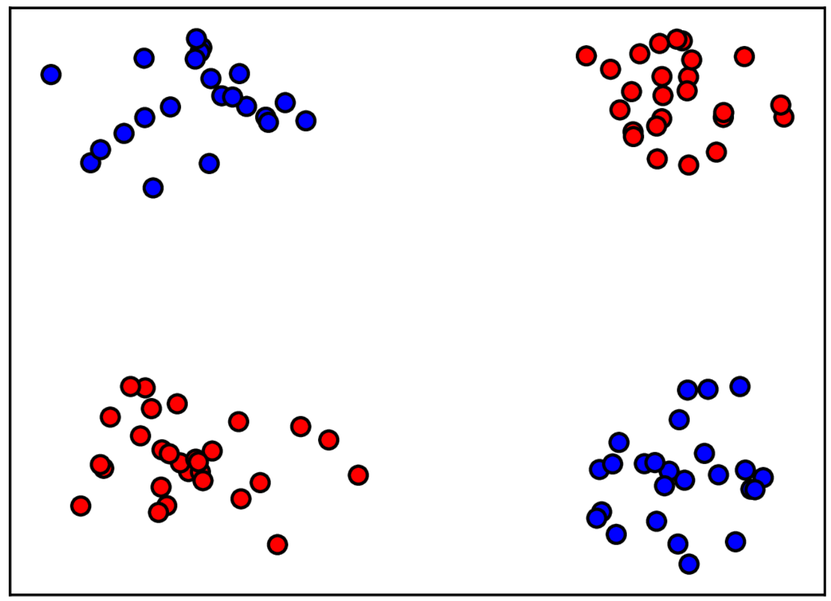


Perceptron: Limitations

- **Quality of the boundary:** That's what SVM are made for (designed around maximizing a *margin* !)
- **Case of Non-linear separability:**
  - The data is *almost* linearly separable: for example, because of noise.
    $\rightarrow$ The *Bayes classifier* (*classifier minimizing the probability of misclassification*) is still an hyperplane
  - The data is not linearly separable.
    $\rightarrow$ The *Bayes classifier* is not an hyperplane

Perceptron: Limitations

- **Quality of the boundary:** That's what SVM are made for (designed around maximizing a *margin* !)
- **Case of Non-linear separability:**
  - The data is *almost* linearly separable: for example, because of noise.
    $\rightarrow$ The *Bayes classifier* (*classifier minimizing the probability of misclassification*) is still an hyperplane
  - The data is not linearly separable.
    $\rightarrow$ The *Bayes classifier* is not an hyperplane



Perceptron: Loss function

What do we need ?

Perceptron: Loss function

What do we need ?

- Be able to deal with uncertainty: quantify how happy we are with the scores given by the model across the dataset with a **loss function**

Perceptron: Loss function

What do we need ?

- Be able to deal with uncertainty: quantify how happy we are with the scores given by the model across the dataset with a **loss function**
- Efficiently find the parameters that minimize this loss function (*optimization*)

Perceptron: Loss function

What do we need ?

- Be able to deal with uncertainty: quantify how happy we are with the scores given by the model across the dataset with a **loss function**
- Efficiently find the parameters that minimize this loss function (*optimization*)

Given a dataset $(\mathbf{x}_i, y_i)_{i=1}^n$, a loss function l tells us how good our classifier is by being averaged over all examples:

$$l((\mathbf{x}_i, y_i)_{i=1}^n | \mathbf{w}) = \frac{1}{n} \sum_{i=1}^{n} l_i(\hat{y}_i, y_i) = \frac{1}{n} \sum_{i=1}^{n} l_i((f(\mathbf{x}_i, \mathbf{w}), y_i)$$

Perceptron: Loss function

What do we need ?

- Be able to deal with uncertainty: quantify how happy we are with the scores given by the model across the dataset with a **loss function**
- Efficiently find the parameters that minimize this loss function (*optimization*)

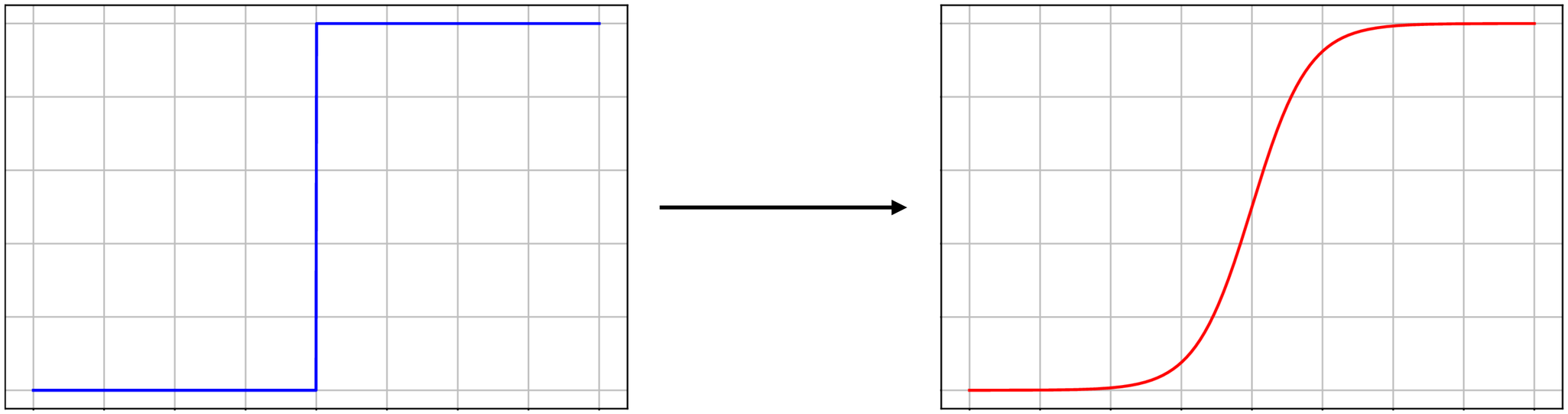
Given a dataset $(\mathbf{x}_i, y_i)_{i=1}^n$, a loss function l tells us how good our classifier is by being averaged over all examples:

$$l((\mathbf{x}_i, y_i)_{i=1}^n | \mathbf{w}) = \frac{1}{n} \sum_{i=1}^{n} l_i(\hat{y}_i, y_i) = \frac{1}{n} \sum_{i=1}^{n} l_i((f(\mathbf{x}_i, \mathbf{w}), y_i)$$

We have seen:

- The zero-one loss: $|y - sign(f(\mathbf{x}, \mathbf{w}))|$
- The hinge loss: $\max(0, 1 - y \cdot f(\mathbf{x}, \mathbf{w}))$
- The MSE loss: $(y - f(\mathbf{x}, \mathbf{w}))^2$

Probabilistic Learning



First, replace the $sign$ function by the *differentiable* $sigmoid$ function:

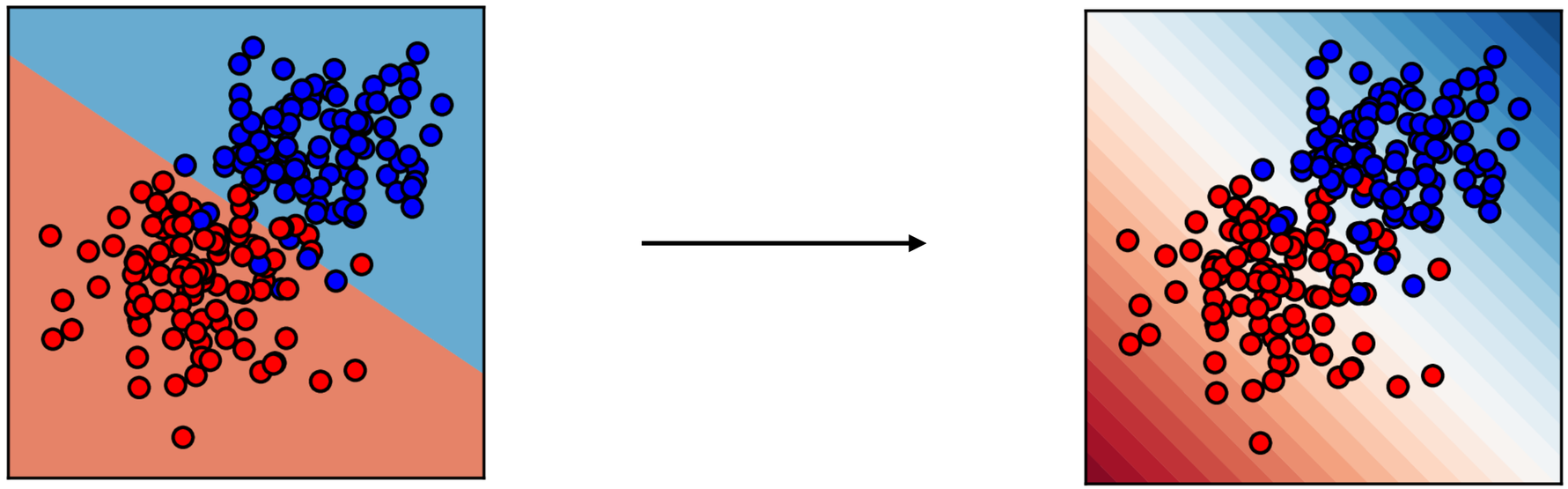
$$\sigma(x) = \frac{\exp(x)}{1+\exp(x)} = \frac{1}{1+\exp(-x)}$$

Probabilistic Learning

First, replace the $sign$ function by the *differentiable* $sigmoid$ function:

$$\sigma(x) = \frac{\exp(x)}{1 + \exp(x)} = \frac{1}{1 + \exp(-x)}$$

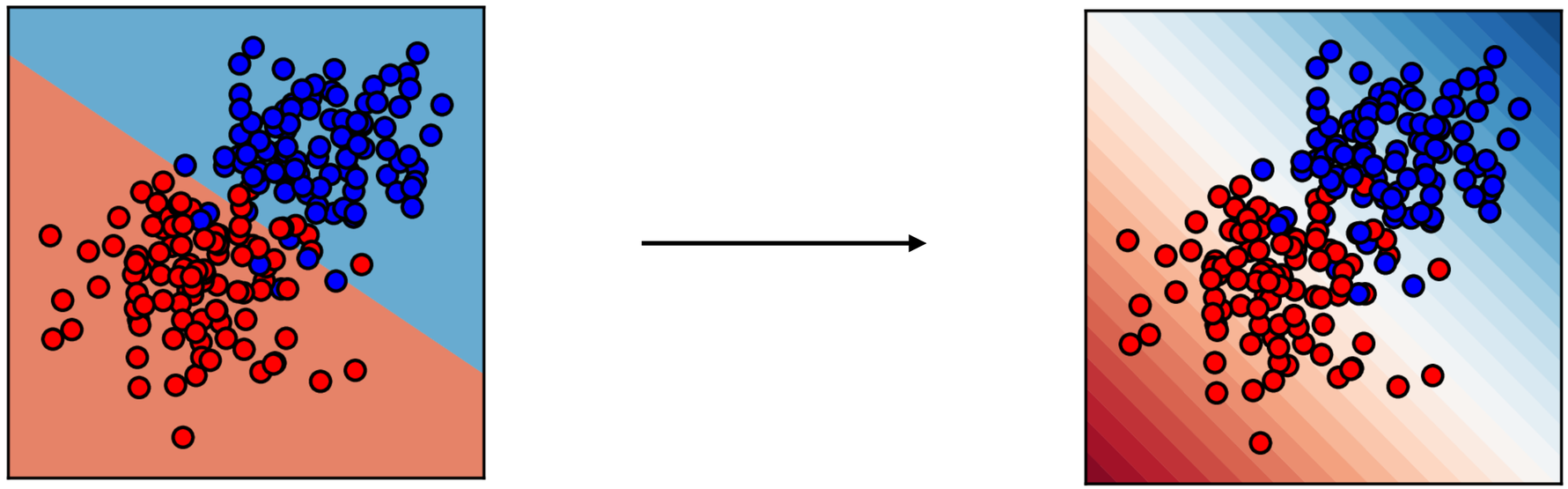
Probabilistic Learning



First, replace the $sign$ function by the *differentiable* $sigmoid$ function:

$$\sigma(x) = \frac{\exp(x)}{1+\exp(x)} = \frac{1}{1+\exp(-x)}$$

Probabilistic Learning



First, replace the $sign$ function by the *differentiable* $sigmoid$ function:

$$\sigma(x) = \frac{\exp(x)}{1+\exp(x)} = \frac{1}{1+\exp(-x)}$$

We now have the following function:

$$\hat{y}_i = f(\mathbf{x}_i, \mathbf{w}) = \sigma(\mathbf{w}^T \mathbf{x}_i)$$

where $\hat{y}_i \in [0,1]$ has a *probabilistic interpretation* as $\hat{P}(y_i = 1 | \mathbf{x}_i, \theta)$.

(Remember: θ is the set of *parameters* of the model, here being $\mathbf{w}$)

Now, how do we get the **probabilistic loss function** ?

Probabilistic Learning with MLE

→ **Maximum Likelihood Estimation (MLE)**

Probabilistic Learning with MLE

$\rightarrow$ Maximum Likelihood Estimation (MLE)

Under our interpretation, the (conditional) *likelihood* of our data $(\mathbf{x}_i, y_i)_{i=1}^n$ according to our model parameters θ is written:

$$\mathcal{L}((\mathbf{x}_i, y_i)_{i=1}^n | \theta) = \prod_{i=1}^n \hat{P}(y_i = 1 | \mathbf{x}_i, \theta)^{y_i} \hat{P}(y_i = 0 | \mathbf{x}_i, \theta)^{1-y_i}$$

Probabilistic Learning with MLE

$\rightarrow$ Maximum Likelihood Estimation (MLE)

Under our interpretation, the (conditional) *likelihood* of our data $(\mathbf{x}_i, y_i)_{i=1}^n$ according to our model parameters θ is written:

$$\mathcal{L}((\mathbf{x}_i, y_i)_{i=1}^n | \theta) = \prod_{i=1}^{n} \hat{P}(y_i = 1 | \mathbf{x}_i, \theta)^{y_i} \hat{P}(y_i = 0 | \mathbf{x}_i, \theta)^{1-y_i}$$

$$= \prod_{i=1}^n f(\mathbf{x}_i, \mathbf{w})^{y_i} \left(1 - f(\mathbf{x}_i, \mathbf{w})\right)^{1-y_i}$$

Probabilistic Learning with MLE

$\rightarrow$ Maximum Likelihood Estimation (MLE)

Under our interpretation, the (conditional) *likelihood* of our data $(\mathbf{x}_i, y_i)_{i=1}^n$ according to our model parameters θ is written:

$$\mathcal{L}((\mathbf{x}_i, y_i)_{i=1}^n | \theta) = \prod_{i=1}^{n} \hat{P}(y_i = 1 | \mathbf{x}_i, \theta)^{y_i} \hat{P}(y_i = 0 | \mathbf{x}_i, \theta)^{1-y_i}$$

$$= \prod_{i=1}^n f(\mathbf{x}_i, \mathbf{w})^{y_i} (1 - f(\mathbf{x}_i, \mathbf{w}))^{1-y_i}$$

You can compare this to the likelihood of success of a sequence of n Bernouilli trials with a varying probability p_i:

$$\prod_{i=1}^{n} p_i^{y_i} (1 - p_i)^{1-y_i}$$

but the **continuity** of our function f will force similar inputs $\mathbf{x}_i$ to have similar output probabilities !

Probabilistic Learning with MLE

$\rightarrow$ We are looking for the θ that will **maximize this likelihood**:

$$\hat{\theta} = \text{argmax}_\theta \; \mathcal{L}((\mathbf{x}_i, y_i)_{i=1}^n | \theta) = \; \text{argmax}_\theta \prod_{i=1}^{n} f(\mathbf{x}_i, \mathbf{w})^{y_i} (1 - f(\mathbf{x}_i, \mathbf{w}))^{1-y_i}$$

Probabilistic Learning with MLE

$\rightarrow$ We are looking for the θ that will **maximize this likelihood**:

$$\hat{\theta} = \text{argmax}_\theta \; \mathcal{L}((\mathbf{x}_i, y_i)_{i=1}^n | \theta) = \; \text{argmax}_\theta \prod_{i=1}^{n} f(\mathbf{x}_i, \mathbf{w})^{y_i} (1 - f(\mathbf{x}_i, \mathbf{w}))^{1-y_i}$$

The equivalent but more convenient optimization problem is to maximize the **log**-likelihood:

$$\log \mathcal{L}((\mathbf{x}_i, y_i)_{i=1}^n | \theta) = \sum_{i=1}^{n} y_i \log f(\mathbf{x}_i, \mathbf{w}) + (1 - y_i) \log(1 - f(\mathbf{x}_i, \mathbf{w}))$$

Probabilistic Learning with MLE

$\rightarrow$ We are looking for the θ that will **maximize this likelihood**:

$$\hat{\theta} = \text{argmax}_\theta \ \mathcal{L}((\mathbf{x}_i, y_i)_{i=1}^n|\theta) = \ \text{argmax}_\theta \prod_{i=1}^{n} f(\mathbf{x}_i, \mathbf{w})^{y_i}(1 - f(\mathbf{x}_i, \mathbf{w}))^{1-y_i}$$

The equivalent but more convenient optimization problem is to maximize the **log**-likelihood:

$$\log \mathcal{L}((\mathbf{x}_i, y_i)_{i=1}^n|\theta) = \sum_{i=1}^{n} y_i \log f(\mathbf{x}_i, \mathbf{w}) + (1 - y_i) \log(1 - f(\mathbf{x}_i, \mathbf{w}))$$

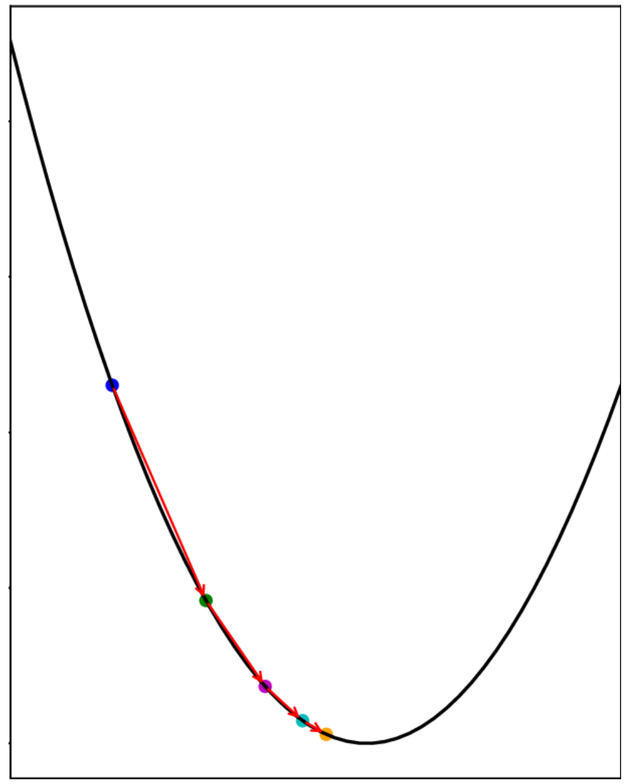
We note the *negative* log-likelihood $l_{MLE}(\theta) = -\log \mathcal{L}(\theta)$ as the loss function to minimize.

It corresponds to the *Kullback-Leibler divergence* between the data distribution $\hat{p}_{data}$ and the model distribution $p_\theta = f(., \mathbf{w})$:

$$l_{MLE}(\theta) = D_{KL}(\hat{p}_{data}, p_\theta) + C$$

Gradient-based Learning

$\rightarrow$ We are looking for the parameters θ^* that will minimize the negative log-likelihood.

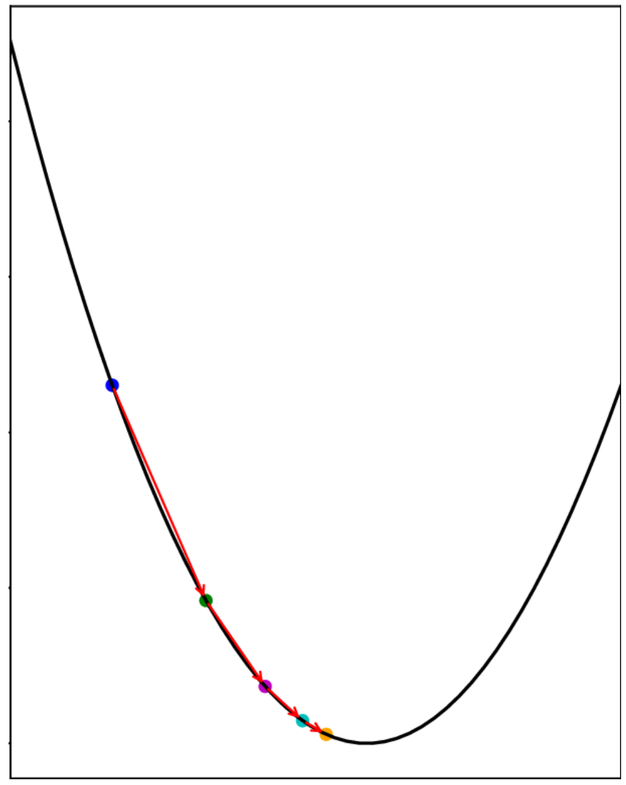


Gradient-based Learning

$\rightarrow$ We are looking for the parameters θ^* that will minimize the negative log-likelihood.

We use the **gradient descent**, which is based on the following update rule:

$$\theta^{t+1} = \theta^t + \epsilon \nabla_\theta l(\theta)$$



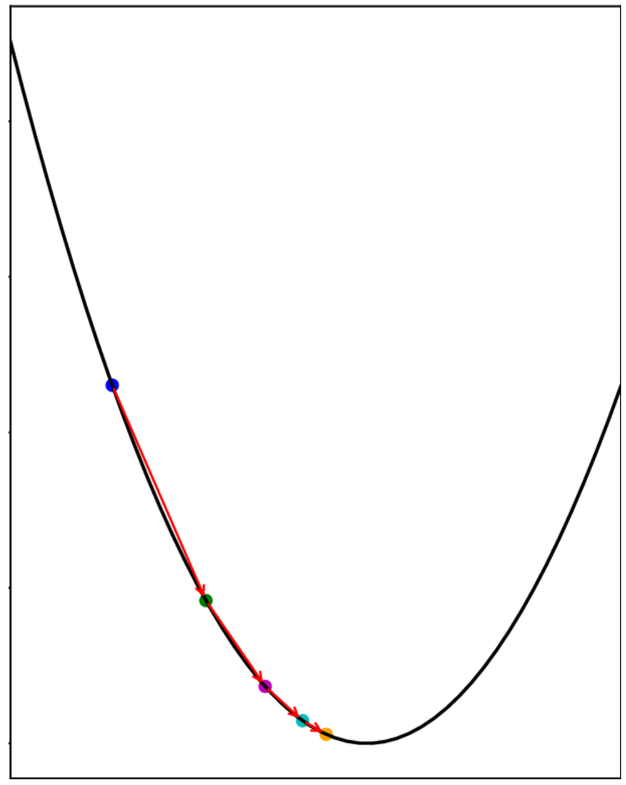
Gradient-based Learning

$\rightarrow$ We are looking for the parameters θ^* that will minimize the negative log-likelihood.

We use the **gradient descent**, which is based on the following update rule:

$$\theta^{t+1} = \theta^t + \epsilon \nabla_\theta l(\theta)$$

The learning rate ϵ dictates how fast we follow the direction of steepest descent



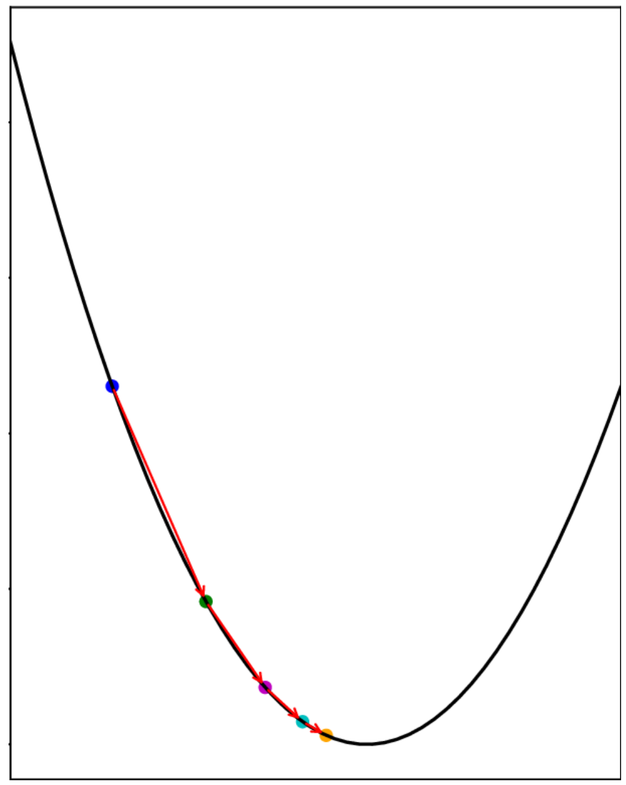
Gradient-based Learning

$\rightarrow$ We are looking for the parameters θ^* that will minimize the negative log-likelihood.

We use the **gradient descent**, which is based on the following update rule:

$$\theta^{t+1} = \theta^t + \epsilon \nabla_\theta l(\theta)$$

The learning rate ϵ dictates how fast we follow the direction of steepest descent



Computing the gradient on all data points is expensive: in practice, we use only a small batch of randomly selected points for an update.

$\rightarrow$ This is **Stochastic Gradient Descent (SGD)**.

Gradient-based Learning

$\rightarrow$ Coming back to our model: the gradient of the loss $l_{MLE}(\theta)$.

The derivative with respect to the j^{th} component of $\mathbf{w}$, w^j is:

$$\frac{\delta l_{MLE}}{\delta w^j} = -\sum_{i=1}^{n} \left[y_i - f(\mathbf{x}_i, \mathbf{w})\right] x_i^j$$

Gradient-based Learning

$\rightarrow$ Coming back to our model: the gradient of the loss $l_{MLE}(\theta)$.

The derivative with respect to the j^{th} component of $\mathbf{w}$, w^j is:

$$\frac{\delta l_{MLE}}{\delta w^j} = -\sum_{i=1}^{n} \left[y_i - f(\mathbf{x}_i, \mathbf{w}) \right] x_i^j$$

Gradient-based learning procedure:

Gradient-based Learning

$\rightarrow$ Coming back to our model: the gradient of the loss $l_{MLE}(\theta)$.

The derivative with respect to the j^{th} component of $\mathbf{w}$, w^j is:

$$\frac{\delta l_{MLE}}{\delta w^j} = -\sum_{i=1}^{n} \left[y_i - f(\mathbf{x}_i, \mathbf{w}) \right] x_i^j$$

Gradient-based learning procedure:

- Start with $t = 1$, $\mathbf{w}_t$ initialized appropriatly;
  Number of iterations n_{iter}, Learning rate $\epsilon > 0$, and $\delta > 0$
  Examples $(\mathbf{x}_i, y_i)_{i=1}^n$;

Gradient-based Learning

$\rightarrow$ Coming back to our model: the gradient of the loss $l_{MLE}(\theta)$.

The derivative with respect to the j^{th} component of $\mathbf{w}$, w^j is:

$$\frac{\delta l_{MLE}}{\delta w^j} = -\sum_{i=1}^{n} \left[y_i - f(\mathbf{x}_i, \mathbf{w})\right] x_i^j$$

Gradient-based learning procedure:

- Start with $t = 1$, $\mathbf{w}_t$ initialized appropriatly;
  Number of iterations n_{iter}, Learning rate $\epsilon > 0$, and $\delta > 0$
  Examples $(\mathbf{x}_i, y_i)_{i=1}^n$;
- While $||l_{ML}(\mathbf{w}_{t+1}) - l_{ML}(\mathbf{w}_t)|| > \delta$ and $t > n_{iter}$:
  - For $j \in [1, d]$ (on a set of d randomly sampled examples in the data):
    - Do $w_{t+1}^j = w_t^j + \epsilon \sum_{i=1}^{d} \left[y_i - f(\mathbf{x}_i, \mathbf{w})\right] x_i^j$

Gradient-based Learning

$\rightarrow$ Coming back to our model: the gradient of the loss $l_{MLE}(\theta)$.

The derivative with respect to the j^{th} component of $\mathbf{w}$, w^j is:

$$\frac{\delta l_{MLE}}{\delta w^j} = -\sum_{i=1}^{n} \left[y_i - f(\mathbf{x}_i, \mathbf{w})\right] x_i^j$$

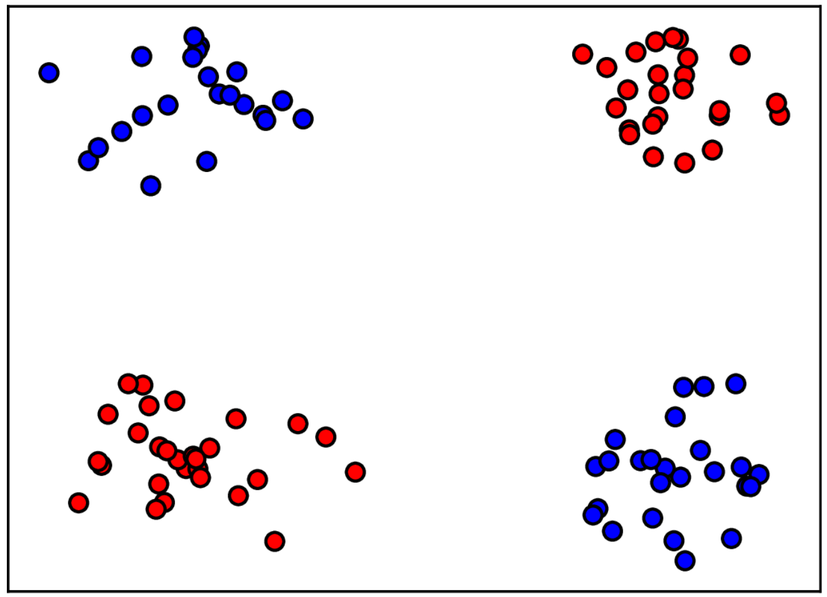
Gradient-based learning procedure:

- Start with $t = 1$, $\mathbf{w}_t$ initialized appropriatly;
  Number of iterations n_{iter}, Learning rate $\epsilon > 0$, and $\delta > 0$
  Examples $(\mathbf{x}_i, y_i)_{i=1}^n$;
- While $||l_{ML}(\mathbf{w}_{t+1}) - l_{ML}(\mathbf{w}_t)|| > \delta$ and $t > n_{iter}$:
  - For $j \in [1, d]$ (on a set of d randomly sampled examples in the data):
    - Do $w_{t+1}^j = w_t^j + \epsilon \sum_{i=1}^{d} \left[y_i - f(\mathbf{x}_i, \mathbf{w})\right] x_i^j$

$\rightarrow$ We now have a well defined **probabilistic** model for binary classification, and **an efficient way to learn it** !

Non-linear Learning

→ Reminder: the **XOR** issue !



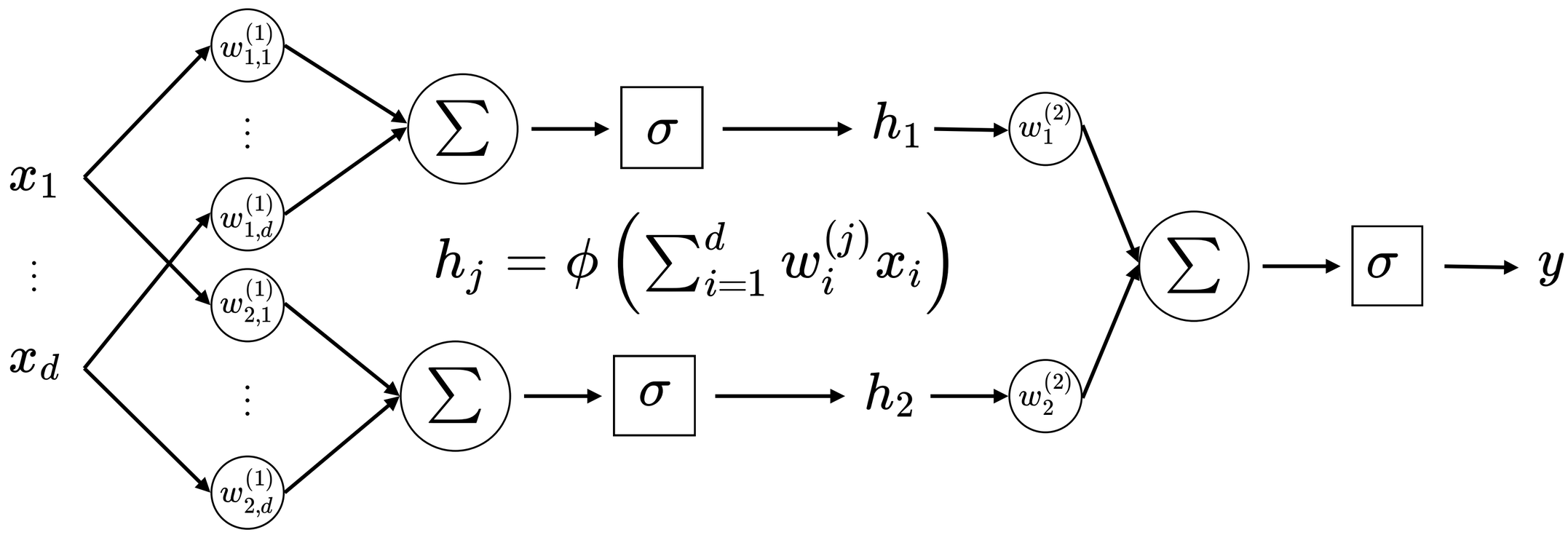
Non-linear Learning

→ Reminder: the **XOR** issue !

Non-linear Learning

→ Reminder: the **XOR** issue !

Solution: *combining* several outputs as inputs to a new neuron, forming a **Multi-Layer Perceptron (MLP)**:



Multi-Layer Perceptron

Intuitions:

- Features are mapped into an *intermediate space*: the model uses an **internal representation** that's the input for the output neuron

Multi-Layer Perceptron

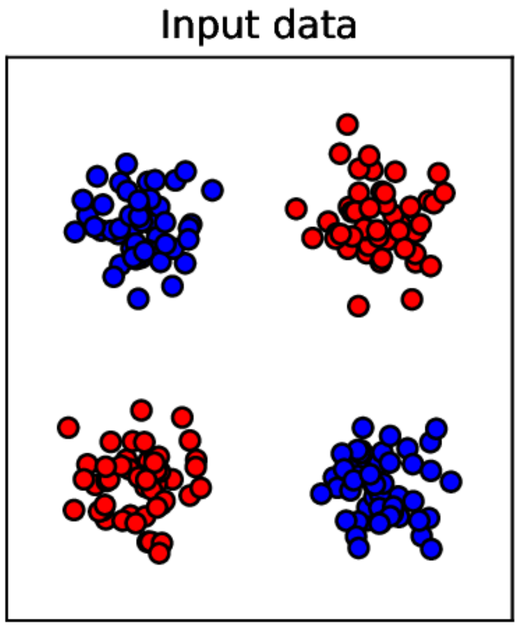
Intuitions:

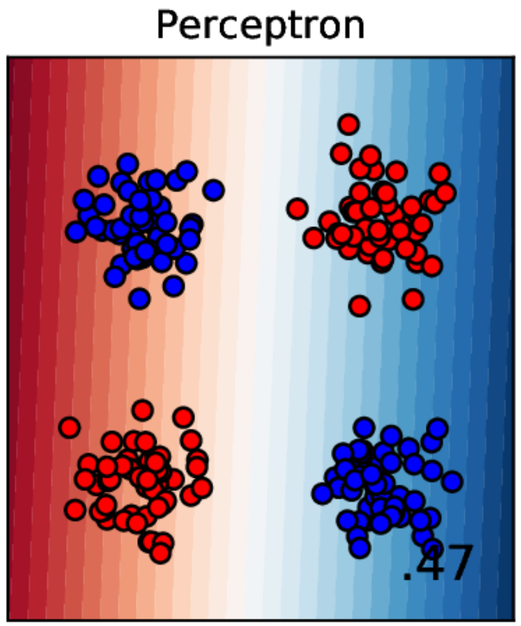
- Features are mapped into an *intermediate space*: the model uses an **internal representation** that's the input for the output neuron
- The input representation $\mathbf{x}$ is transformed/compressed in a new representation $\mathbf{h}$

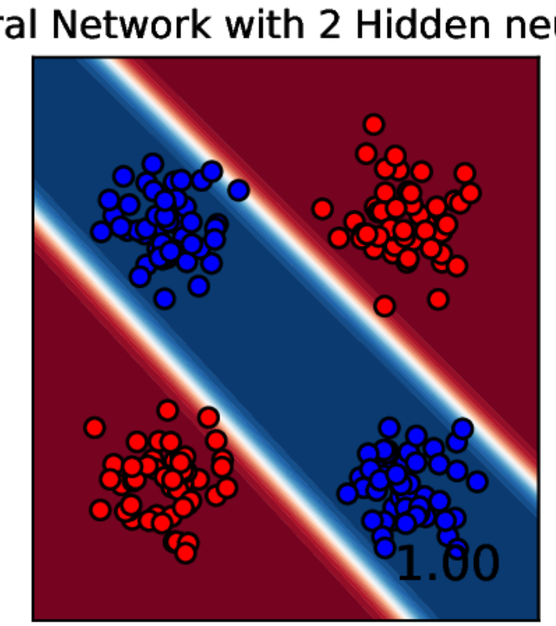
Multi-Layer Perceptron

Intuitions:

- Features are mapped into an *intermediate space*: the model uses an **internal representation** that's the input for the output neuron
- The input representation $\mathbf{x}$ is transformed/compressed in a new representation $\mathbf{h}$







Multi-Layer Perceptron: Architecture

Usually, neurons are grouped into **layers**:

$\rightarrow$ We *vectorialize* the neurons

Multi-Layer Perceptron: Architecture

Usually, neurons are grouped into **layers**:

$\rightarrow$ We *vectorialize* the neurons

$$h_1^{(1)} = \phi^{(1)}\left({\mathbf{w}_1^{(1)}}^T \mathbf{x} + b_1^{(1)}\right)$$

$$h_2^{(1)} = \phi^{(1)}\left({\mathbf{w}_2^{(1)}}^T \mathbf{x} + b_2^{(1)}\right)$$

$$\vdots$$

$$h_{d_h}^{(1)} = \phi^{(1)}\left({\mathbf{w}_{d_h}^{(1)}}^T \mathbf{x} + b_{d_h}^{(1)}\right)$$

Multi-Layer Perceptron: Architecture

Usually, neurons are grouped into **layers**:

$\rightarrow$ We *vectorialize* the neurons

.... Obtaining a **fully connected** layer:

Multi-Layer Perceptron: Architecture

Usually, neurons are grouped into **layers**:

$\rightarrow$ We *vectorialize* the neurons

.... Obtaining a **fully connected** layer:

$$\mathbf{h}^{(1)} = \sigma\left(\mathbf{W}^{(1)^T}\mathbf{x} + \mathbf{b}^{(1)}\right)$$

Multi-Layer Perceptron: Architecture

Usually, neurons are grouped into **layers**:

$\rightarrow$ We *vectorialize* the neurons

.... Obtaining a **fully connected** layer:

$$\mathbf{h}^{(1)} = \phi^{(1)}\left({\mathbf{W}^{(1)}}^T\mathbf{x} + \mathbf{b}^{(1)}\right)$$

$\phi^{(1)}$ can be any **non-linear activation function**

Multi-Layer Perceptron: Architecture

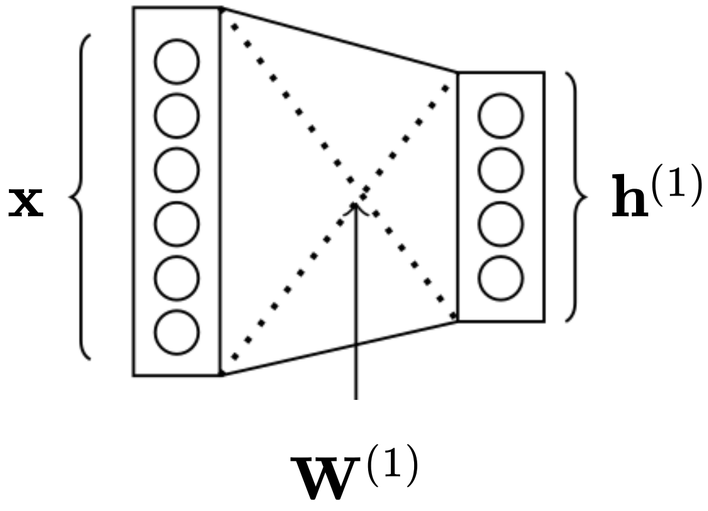
Usually, neurons are grouped into **layers**:

$\rightarrow$ We *vectorialize* the neurons

.... Obtaining a **fully connected** layer:

$$\mathbf{h}^{(1)} = \phi^{(1)}\left(\mathbf{W}^{(1)^T}\mathbf{x} + \mathbf{b}^{(1)}\right)$$

$\phi^{(1)}$ can be any **non-linear activation function**



Multi-Layer Perceptron: Architecture

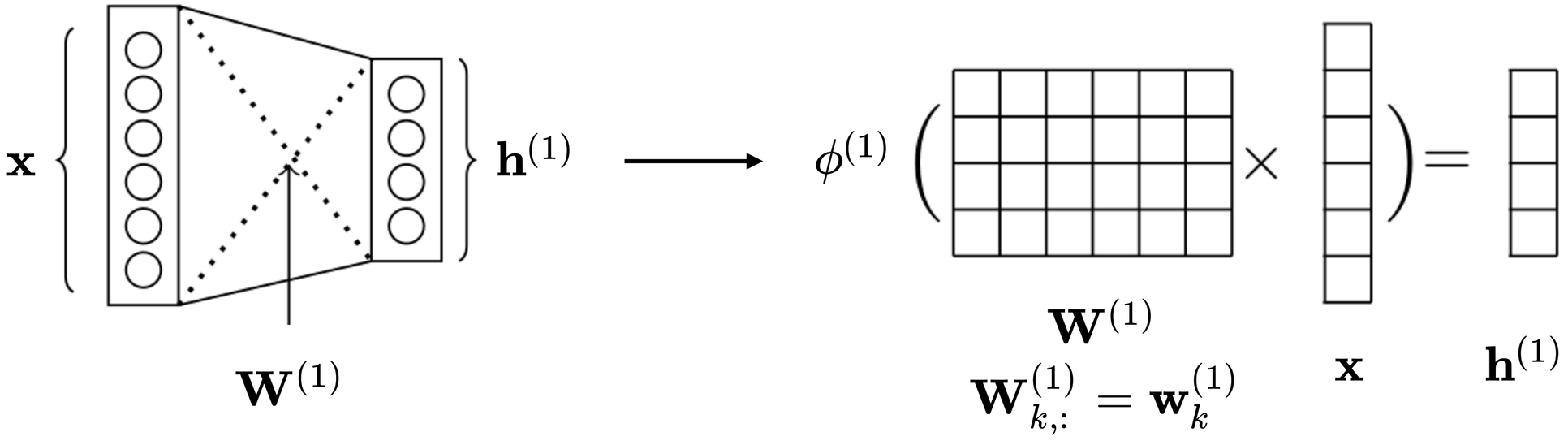
Usually, neurons are grouped into **layers**:

$\rightarrow$ We *vectorialize* the neurons

.... Obtaining a **fully connected** layer:

$$\mathbf{h}^{(1)} = \phi^{(1)}\left(\mathbf{W}^{(1)^T}\mathbf{x} + \mathbf{b}^{(1)}\right)$$

$\phi^{(1)}$ can be any **non-linear activation function**



Multi-Layer Perceptron: Architecture

Layers are organized in a **chain structure**:

$\rightarrow$ Each layer is a function of the previous one

Multi-Layer Perceptron: Architecture

Layers are organized in a **chain structure**:

$\rightarrow$ Each layer is a function of the previous one

$$\mathbf{h}^{(1)} = \phi^{(1)}\left(\mathbf{W}^{(1)^T}\mathbf{x} + \mathbf{b}^{(1)}\right)$$

Multi-Layer Perceptron: Architecture

Layers are organized in a **chain structure**:

$\rightarrow$ Each layer is a function of the previous one

$$\mathbf{h}^{(1)} = \phi^{(1)}\left({\mathbf{W}^{(1)}}^{T}\mathbf{x} + \mathbf{b}^{(1)}\right)$$

$$\mathbf{h}^{(2)} = \phi^{(2)}\left({\mathbf{W}^{(2)}}^{T}\mathbf{h}^{(1)} + \mathbf{b}^{(2)}\right)$$

Multi-Layer Perceptron: Architecture

Layers are organized in a **chain structure**:

$\rightarrow$ Each layer is a function of the previous one

$$\mathbf{h}^{(1)} = \phi^{(1)} \left({\mathbf{W}^{(1)}}^T \mathbf{x} + \mathbf{b}^{(1)} \right)$$

$$\mathbf{h}^{(2)} = \phi^{(2)} \left({\mathbf{W}^{(2)}}^T \mathbf{h}^{(1)} + \mathbf{b}^{(2)} \right)$$

And so on, until the layer l:

$$\mathbf{h}^{(l)} = \phi^{(l)} \left({\mathbf{W}^{(l)}}^T \mathbf{h}^{(l-1)} + \mathbf{b}^{(l)} \right)$$

Multi-Layer Perceptron: Activations

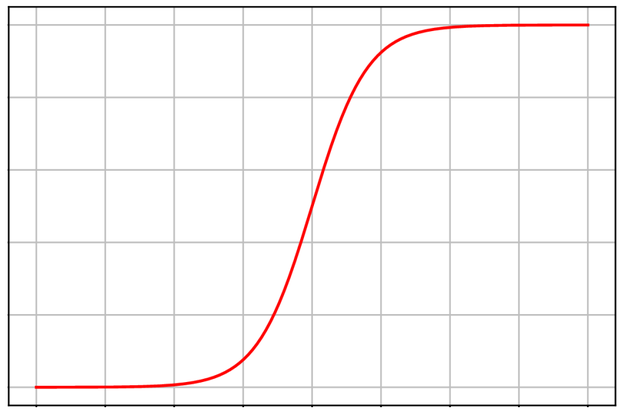
Activations for the hidden layers have various (dis)advantages:

$\rightarrow$ Which one to choose depends on the data and task !

Multi-Layer Perceptron: Activations

Activations for the hidden layers have various (dis)advantages:

$\rightarrow$ Which one to choose depends on the data and task !

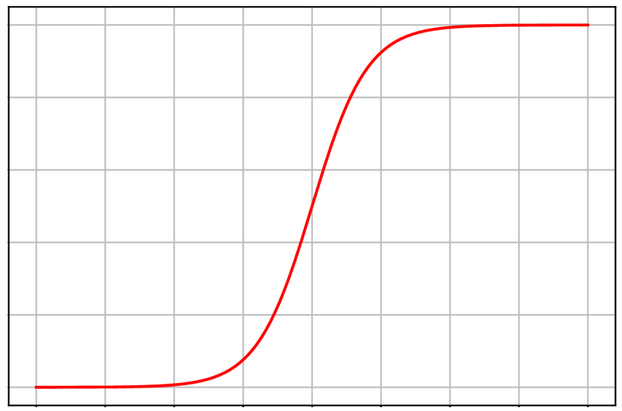


$$\sigma(x) = \frac{1}{1+e^{-x}}$$

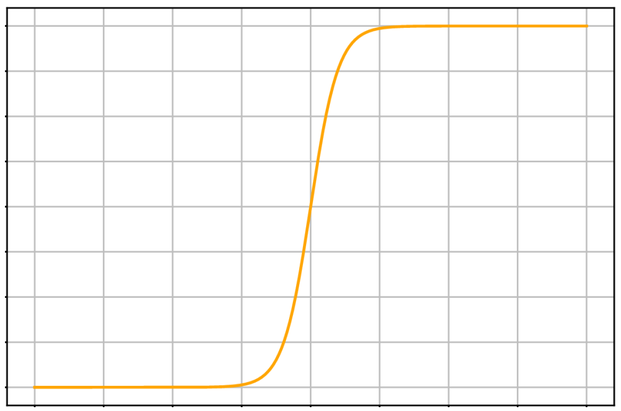
Multi-Layer Perceptron: Activations

Activations for the hidden layers have various (dis)advantages:

$\rightarrow$ Which one to choose depends on the data and task !



$$\sigma(x) = \frac{1}{1+e^{-x}}$$



$$\tanh(x) = \frac{e^{x}-e^{-x}}{e^{x}+e^{-x}}$$

Multi-Layer Perceptron: Multi-outputs

We can also have an arbitrary number of output neurons: for multi-class classification with K classes, we have $y_i \in [1, K]$.

Equivalently, we write the corresponding output vector $\mathbf{o}_i \in \mathbb{R}^K$:

$$y_i = k \iff \mathbf{o}_i = [0, ..., 1, ..., 0]$$

$k^{th}\, component$

Multi-Layer Perceptron: Multi-outputs

We can also have an arbitrary number of output neurons: for multi-class classification with K classes, we have $y_i \in [1, K]$.

Equivalently, we write the corresponding output vector $\mathbf{o}_i \in \mathbb{R}^K$:

$$y_i = k \iff \mathbf{o}_i = [0, ..., \underset{\substack{\uparrow \\ k^{th} component}}{1}, ..., 0]$$

$\rightarrow$ We use the **softmax** activation function, which generalizes the sigmoid to k outputs:

$$\hat{\mathbf{o}}_i = softmax(\mathbf{h}^{(l)}) = [\frac{e^{\mathbf{h}^{(l),1}}}{\sum_{k=1}^{K} e^{\mathbf{h}^{(l),k}}}, ..., \frac{e^{\mathbf{h}^{(l),K}}}{\sum_{k=1}^{K} e^{\mathbf{h}^{(l),k}}}]$$

Multi-Layer Perceptron: Multi-outputs

We can also have an arbitrary number of output neurons: for multi-class classification with K classes, we have $y_i \in [1, K]$.

Equivalently, we write the corresponding output vector $\mathbf{o}_i \in \mathbb{R}^K$:

$$y_i = k \iff \mathbf{o}_i = [0, ..., 1, ..., 0]$$

$k^{th} component$

$\rightarrow$ We use the **softmax** activation function, which generalizes the sigmoid to k outputs:

$$\hat{\mathbf{o}}_i = softmax(\mathbf{h}^{(l)}) = [\frac{e^{\mathbf{h}^{(l),1}}}{\sum_{k=1}^{K} e^{\mathbf{h}^{(l),k}}}, ..., \frac{e^{\mathbf{h}^{(l),K}}}{\sum_{k=1}^{K} e^{\mathbf{h}^{(l),k}}}]$$

The components of $\hat{\mathbf{o}}_i$ sum to 1 and can be interpreted as probabilities over a **multinomial** distribution

Multi-Layer Perceptron: Optimization

The parameters of the MLP are $\theta = (\mathbf{W}^{(1)}, \mathbf{b}^{(1)}, ..., \mathbf{W}^{(l)}, \mathbf{b}^{(l)})$

Multi-Layer Perceptron: Optimization

The parameters of the MLP are $\theta = (\mathbf{W}^{(1)}, \mathbf{b}^{(1)}, ..., \mathbf{W}^{(l)}, \mathbf{b}^{(l)})$

As for the binary case, we use the negative log-likelihood as loss to minimize, following a **probabilistic interpretation of the softmax**:

$$l_{MLE}((\mathbf{x}_i, y_i)_{i=1}^n|\theta) = -\sum_{i=1}^{n} \log \prod_{k=1}^{K} \hat{P}(y_i = k|\mathbf{x}_i, \theta)^{o_i^k} = -\sum_{i=1}^{n} \sum_{k=1}^{K} o_i^k \log \hat{o}_i^k$$

Multi-Layer Perceptron: Optimization

The parameters of the MLP are $\theta = (\mathbf{W}^{(1)}, \mathbf{b}^{(1)}, ..., \mathbf{W}^{(l)}, \mathbf{b}^{(l)})$

As for the binary case, we use the negative log-likelihood as loss to minimize, following a **probabilistic interpretation of the softmax**:

$$l_{MLE}((\mathbf{x}_i, y_i)_{i=1}^n | \theta) = -\sum_{i=1}^{n} \log \prod_{k=1}^{K} \hat{P}(y_i = k | \mathbf{x}_i, \theta)^{o_i^k} = -\sum_{i=1}^{n} \sum_{k=1}^{K} o_i^k \log \hat{o}_i^k$$

Since $o_i^k = 1 \iff y_i = k$, we end up with:

$$l_{MLE}((\mathbf{x}_i, y_i)_{i=1}^n | \theta) = -\sum_{i=1}^{n} \log \hat{o}_i^{y_i} = -\sum_{i=1}^{n} \log \left(\frac{e^{\mathbf{h}^{(l),y_i}}}{\sum_{k=1}^{K} e^{\mathbf{h}^{(l),k}}} \right)$$

Multi-Layer Perceptron: Optimization

The parameters of the MLP are $\theta = (\mathbf{W}^{(1)}, \mathbf{b}^{(1)}, ..., \mathbf{W}^{(l)}, \mathbf{b}^{(l)})$

As for the binary case, we use the negative log-likelihood as loss to minimize, following a **probabilistic interpretation of the softmax**:

$$l_{MLE}((\mathbf{x}_i, y_i)_{i=1}^n|\theta) = -\sum_{i=1}^{n} \log \prod_{k=1}^{K} \hat{P}(y_i = k|\mathbf{x}_i, \theta)^{o_i^k} = -\sum_{i=1}^{n}\sum_{k=1}^{K} o_i^k \log \hat{o}_i^k$$

Since $o_i^k = 1 \iff y_i = k$, we end up with:

$$l_{MLE}((\mathbf{x}_i, y_i)_{i=1}^n|\theta) = -\sum_{i=1}^{n} \log \hat{o}_i^{y_i} = -\sum_{i=1}^{n} \log \left(\frac{e^{\mathbf{h}^{(l),y_i}}}{\sum_{k=1}^{K} e^{\mathbf{h}^{(l),k}}} \right)$$

But here, it is not as easy to compute the derivative $\frac{\delta l_{MLE}}{\delta w}$ for all parameters $w \in \theta$ ...

$\rightarrow$ To do so, we will use **Backpropagation**

MLP: Backpropagation

Backpropagation was proposed by Rumelhart (*Learning representations by back-propagating errors*, 1986)

MLP: Backpropagation

Backpropagation was proposed by Rumelhart (*Learning representations by back-propagating errors*, 1986)

$\rightarrow$ It is based on the **chain rule**:

MLP: Backpropagation

Backpropagation was proposed by Rumelhart (*Learning representations by back-propagating errors*, 1986)

$\rightarrow$ It is based on the **chain rule**:

In the scalar case:

$$y = g(x) \text{ and } z = f(g(x)) = f(y)$$

MLP: Backpropagation

Backpropagation was proposed by Rumelhart (*Learning representations by back-propagating errors*, 1986)

$\rightarrow$ It is based on the **chain rule**:

In the scalar case:

$$y = g(x) \text{ and } z = f(g(x)) = f(y)$$

$$\frac{\delta z}{\delta x} = \frac{\delta z}{\delta y} \frac{\delta y}{\delta x}$$

MLP: Backpropagation

Backpropagation was proposed by Rumelhart (*Learning representations by back-propagating errors*, 1986)

$\rightarrow$ It is based on the **chain rule**:

In the scalar case:

$$y = g(x) \text{ and } z = f(g(x)) = f(y)$$

$$\frac{\delta z}{\delta x} = \frac{\delta z}{\delta y} \frac{\delta y}{\delta x}$$

$\rightarrow$ Allows to **recursively** compute gradients for all the parameters in the network from a **computational graph**

MLP: Backpropagation

Backpropagation was proposed by Rumelhart (*Learning representations by back-propagating errors*, 1986)

$\rightarrow$ It is based on the **chain rule**:

In the scalar case:

$$y = g(x) \text{ and } z = f(g(x)) = f(y)$$

$$\frac{\delta z}{\delta x} = \frac{\delta z}{\delta y} \frac{\delta y}{\delta x}$$

$\rightarrow$ Allows to **recursively** compute gradients for all the parameters in the network from a **computational graph**

(But parameters are vectors and tensors: it quickly becomes complicated)

MLP: Backpropagation

Backpropagation was proposed by Rumelhart (*Learning representations by back-propagating errors*, 1986)

$\rightarrow$ It is based on the **chain rule**:

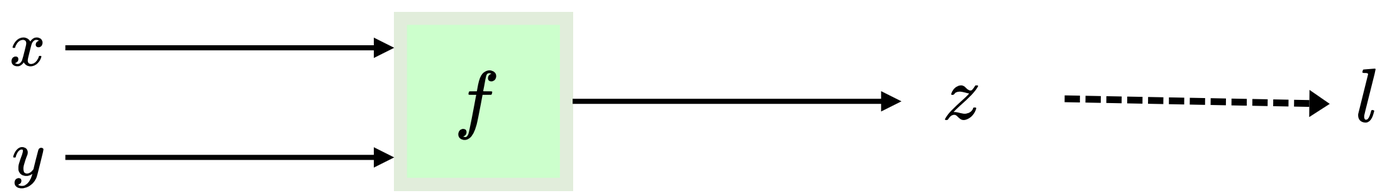
In the scalar case:

$$y = g(x) \text{ and } z = f(g(x)) = f(y)$$

$$\frac{\delta z}{\delta x} = \frac{\delta z}{\delta y} \frac{\delta y}{\delta x}$$

$\rightarrow$ Allows to **recursively** compute gradients for all the parameters in the network from a **computational graph**

(But parameters are vectors and tensors: it quickly becomes complicated)



$$z = f(x, y)$$

MLP: Backpropagation

Backpropagation was proposed by Rumelhart (*Learning representations by back-propagating errors*, 1986)

$\rightarrow$ It is based on the **chain rule**:

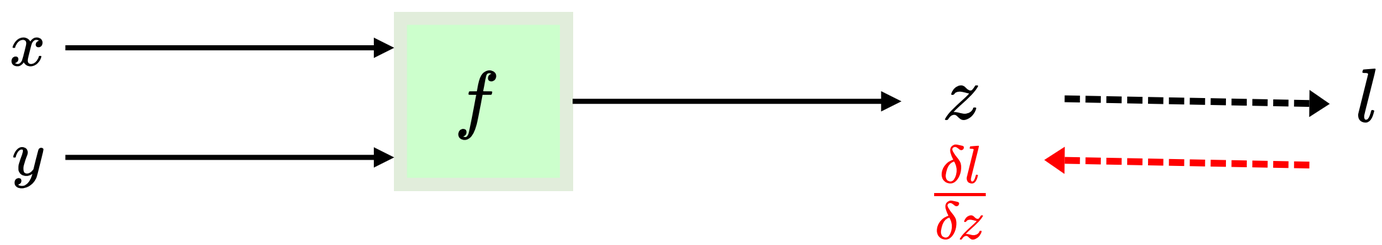
In the scalar case:

$$y = g(x) \text{ and } z = f(g(x)) = f(y)$$

$$\frac{\delta z}{\delta x} = \frac{\delta z}{\delta y} \frac{\delta y}{\delta x}$$

$\rightarrow$ Allows to **recursively** compute gradients for all the parameters in the network from a **computational graph**

(But parameters are vectors and tensors: it quickly becomes complicated)



$$z = f(x, y)$$

MLP: Backpropagation

Backpropagation was proposed by Rumelhart (*Learning representations by back-propagating errors*, 1986)

$\rightarrow$ It is based on the **chain rule**:

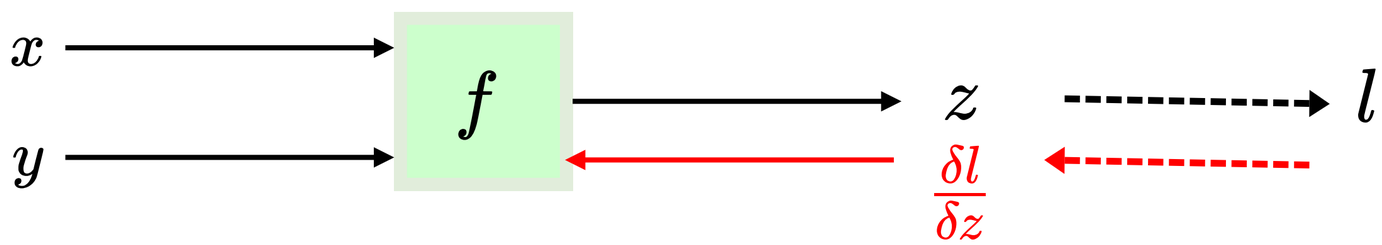
In the scalar case:

$$y = g(x) \text{ and } z = f(g(x)) = f(y)$$

$$\frac{\delta z}{\delta x} = \frac{\delta z}{\delta y} \frac{\delta y}{\delta x}$$

$\rightarrow$ Allows to **recursively** compute gradients for all the parameters in the network from a **computational graph**

(But parameters are vectors and tensors: it quickly becomes complicated)



$$z = f(x, y)$$

MLP: Backpropagation

Backpropagation was proposed by Rumelhart (*Learning representations by back-propagating errors*, 1986)

$\rightarrow$ It is based on the **chain rule**:

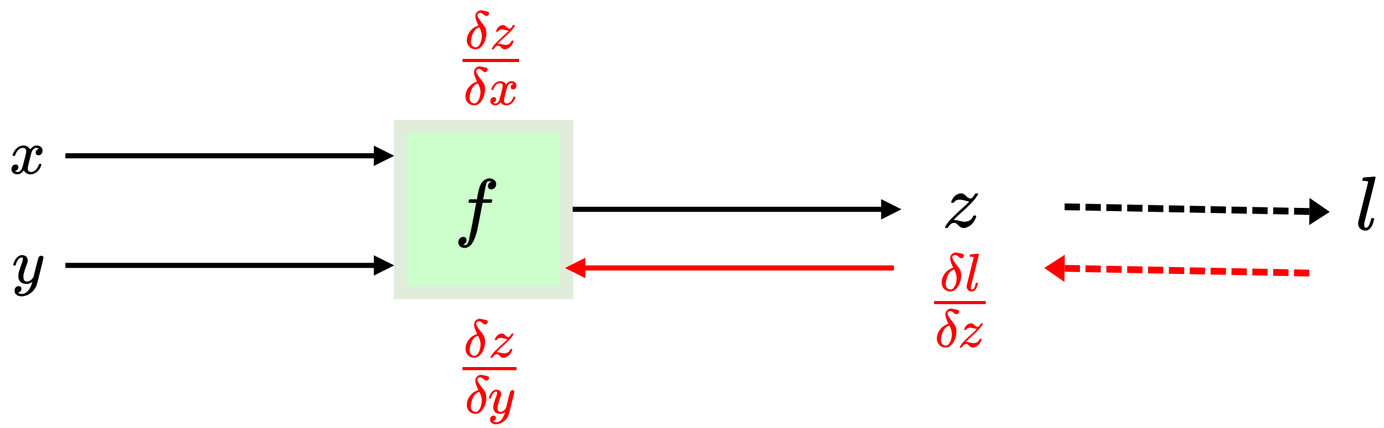
In the scalar case:

$$y = g(x) \text{ and } z = f(g(x)) = f(y)$$

$$\frac{\delta z}{\delta x} = \frac{\delta z}{\delta y} \frac{\delta y}{\delta x}$$

$\rightarrow$ Allows to **recursively** compute gradients for all the parameters in the network from a **computational graph**

(But parameters are vectors and tensors: it quickly becomes complicated)



$$z = f(x, y)$$

MLP: Backpropagation

Backpropagation was proposed by Rumelhart (*Learning representations by back-propagating errors*, 1986)

$\rightarrow$ It is based on the **chain rule**:

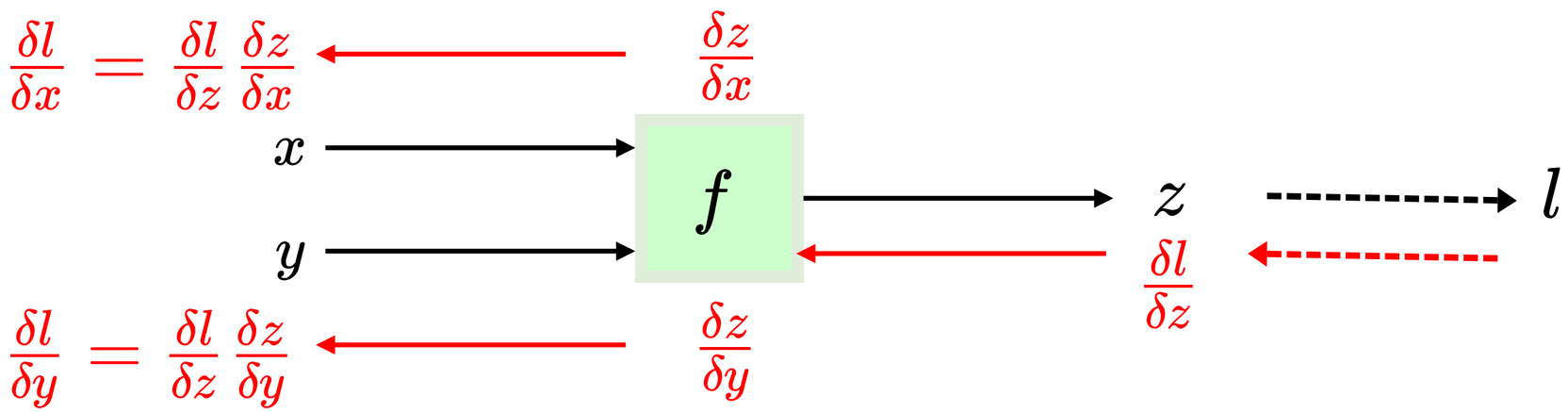
In the scalar case:

$$y = g(x) \text{ and } z = f(g(x)) = f(y)$$

$$\frac{\delta z}{\delta x} = \frac{\delta z}{\delta y}\frac{\delta y}{\delta x}$$

$\rightarrow$ Allows to **recursively** compute gradients for all the parameters in the network from a **computational graph**

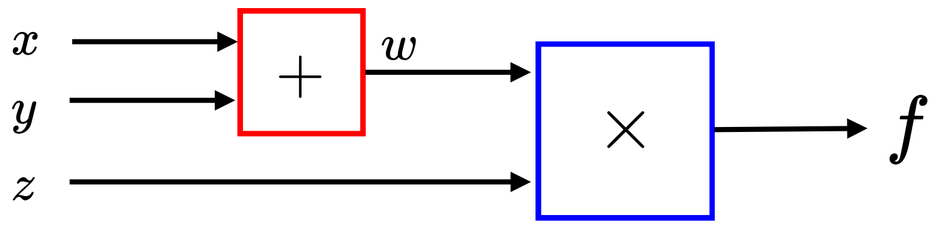
(But parameters are vectors and tensors: it quickly becomes complicated)



$$z = f(x, y)$$

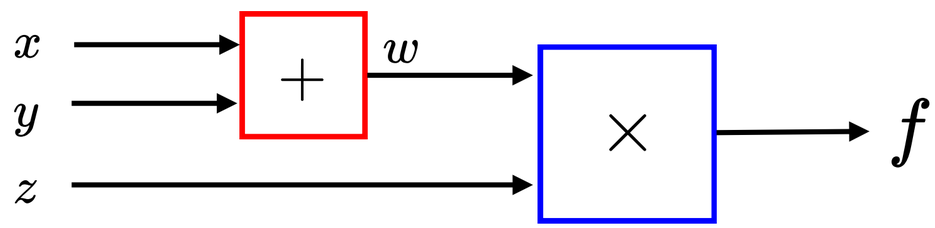
Backpropagation : simple example

$$f\left(x,y,z\right)=\left(x+y\right)z$$



Backpropagation : simple example

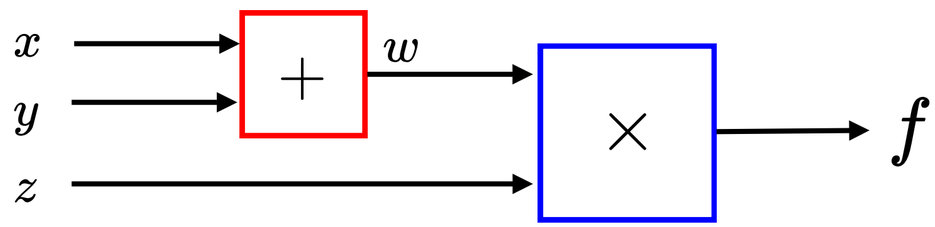
$$f\left(x,y,z\right)=\left(x+y\right)z$$



$$w=x+y$$

Backpropagation : simple example

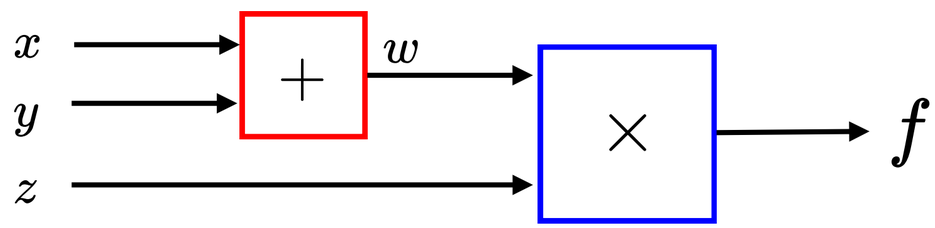
$$f\left(x,y,z\right)=\left(x+y\right)z$$



$$w=x+y \quad \rightarrow \quad \frac{\delta w}{\delta x}=1 \quad \frac{\delta w}{\delta y}=1$$

Backpropagation : simple example

$$f\left(x,y,z\right)=\left(x+y\right)z$$

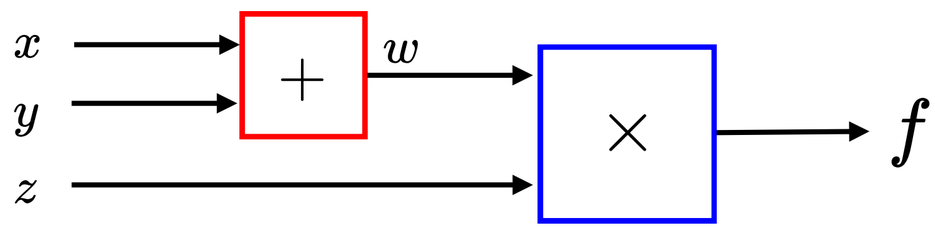


$$w=x+y \quad \rightarrow \quad \frac{\delta w}{\delta x}=1 \quad \frac{\delta w}{\delta y}=1$$

$$f=wz$$

Backpropagation : simple example

$$f\left(x,y,z\right)=\left(x+y\right)z$$

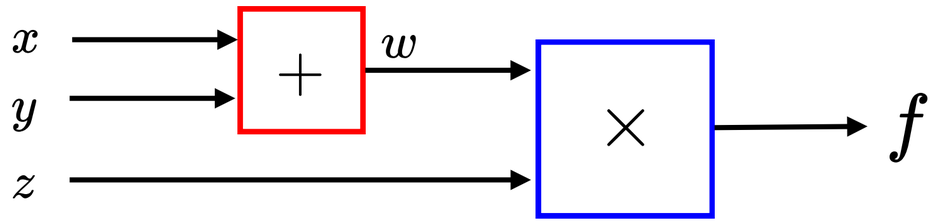


$$w=x+y \quad \rightarrow \quad \frac{\delta w}{\delta x}=1 \quad \frac{\delta w}{\delta y}=1$$

$$f=wz \quad \rightarrow \quad \frac{\delta f}{\delta w}=z \quad \frac{\delta f}{\delta z}=w$$

Backpropagation : simple example

$$f\left(x,y,z\right)=\left(x+y\right)z$$



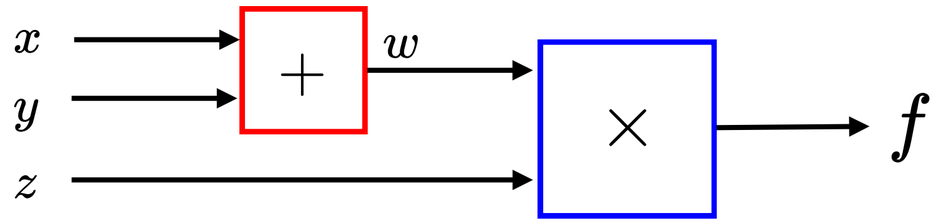
$$w=x+y \quad \rightarrow \quad \frac{\delta w}{\delta x}=1 \quad \frac{\delta w}{\delta y}=1$$

$$f=wz \quad \rightarrow \quad \frac{\delta f}{\delta w}=z \quad \frac{\delta f}{\delta z}=w$$

What are the gradients $\frac{\delta f}{\delta x}, \frac{\delta f}{\delta y}, \frac{\delta f}{\delta z}$?

Backpropagation : simple example

$$f\left(x,y,z\right)=\left(x+y\right)z$$



$$w=x+y \quad \rightarrow \quad \frac{\delta w}{\delta x}=1 \quad \frac{\delta w}{\delta y}=1$$

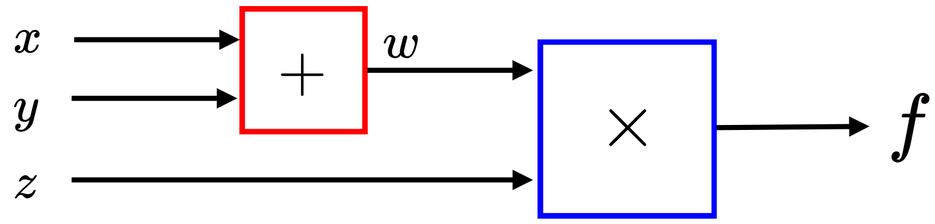
$$f=wz \quad \rightarrow \quad \frac{\delta f}{\delta w}=z \quad \frac{\delta f}{\delta z}=w$$

What are the gradients $\frac{\delta f}{\delta x}, \frac{\delta f}{\delta y}, \frac{\delta f}{\delta z}$?

$\rightarrow$ **Forward**: with $x=-2, y=5, z=-4$: $\rightarrow w=3$ and $f=-12$

Backpropagation : simple example

$$f\left(x,y,z\right)=\left(x+y\right)z$$



$$w=x+y \quad \rightarrow \quad \frac{\delta w}{\delta x}=1 \quad \frac{\delta w}{\delta y}=1$$

$$f=wz \quad \rightarrow \quad \frac{\delta f}{\delta w}=z \quad \frac{\delta f}{\delta z}=w$$

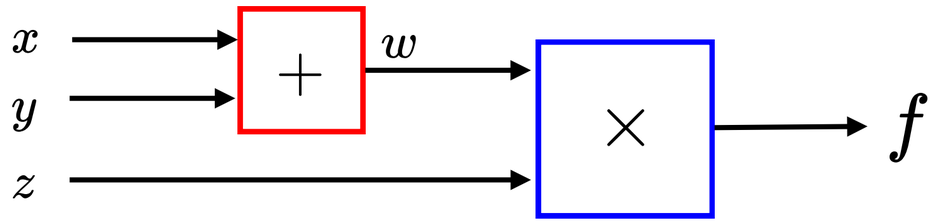
What are the gradients $\frac{\delta f}{\delta x}, \frac{\delta f}{\delta y}, \frac{\delta f}{\delta z}$?

$\rightarrow$ **Forward**: with $x=-2, y=5, z=-4$: $\rightarrow w=3$ and $f=-12$

$\rightarrow$ **Backward**: $\frac{\delta f}{\delta z}=w=3$

Backpropagation : simple example

$$f\left(x,y,z\right)=\left(x+y\right)z$$



$$w=x+y \quad \rightarrow \quad \frac{\delta w}{\delta x}=1 \quad \frac{\delta w}{\delta y}=1$$

$$f=wz \quad \rightarrow \quad \frac{\delta f}{\delta w}=z \quad \frac{\delta f}{\delta z}=w$$

What are the gradients $\frac{\delta f}{\delta x}, \frac{\delta f}{\delta y}, \frac{\delta f}{\delta z}$?

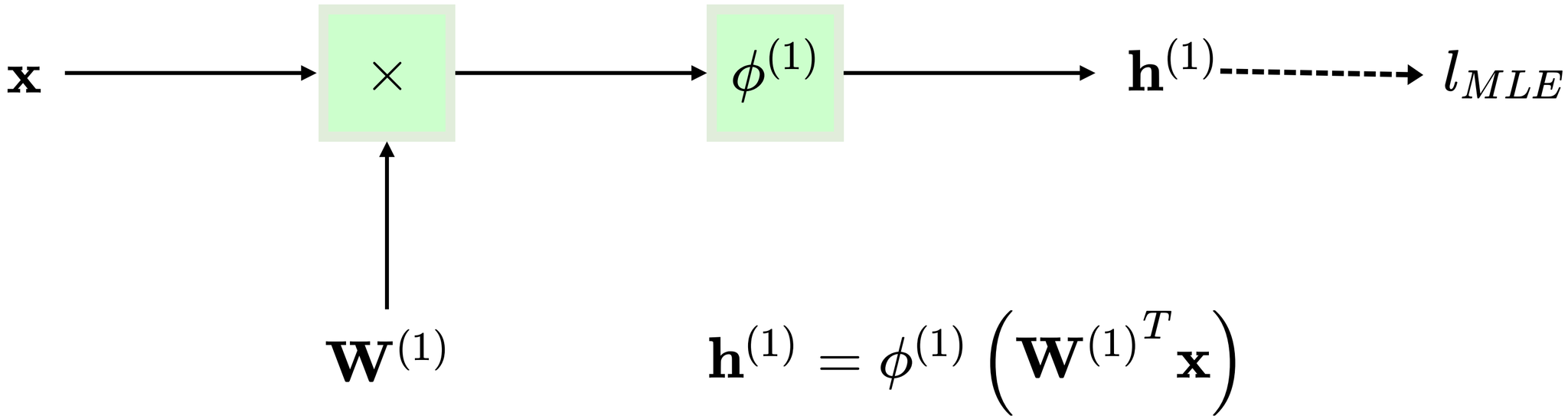
$\rightarrow$ **Forward**: with $x=-2, y=5, z=-4$: $\rightarrow w=3$ and $f=-12$

$\rightarrow$ **Backward**: $\frac{\delta f}{\delta z}=w=3$

$$\frac{\delta f}{\delta x}=\frac{\delta f}{\delta w}\frac{\delta w}{\delta x}=z\times 1=-4$$

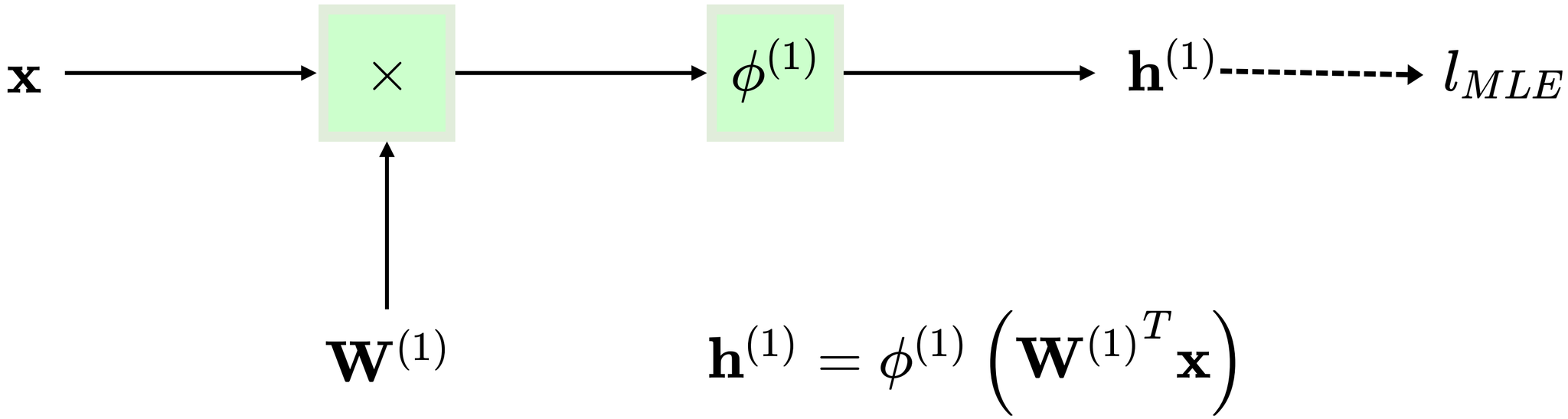
$$\frac{\delta f}{\delta y}=\frac{\delta f}{\delta x}=-4$$

MLP: Computational graph



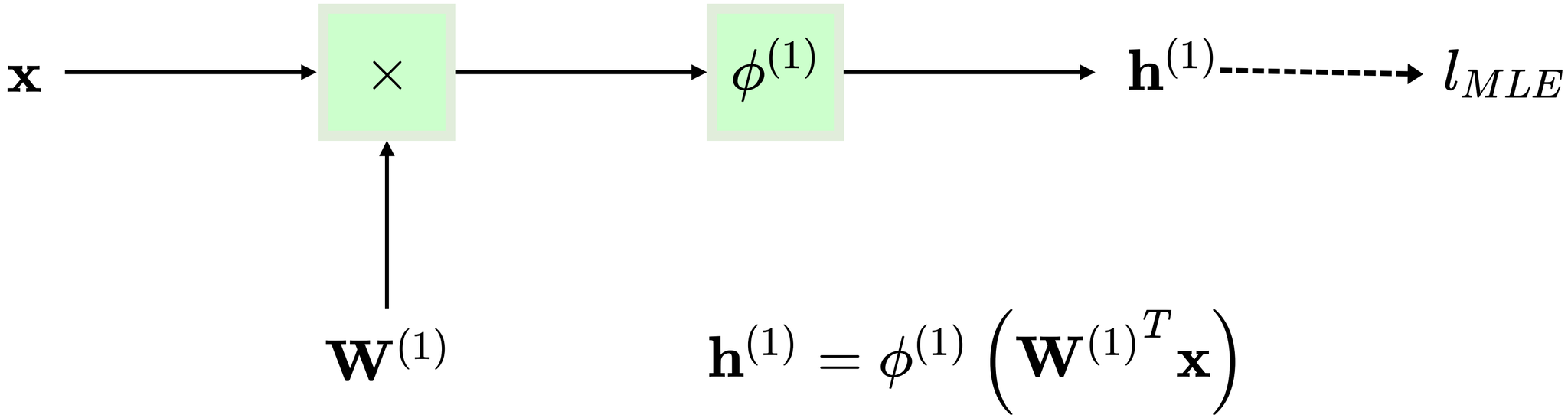
- Each node is an **operation** or a **variable**

MLP: Computational graph



- Each node is an **operation** or a **variable**
- An *operation* has some inputs/outputs made of *variables*

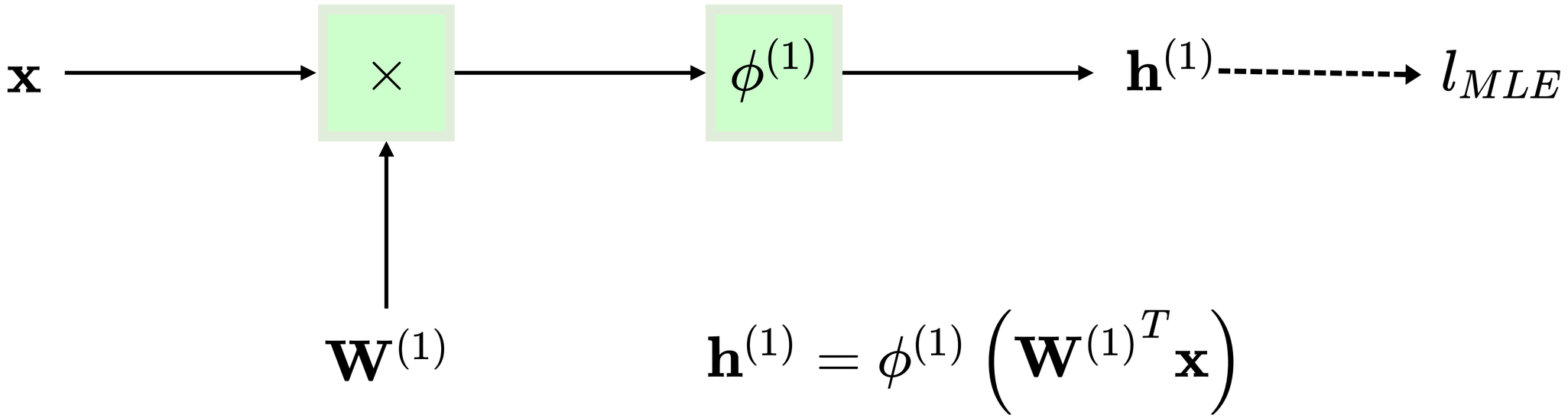
MLP: Computational graph



- Each node is an **operation** or a **variable**
- An *operation* has some inputs/outputs made of *variables*

- The **forward pass** computes the output for a given input

MLP: Computational graph



- Each node is an **operation** or a **variable**
- An *operation* has some inputs/outputs made of *variables*

- The **forward pass** computes the output for a given input
- The **backward pass** computes the gradient of the loss with respect to the parameters (here, $\mathbf{W}^{(1)}$)

Backpropagation : vector derivatives

→ As mentionned before**,** computing gradients rapidly becomes complicated when we work with **vectors**:

Backpropagation : vector derivatives

$\rightarrow$ As mentionned before**,** computing gradients rapidly becomes complicated when we work with **vectors**:

$\rightarrow$ **Vector to scalar**:

If $\mathbf{x} \in \mathbb{R}^n$, $y \in \mathbb{R}$:

$\frac{\delta y}{\delta \mathbf{x}}$ is a vector noted $\nabla_{\mathbf{x}} y(\mathbf{x}) \in \mathbb{R}^n$ that we call a **gradient.**

Backpropagation : vector derivatives

$\rightarrow$ As mentionned before**,** computing gradients rapidly becomes complicated when we work with **vectors**:

$\rightarrow$ **Vector to scalar**:

If $\mathbf{x} \in \mathbb{R}^n$, $y \in \mathbb{R}$:

$\frac{\delta y}{\delta \mathbf{x}}$ is a vector noted $\nabla_{\mathbf{x}} y(\mathbf{x}) \in \mathbb{R}^n$ that we call a **gradient.**

$\rightarrow$ **Vector to vector**:

If $\mathbf{x} \in \mathbb{R}^n$, $\mathbf{y} \in \mathbb{R}^m$:

$\frac{\delta \mathbf{y}}{\delta \mathbf{x}}$ is a matrix noted $\mathbf{J}_{\mathbf{y}}(\mathbf{x}) \in \mathbb{R}^{n \times m}$ that we call a **jacobian.**

Backpropagation : vector derivatives

$\rightarrow$ As mentionned before**,** computing gradients rapidly becomes complicated when we work with **vectors**:

$\rightarrow$ **Vector to scalar**:

If $\mathbf{x} \in \mathbb{R}^n$, $y \in \mathbb{R}$:

$\frac{\delta y}{\delta \mathbf{x}}$ is a vector noted $\nabla_{\mathbf{x}} y(\mathbf{x}) \in \mathbb{R}^n$ that we call a **gradient.**

$\rightarrow$ **Vector to vector**:

If $\mathbf{x} \in \mathbb{R}^n$, $\mathbf{y} \in \mathbb{R}^m$:

$\frac{\delta \mathbf{y}}{\delta \mathbf{x}}$ is a matrix noted $\mathbf{J}_{\mathbf{y}}(\mathbf{x}) \in \mathbb{R}^{n \times m}$ that we call a **jacobian.**

$\rightarrow$ **For example**:

Backpropagation : vector derivatives

$\rightarrow$ As mentionned before**,** computing gradients rapidly becomes complicated when we work with **vectors**:

$\rightarrow$ **Vector to scalar**:

If $\mathbf{x} \in \mathbb{R}^n$, $y \in \mathbb{R}$:

$\frac{\delta y}{\delta \mathbf{x}}$ is a vector noted $\nabla_{\mathbf{x}} y(\mathbf{x}) \in \mathbb{R}^n$ that we call a **gradient.**

$\rightarrow$ **Vector to vector**:

If $\mathbf{x} \in \mathbb{R}^n$, $\mathbf{y} \in \mathbb{R}^m$:

$\frac{\delta \mathbf{y}}{\delta \mathbf{x}}$ is a matrix noted $\mathbf{J}_{\mathbf{y}}(\mathbf{x}) \in \mathbb{R}^{n \times m}$ that we call a **jacobian.**

$\rightarrow$ **For example**:

If $\mathbf{x} \in \mathbb{R}^n$, $\mathbf{y} \in \mathbb{R}^m$, $z \in \mathbb{R}$:

$$\mathbf{y} = g(\mathbf{x}) \text{ and } z = f(\mathbf{y})$$

Backpropagation : vector derivatives

$\rightarrow$ As mentionned before**,** computing gradients rapidly becomes complicated when we work with **vectors**:

$\rightarrow$ **Vector to scalar**:

If $\mathbf{x} \in \mathbb{R}^n$, $y \in \mathbb{R}$:

$\frac{\delta y}{\delta \mathbf{x}}$ is a vector noted $\nabla_{\mathbf{x}} y(\mathbf{x}) \in \mathbb{R}^n$ that we call a **gradient.**

$\rightarrow$ **Vector to vector**:

If $\mathbf{x} \in \mathbb{R}^n$, $\mathbf{y} \in \mathbb{R}^m$:

$\frac{\delta \mathbf{y}}{\delta \mathbf{x}}$ is a matrix noted $\mathbf{J}_{\mathbf{y}}(\mathbf{x}) \in \mathbb{R}^{n \times m}$ that we call a **jacobian.**

$\rightarrow$ **For example**:

If $\mathbf{x} \in \mathbb{R}^n$, $\mathbf{y} \in \mathbb{R}^m$, $z \in \mathbb{R}$:

$$\mathbf{y} = g(\mathbf{x}) \text{ and } z = f(\mathbf{y})$$

Then $\frac{\delta z}{\delta \mathbf{x}} \in \mathbb{R}^n$, and

Backpropagation : vector derivatives

$\rightarrow$ As mentionned before**,** computing gradients rapidly becomes complicated when we work with **vectors**:

$\rightarrow$ **Vector to scalar**:

If $\mathbf{x} \in \mathbb{R}^n$, $y \in \mathbb{R}$:

$\frac{\delta y}{\delta \mathbf{x}}$ is a vector noted $\nabla_{\mathbf{x}} y(\mathbf{x}) \in \mathbb{R}^n$ that we call a **gradient.**

$\rightarrow$ **Vector to vector**:

If $\mathbf{x} \in \mathbb{R}^n$, $\mathbf{y} \in \mathbb{R}^m$:

$\frac{\delta \mathbf{y}}{\delta \mathbf{x}}$ is a matrix noted $\mathbf{J}_{\mathbf{y}}(\mathbf{x}) \in \mathbb{R}^{n \times m}$ that we call a **jacobian.**

$\rightarrow$ **For example**:

If $\mathbf{x} \in \mathbb{R}^n$, $\mathbf{y} \in \mathbb{R}^m$, $z \in \mathbb{R}$:

$$\mathbf{y} = g(\mathbf{x}) \text{ and } z = f(\mathbf{y})$$

Then $\frac{\delta z}{\delta \mathbf{x}} \in \mathbb{R}^n$, and $\frac{\delta z}{\delta \mathbf{x}} = \left[\frac{\delta z}{\delta x_i} \right]_{i=1}^{n}$ with $\frac{\delta z}{\delta x_i} = \sum_{j=1}^{m} \frac{\delta z}{\delta y_j} \frac{\delta y_j}{\delta x_i}$

Backpropagation : vector derivatives

$\rightarrow$ As mentionned before**,** computing gradients rapidly becomes complicated when we work with **vectors**:

$\rightarrow$ **Vector to scalar**:

If $\mathbf{x} \in \mathbb{R}^n$, $y \in \mathbb{R}$:

$\frac{\delta y}{\delta \mathbf{x}}$ is a vector noted $\nabla_{\mathbf{x}} y(\mathbf{x}) \in \mathbb{R}^n$ that we call a **gradient.**

$\rightarrow$ **Vector to vector**:

If $\mathbf{x} \in \mathbb{R}^n$, $\mathbf{y} \in \mathbb{R}^m$:

$\frac{\delta \mathbf{y}}{\delta \mathbf{x}}$ is a matrix noted $\mathbf{J}_{\mathbf{y}}(\mathbf{x}) \in \mathbb{R}^{n \times m}$ that we call a **jacobian.**

$\rightarrow$ **For example**:

If $\mathbf{x} \in \mathbb{R}^n$, $\mathbf{y} \in \mathbb{R}^m$, $z \in \mathbb{R}$:

$$\mathbf{y} = g(\mathbf{x}) \text{ and } z = f(\mathbf{y})$$

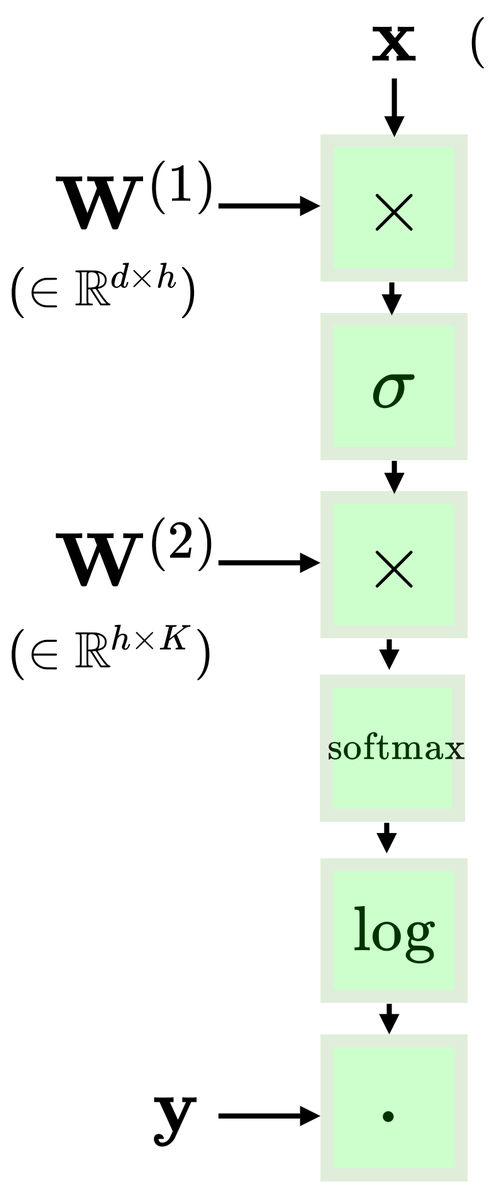
Then $\frac{\delta z}{\delta \mathbf{x}} \in \mathbb{R}^n$, and $\frac{\delta z}{\delta \mathbf{x}} = \left[\frac{\delta z}{\delta x_i} \right]_{i=1}^{n}$ with $\frac{\delta z}{\delta x_i} = \sum_{j=1}^{m} \frac{\delta z}{\delta y_j} \frac{\delta y_j}{\delta x_i}$

Hence, $\frac{\delta z}{\delta \mathbf{x}} = \frac{\delta z}{\delta \mathbf{y}} \times \frac{\delta \mathbf{y}}{\delta \mathbf{x}}^T \leftarrow$ Product of matrices !

$[1 \times n] = [1 \times m] \times [m \times n]$

Backpropagation for a MLP

Example with a **one-hidden layer MLP** which outputs a prediction over K classes: **compute the gradients** of the weights ?



$$\mathbf{a}^{(1)} = \mathbf{W}^{(1)^T}\mathbf{x}$$

$$\mathbf{h}^{(1)} = \sigma\left(\mathbf{a}^{(1)}\right) \quad (\in \mathbb{R}^h)$$

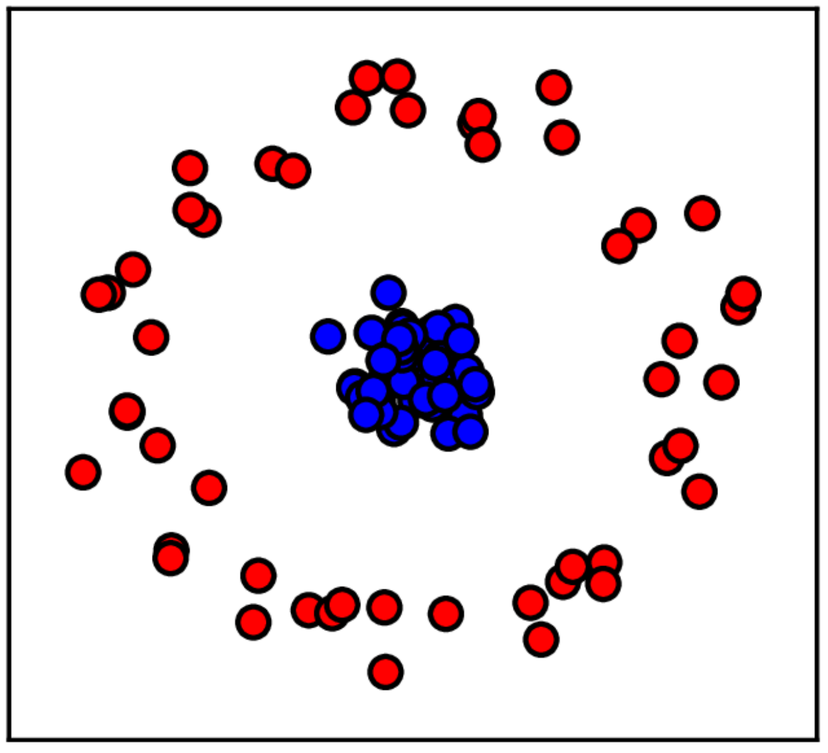
$$\mathbf{a}^{(2)} = \mathbf{W}^{(2)^T}\mathbf{h}^{(1)}$$

$$\mathbf{o} = \text{softmax}\left(\mathbf{a}^{(2)}\right) (\in \mathbb{R}^K)$$

$$l_{MLE}(\mathbf{x}, \mathbf{y}) = -\sum_{k=1}^{K} \mathbf{y}_k \log \mathbf{o}_k$$

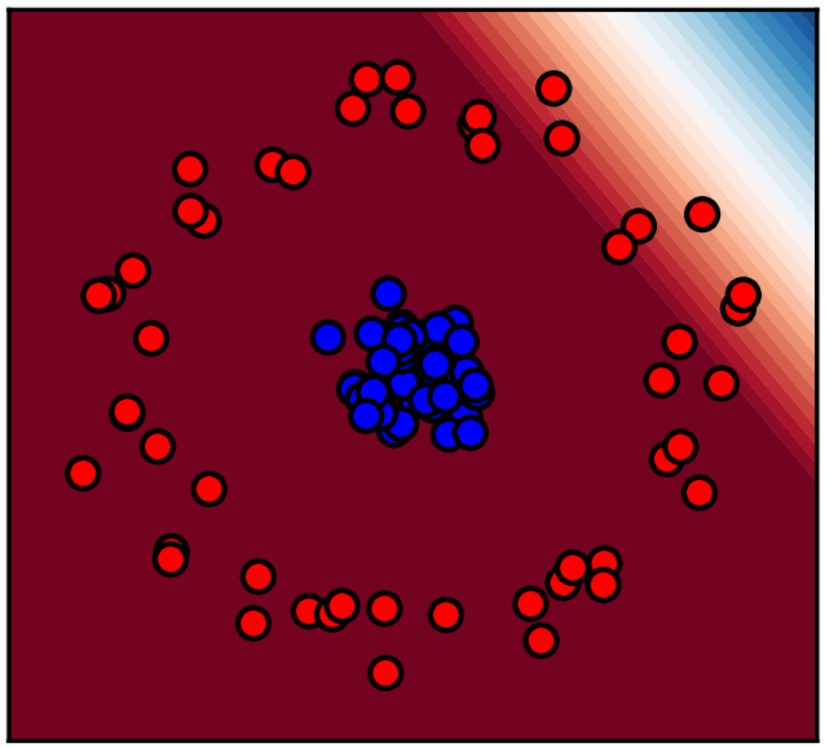
What can Neural Networks do ?

We now have a way to efficiently train neural networks. But **how many neurons** are needed for a one-layer NN to successfully separate these two classes ?



What can Neural Networks do ?

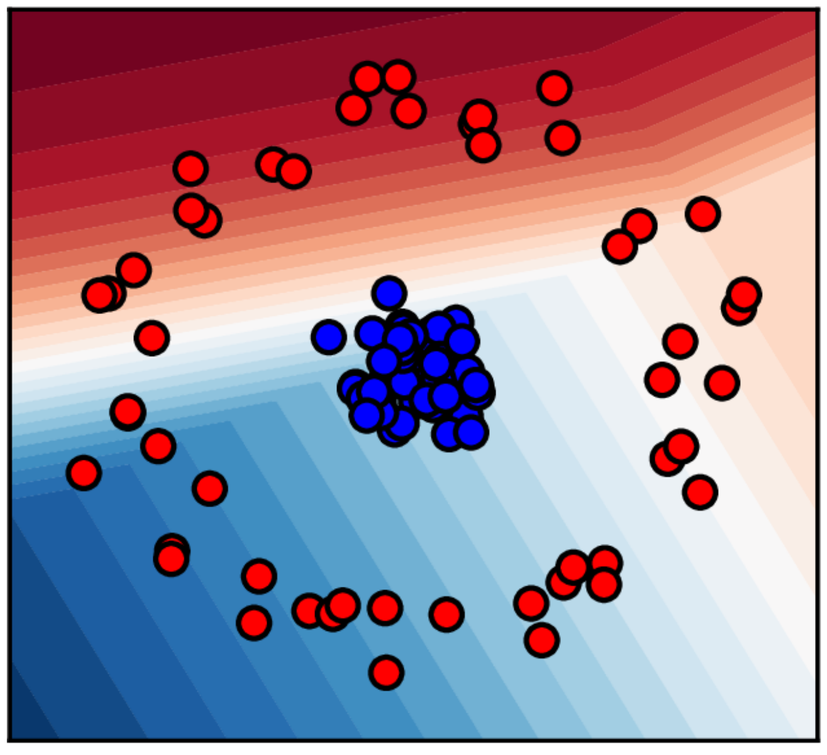
We now have a way to efficiently train neural networks. But **how many neurons** are needed for a one-layer NN to successfully separate these two classes ?



Hidden neuron: **1**

What can Neural Networks do ?

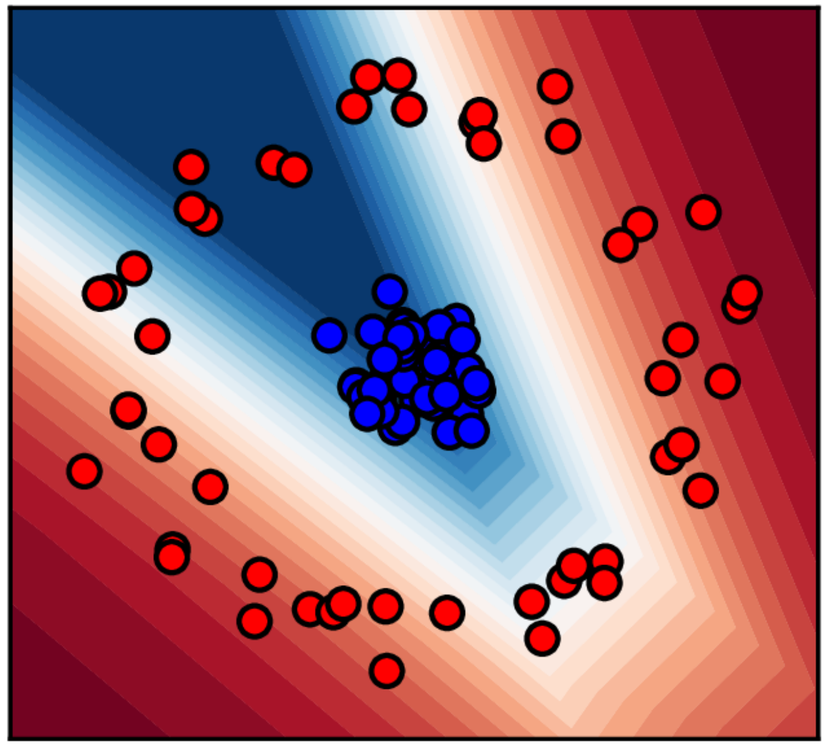
We now have a way to efficiently train neural networks. But **how many neurons** are needed for a one-layer NN to successfully separate these two classes ?



Hidden neuron: **2**

What can Neural Networks do ?

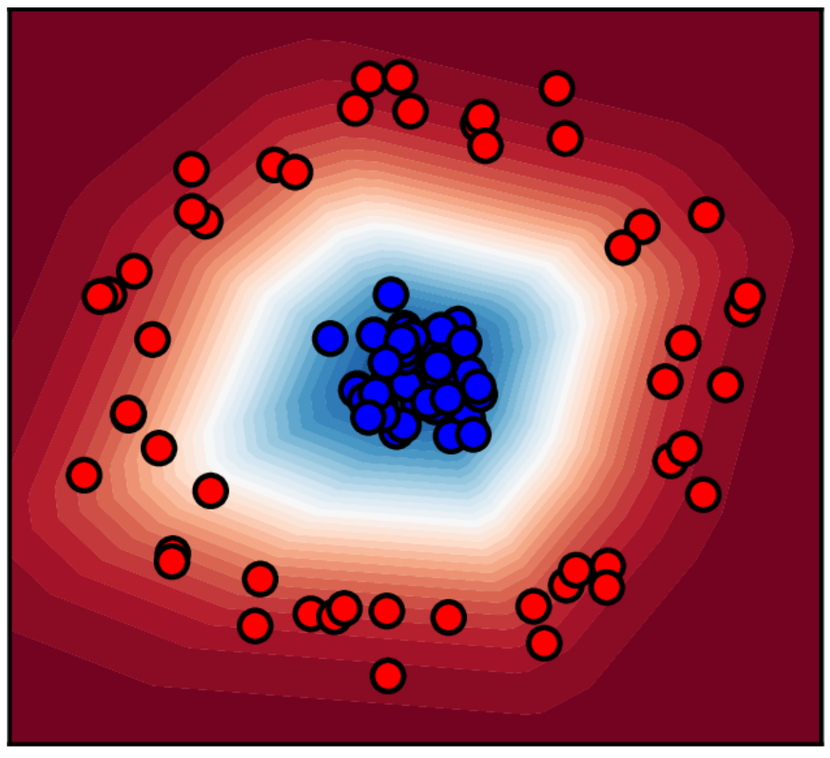
We now have a way to efficiently train neural networks. But **how many neurons** are needed for a one-layer NN to successfully separate these two classes ?



Hidden neuron: **4**

What can Neural Networks do ?

We now have a way to efficiently train neural networks. But **how many neurons** are needed for a one-layer NN to successfully separate these two classes ?



Hidden neuron: **20**

What can Neural Networks do ?

One-layer NN were proved to be **universal approximators** by Hornik et al. (*Multilayer feedforward networks are universal approximators*, 1989)

What can Neural Networks do ?

One-layer NN were proved to be **universal approximators** by Hornik et al. (*Multilayer feedforward networks are universal approximators*, 1989)

Theorem:

The family of multi-layer perceptrons with one hidden layer of $p+1$ inputs is **dense** in the space of continuous functions from a compact subset of $\mathbb{R}^p$ to $\mathbb{R}$

What can Neural Networks do ?

One-layer NN were proved to be **universal approximators** by Hornik et al. (*Multilayer feedforward networks are universal approximators*, 1989)

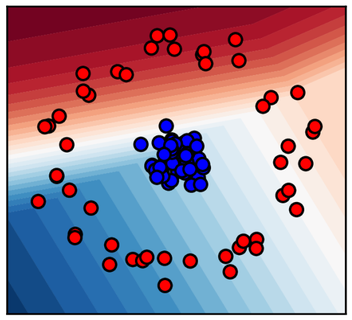
Theorem:

The family of multi-layer perceptrons with one hidden layer of $p+1$ inputs is **dense** in the space of continuous functions from a compact subset of $\mathbb{R}^p$ to $\mathbb{R}$

$\rightarrow$ For any function f in that space, there exist a number of hidden neurons N and corresponding parameters θ such that the resulting MLP is arbiratrily close to f. (Read more)

Model and hyperparameter selection

Model and hyperparameter selection



Model not able to obtain a satisfying result on the dataset

$\rightarrow$ Not enough *capacity* !

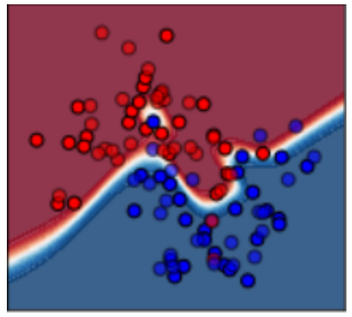
$\rightarrow$ **Underfitting**

Model and hyperparameter selection

Model obtaining great results but adapts too much to outliers

$\rightarrow$ Too much *capacity* !

$\rightarrow$ **Overfitting**



Model and hyperparameter selection

How to verify in which case we are ?

$\rightarrow$ Split data into **train** and **test** data - and choose the *hyperparameters* (here, the number of neurons, determining the capacity of the model) giving the best result on test data.

Model and hyperparameter selection

How to verify in which case we are ?

$\rightarrow$ Split data into **train** and **test** data - and choose the *hyperparameters* (here, the number of neurons, determining the capacity of the model) giving the best result on test data.

Not enough ! How will it behave on new data ?

$\rightarrow$ Split data into **train**, **validation** and **test** data - use the validation to select the best hyperparameters and verify the performance on test data.

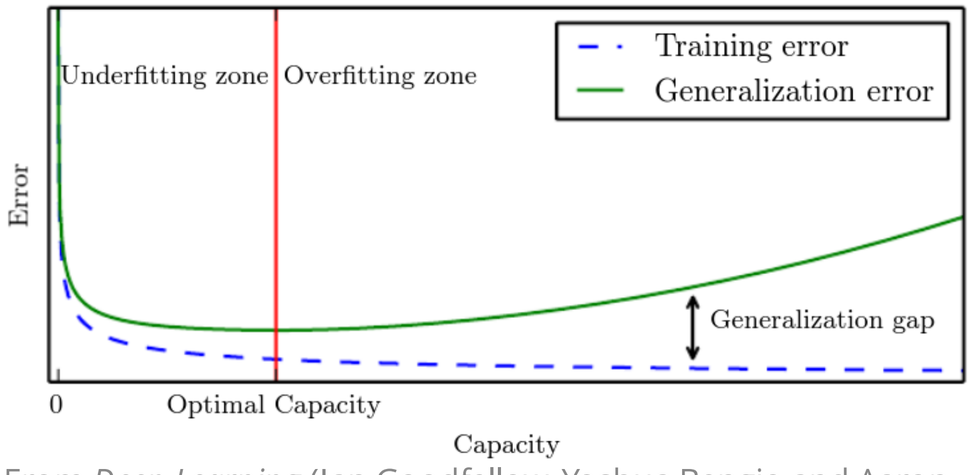
Model and hyperparameter selection

How to verify in which case we are ?

$\rightarrow$ Split data into **train** and **test** data - and choose the *hyperparameters* (here, the number of neurons, determining the capacity of the model) giving the best result on test data.

Not enough ! How will it behave on new data ?

$\rightarrow$ Split data into **train**, **validation** and **test** data - use the validation to select the best hyperparameters and verify the performance on test data.

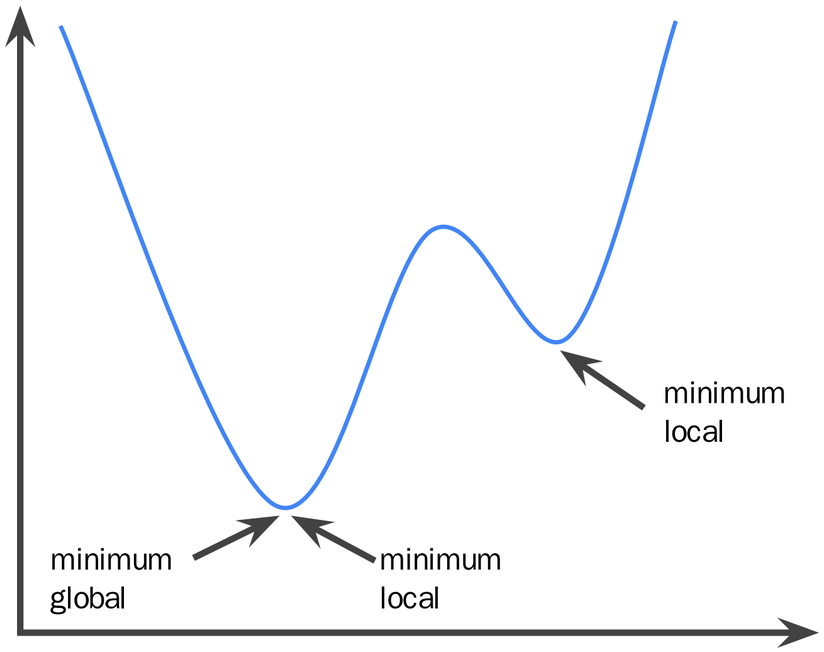


From *Deep Learning* (Ian Goodfellow, Yoshua Bengio and Aaron Courville, 2016)

$\rightarrow$ **Monitoring the error** on training and validation sets allows you to choose the capacity - but also **other hyperparameters** !

Optimization hyperparameters

Composing non-linear activations makes the loss **non-convex**
$\rightarrow$ We will probably end-up on a local minima (which can be good !)



Optimization hyperparameters

Composing non-linear activations makes the loss **non-convex**
$\rightarrow$ We will probably end-up on a local minima (which can be good !)

$\rightarrow$ How to choose the **learning rate** ϵ - a very important hyperparameter during training ?

- In case of convex optimization, we have exact search strategies.

Optimization hyperparameters

Composing non-linear activations makes the loss **non-convex**
$\rightarrow$ We will probably end-up on a local minima (which can be good !)

$\rightarrow$ How to choose the **learning rate** ϵ - a very important hyperparameter during training ?

- In case of convex optimization, we have exact search strategies.
- Simple heuristic:
  - Choose a small initial ϵ
  - Monitor the performance on validation data: if it does not increase, decay the learning rate with a value α : $\epsilon = \epsilon * \alpha$

Optimization hyperparameters

Composing non-linear activations makes the loss **non-convex**
$\rightarrow$ We will probably end-up on a local minima (which can be good !)

$\rightarrow$ How to choose the **learning rate** ϵ - a very important hyperparameter during training ?

- In case of convex optimization, we have exact search strategies.
- Simple heuristic:
  - Choose a small initial ϵ
  - Monitor the performance on validation data: if it does not increase, decay the learning rate with a value α : $\epsilon = \epsilon * \alpha$
- Other strategies:
  - Step decay: $\times \alpha \in [0, 1]$ every N epochs
  - Exponential decay: $\epsilon^{(t)} = \epsilon^{(0)} e^{(-\alpha t)}$

Regularization

Since we can not change the model capacity during training, we use an artificial constraint, **regularization**, to avoid the model *overfitting* the data

$\rightarrow$ **Weight decay** adds a tradeoff between fitting the training data and keeping the parameters small - if $\theta = \mathbf{w}$:

$$l_{Reg}(\mathbf{w}) = l_{MLE}(\mathbf{w}) + \lambda \mathbf{w}^T \mathbf{w}$$

The tradeoff is controlled by λ.

$\rightarrow$ Constraining the norm of the weights keep the model from adapting too much to the training data !

$\rightarrow$ The update rule becomes:

$$\mathbf{w}^{t+1} = (1 - 2\lambda)\mathbf{w}^t - \epsilon \nabla_{\mathbf{w}} l_{MLE}(\mathbf{w})$$

Initialization

Initialization defines the way we choose the initial values of our parameters

$\rightarrow$ This choice is highly experimental and what works will depend on the activations and the optimization procedure. Usually,

$$\mathbf{w^{(i)}} \sim \mathcal{N}(0, \frac{1}{\sqrt{d_i}})$$

Another possibility is:

$$\mathbf{w^{(i)}} \sim \mathcal{U}\left[-\frac{\sqrt{6}}{\sqrt{d_i + d_{i+1}}}, \frac{\sqrt{6}}{\sqrt{d_i + d_{i+1}}}\right]$$

$\rightarrow$ In practice, most frameworks will nowadays offer alternative solutions brought by progress on other aspects (optimization, architecture, regularization ...)

Advantages and difficulties

- Multi-layer perceptrons are very flexible in terms of possible *inputs* and *outputs*

Advantages and difficulties

- Multi-layer perceptrons are very flexible in terms of possible *inputs* and *outputs*
- With **backpropagation**, we can efficiently compute updates for a large number of parameters

Advantages and difficulties

- Multi-layer perceptrons are very flexible in terms of possible *inputs* and *outputs*
- With **backpropagation**, we can efficiently compute updates for a large number of parameters
- With **stochastic gradient descent**, we have an efficient training procedure that is adapted to a large quantity of data

Advantages and difficulties

- Multi-layer perceptrons are very flexible in terms of possible *inputs* and *outputs*
- With **backpropagation**, we can efficiently compute updates for a large number of parameters
- With **stochastic gradient descent**, we have an efficient training procedure that is adapted to a large quantity of data

However,

Advantages and difficulties

- Multi-layer perceptrons are very flexible in terms of possible *inputs* and *outputs*
- With **backpropagation**, we can efficiently compute updates for a large number of parameters
- With **stochastic gradient descent**, we have an efficient training procedure that is adapted to a large quantity of data

However,

- Gradient descent is not easy to execute
  - + Vanishing gradients, saturated gradients

Advantages and difficulties

- Multi-layer perceptrons are very flexible in terms of possible *inputs* and *outputs*
- With **backpropagation**, we can efficiently compute updates for a large number of parameters
- With **stochastic gradient descent**, we have an efficient training procedure that is adapted to a large quantity of data

However,

- Gradient descent is not easy to execute
  - + Vanishing gradients, saturated gradients
- A lot of model selection ! (Many hyperparameters)

Advantages and difficulties

- Multi-layer perceptrons are very flexible in terms of possible *inputs* and *outputs*
- With **backpropagation**, we can efficiently compute updates for a large number of parameters
- With **stochastic gradient descent**, we have an efficient training procedure that is adapted to a large quantity of data

However,

- Gradient descent is not easy to execute
  - + Vanishing gradients, saturated gradients
- A lot of model selection ! (Many hyperparameters)

$\rightarrow$ We may have may parameters and not too much data: **Overfitting !**

Advantages and difficulties

- Multi-layer perceptrons are very flexible in terms of possible *inputs* and *outputs*
- With **backpropagation**, we can efficiently compute updates for a large number of parameters
- With **stochastic gradient descent**, we have an efficient training procedure that is adapted to a large quantity of data

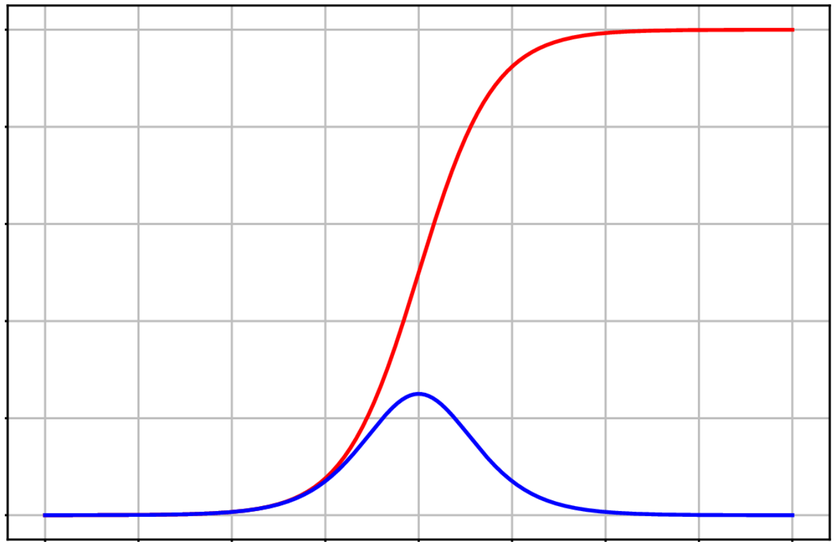
However,

- Gradient descent is not easy to execute
  - + Vanishing gradients, saturated gradients
- A lot of model selection ! (Many hyperparameters)

$\rightarrow$ Optimization is hard: **Underfitting** !

$\rightarrow$ We may have may parameters and not too much data: **Overfitting !**

Vanishing/saturated gradient: intuition



- The derivative of the activation function is:

$$\sigma' = \sigma(1 - \sigma)$$

- From the chain rule, we can see that gradients will get smaller and smaller as we go back through the layers (**vanishing**)
- When the input values are far from 0, the gradient is very small (**saturated**)
- Higher layers will learn far better than the lower ones, which will often get stuck during training

Deep Learning

Given these issues, what made Neural Networks so prevalent ?

Deep Learning

Deep Learning

- If **underfitting**:
  $\rightarrow$ Use more data\better optimization !
- If **overfitting**:
  $\rightarrow$ Find a better way to regularize !
  - **Unsupervised learning**:
    Initialize hidden layers using *unsupervised learning* to have the network represent the latent structure of the input.
    $\rightarrow$ Harder task, less overfitting !
    $\rightarrow$ Hidden layers encode the 'general' structure of the data before the supervised training !
  - **Dropout**:
    Randomly remove parts of the hidden layers.
    $\rightarrow$ Stops the network from 'copying' data !

Better optimization: Adaptive Gradient

- Choosing a learning rate is difficult: learning rate schedules adjust the learning rate during training but have to be defined in advance
- The same learning rate applies to all parameter updates

$\rightarrow$ Adapt the rate of learning to the gradient - for example, with:

$$\theta^{t+1} = \theta^t - \epsilon \frac{\delta l_{MLE}}{\delta \theta}$$

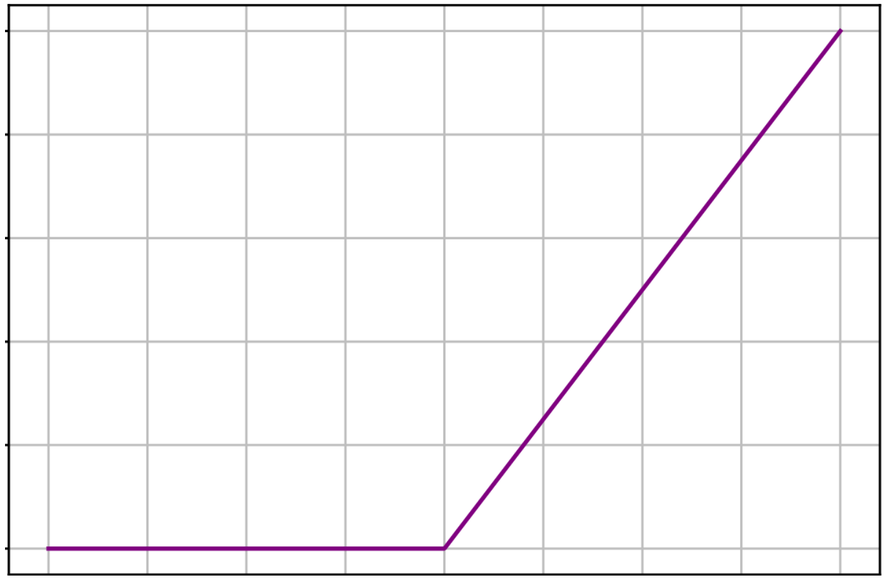
$$\downarrow$$

$$g^{t+1} = g^t + \left(\frac{\delta l_{MLE}}{\delta \theta} \right)^2$$

$$\theta^{t+1} = \theta^t - \frac{\epsilon}{\sqrt{g^{t+1}}} \times \frac{\delta l_{MLE}}{\delta \theta}$$

Which is close to **Adagrad** (Duchi et al, 2011), while **Adadelta** (Zeiler et al, 2012) and especially **Adam** (Kingma et al, 2015) are often used.

Better activation: ReLU



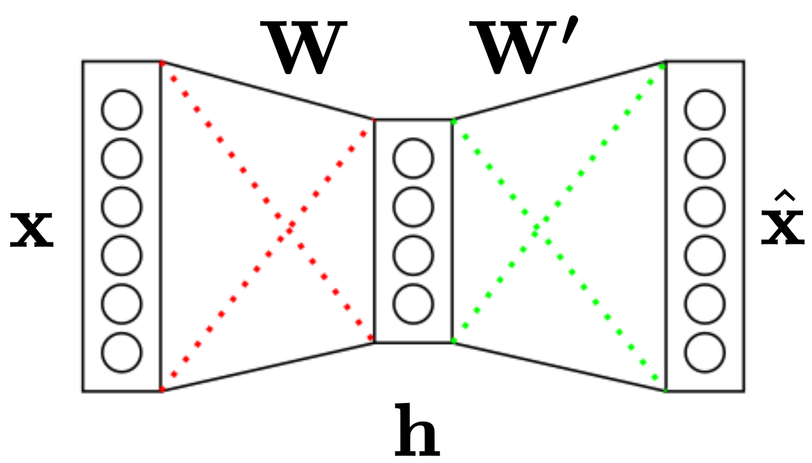
$$relu(x) = max(0, x)$$

$\rightarrow$ **ReLU** (Glorot et al.2011) allows for efficient gradient passing, avoiding saturated and vanishing gradients !

$\rightarrow$ There exists many more recent variants.

Parenthesis: Autoencoders

- *Autoencoder*: Feed-forward neural network trained to re-build its input through a hidden representation.
  $\rightarrow$ **Unsupervised learning** !



- Encoder:

$$\mathbf{h} = \phi\left(\mathbf{W}^T\mathbf{x} + \mathbf{b}\right)$$

- Decoder:

$$\hat{\mathbf{x}} = \mathbf{W}'^T\mathbf{h} + \mathbf{b}'$$

- Loss function: sum of squared differences ($\theta = \{\mathbf{W}, \mathbf{W}', \mathbf{b}, \mathbf{b}'\}$)

$$l_{L2}(\mathbf{x}|\theta) = \frac{1}{2}\sum_k (\hat{x}^k - x^k)^2$$

- Weights $\mathbf{W}$ and $\mathbf{W}'$ can also be tied: $\mathbf{W}' = \mathbf{W}^T$

Parenthesis: Autoencoders

From Hugo Larochelle's class on neural networks, part [6.2]

- Important remark: The squared distance loss assumes that data is coming from an **isotropic gaussian** !

Parenthesis: Autoencoders

From Hugo Larochelle's class on neural networks, part [6.2]

- Important remark: The squared distance loss assumes that data is coming from an **isotropic gaussian** !
- Why ? Assuming this data $\mathbf{x}$ comes from a distribution $p(\mathbf{x}|\mu)$ with parameters μ:
  - Autoencoder = choose the relationship between μ and the hidden representation $\mathbf{h}$ to be ...
    $\rightarrow$ linear transformation + non-linearity !
  - Noting $l(\mathbf{x}) = -\log p(\mathbf{x}|\mu)$ the likelihood of the data being generated from this transformation of $\mathbf{h}$

Parenthesis: Autoencoders

From Hugo Larochelle's class on neural networks, part [6.2]

- Important remark: The squared distance loss assumes that data is coming from an **isotropic gaussian** !
- Why ? Assuming this data $\mathbf{x}$ comes from a distribution $p(\mathbf{x}|\mu)$ with parameters μ:
  - Autoencoder = choose the relationship between μ and the hidden representation $\mathbf{h}$ to be ...
    $\rightarrow$ linear transformation + non-linearity !
  - Noting $l(\mathbf{x}) = -\log p(\mathbf{x}|\mu)$ the likelihood of the data being generated from this transformation of $\mathbf{h}$

- Now, assuming data from an isotropic gaussian with mean μ:
  - $p(\mathbf{x}|\mu) = \frac{1}{(2\pi)^{D/2}} \exp\left(-\frac{1}{2}\sum_k (x^k - \mu^k)^2\right)$
  - We choose $\mu = \mathbf{W}^T\mathbf{h} + \mathbf{b}$; and obtain the squarred error loss !

Parenthesis: Autoencoders

From Hugo Larochelle's class on neural networks, part [6.4]

- Important remark: assuming a linear decoder, the **linear** encoder (no activation function for $\mathbf{h}$) is **actually optimal** for minimizing the training square error !

Parenthesis: Autoencoders

From Hugo Larochelle's class on neural networks, part [6.4]

- Important remark: assuming a linear decoder, the **linear** encoder (no activation function for $\mathbf{h}$) is **actually optimal** for minimizing the training square error !
- The proof relies on the result that the SVD decomposition of a matrix where we keep only the k largest singular values produces the closest matrix of rank k to the original matrix
  - We show that, with k the hidden layer size, **the encoder minimizing the square error comes from the SVD decomposition limited to the k largest singular values**, hence is linear.
  - Intuitive result: if the data is standardized, the encoder coresponds to the Principal Component Analysis (PCA)

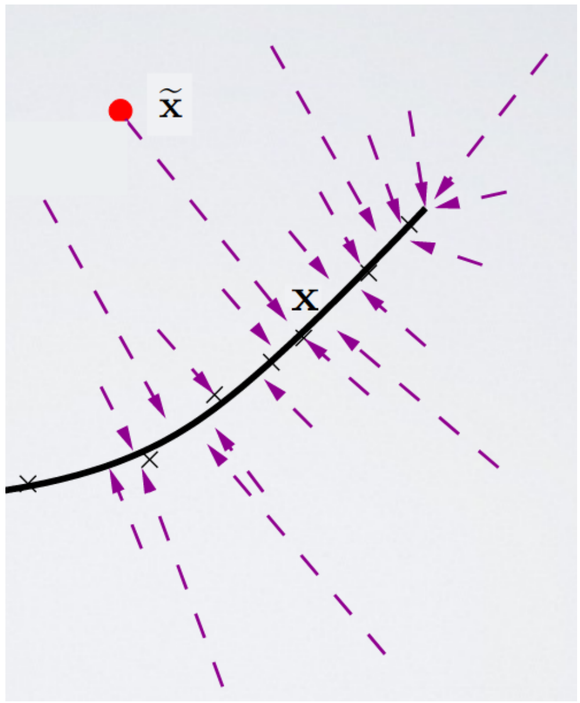
Parenthesis: Autoencoders

- Then, what's the point of using an autoencoder ?
  - If we choose a **smaller hidden size**, we compress the data, but that works only for the training distribution
  - If we choose a **larger hidden size**, the autoencoder could just copy each input component and not extract anything

Parenthesis: Autoencoders

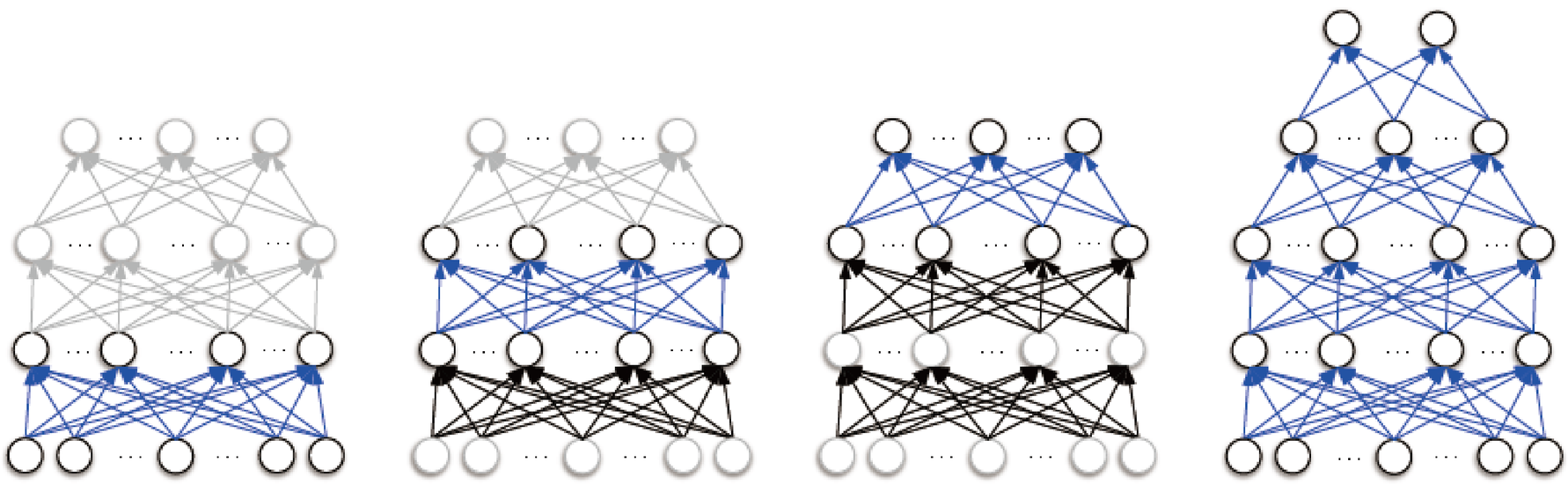
- Then, what's the point of using an autoencoder ?
  - If we choose a **smaller hidden size**, we compress the data, but that works only for the training distribution
  - If we choose a **larger hidden size**, the autoencoder could just copy each input component and not extract anything
- Idea: make the hidden representation robust to noise !
  - Use noise to create corrupted $\tilde{\mathbf{x}}$, and reconstruct $\hat{\mathbf{x}}$.
  - The loss function compares $\hat{\mathbf{x}}$ to the noiseless $\mathbf{x}$!

$\rightarrow$ **Denoising autoencoder** (Vincent et al, 2008) : forces the model to learn about the structure of data !



From Hugo Larochelle's class on neural networks, part [6.6]

Better initialization: Unsupervised pre-training



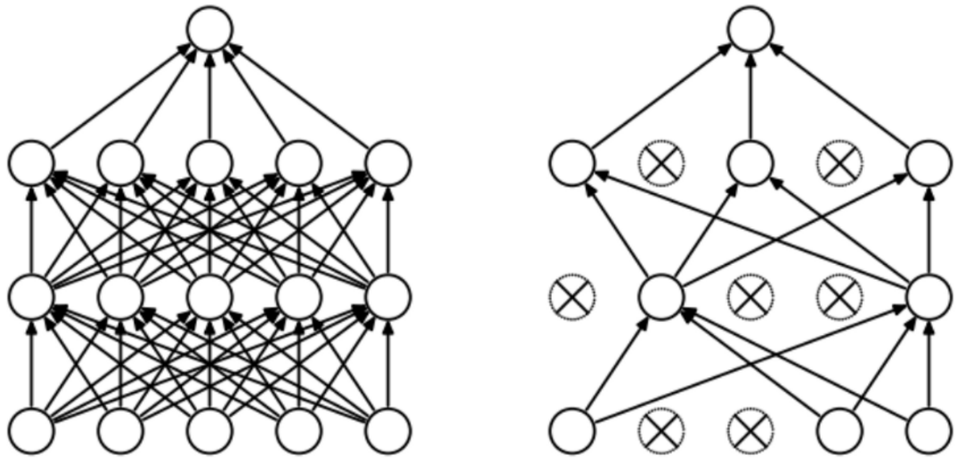
Layer-wise Pre-training followed by **Training the whole network**

- Intuition: when you cannot really escape from the initial (random) point, find a good starting point $\rightarrow$ **unsupervised** learning !
- This is done by training a **denoising auto-encoder** (but later, other methods !) layer by layer to rebuild the altered input of the layer.
- After unsupervised **pre-training**, add an output layer and train with supervised learning: this is called **fine-tuning**.

Better regularization: Dropout

- For each training example : randomly turn-off hidden units with probability p
- At test time, use each unit scaled down by p

From (Srivastava et al, 2014)



- Intuition: similar idea to denoising autoencoders.
- In practice: do backpropagation with **random masks** and replace them by their expectation at test time.
- Dropout aims to **separate effects** from strongly correlated features: each unit needs to be useful on its own.
- It can be seen as averaging different models that share parameters

$\rightarrow$ It acts as powerful **regularization** scheme

Deep Learning

- 1995: **Convolutionnal** Neural Networks (Lecun, Bengio)

Deep Learning

- 1995: **Convolutionnal** Neural Networks (Lecun, Bengio)
- 1997: **Long-Short Term Memory** NN (Hochreiter, Schmidhuber)

Deep Learning

- 1995: **Convolutionnal** Neural Networks (Lecun, Bengio)
- 1997: **Long-Short Term Memory** NN (Hochreiter, Schmidhuber)
- Early 2000s: Development of **GPUs**

Deep Learning

- 1995: **Convolutionnal** Neural Networks (Lecun, Bengio)
- 1997: **Long-Short Term Memory** NN (Hochreiter, Schmidhuber)
- Early 2000s: Development of **GPUs**
- Late 2000s:
  - Very large datasets of Image are created (**Imagenet**)
    $\rightarrow$ Deeper models can be trained
  - Efficient **initialization** with unsupervised learning (**pre-training**)
    $\rightarrow$ Deeper models can avoid vanishing gradients

Deep Learning

Besides, improvements such as:

- **Dropout** (Regularization technique)
- **Re**ctified **L**inear **U**nit (activation)

Deep Learning

Besides, improvements such as:

- **Dropout** (Regularization technique)
- **Re**ctified **L**inear **U**nit (activation)

.... helped deep neural models to win challenges:

- ImageNet - since 2012 (Krizhevsky et al, 2012)

Deep Learning

Besides, improvements such as:

- **Dropout** (Regularization technique)
- **Re**ctified **L**inear **U**nit (activation)

.... helped deep neural models to win challenges:

- ImageNet - since 2012 (Krizhevsky et al, 2012)
- Traffic signs Recognition : in 2011 (Ciresan et al, 2012)

Deep Learning

Besides, improvements such as:

- **Dropout** (Regularization technique)
- **Re**ctified **L**inear **U**nit (activation)

.... helped deep neural models to win challenges:

- ImageNet - since 2012 (Krizhevsky et al, 2012)
- Traffic signs Recognition : in 2011 (Ciresan et al, 2012)
- Handwritting recognition - since 2009 (Graves et al, 2009)

Deep Learning

Besides, improvements such as:

- **Dropout** (Regularization technique)
- **Re**ctified **L**inear **U**nit (activation)

.... helped deep neural models to win challenges:

- ImageNet - since 2012 (Krizhevsky et al, 2012)
- Traffic signs Recognition : in 2011 (Ciresan et al, 2012)
- Handwritting recognition - since 2009 (Graves et al, 2009)
- Automatic Speech Recognition (Hinton et al, 2012)

Deep Learning

Besides, improvements such as:

- **Dropout** (Regularization technique)
- **Re**ctified **L**inear **U**nit (activation)

.... helped deep neural models to win challenges:

- ImageNet - since 2012 (Krizhevsky et al, 2012)
- Traffic signs Recognition : in 2011 (Ciresan et al, 2012)
- Handwritting recognition - since 2009 (Graves et al, 2009)
- Automatic Speech Recognition (Hinton et al, 2012)

The expression "*Deep Learning*" was coined around 2006 from work on unsupervised pre-training (Hinton et al, 2006; Bengio et al, 2007)

What else is new ?

Architectures !

- *Convolutional networks*, specialized for processing a grid of values, like time-series and images
- *Recurrent networks*, specialized for processing sequences of values of arbitrary sizes
- Networks adapted to more specific structures: Recursive networks, Tree-Recurrent networks, *Graph Neural Networks*
- *Attention mechanism* and its adaptation to create faster layers for processing sequences: the *transformer* layers.

→ **Idea** : use a model that will:

- Take advantage of the **structure** of the data
- **Capture the invariance** of a problem

Deep Learning

And besides innovations in **Architecture**, **Regularization**, **and Optimization** ...

- Tremendous improvement of computational capacity
- Availability of huge datasets

Deep Learning

And besides innovations in **Architecture**, **Regularization**, **and Optimization** ...

- Tremendous improvement of computational capacity
- Availability of huge datasets

Why does it work ?

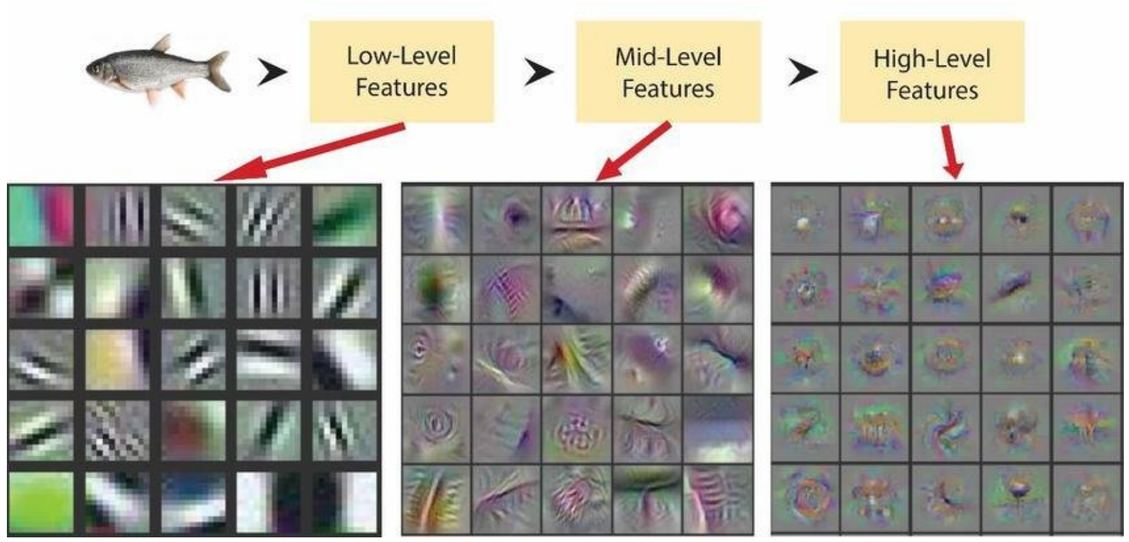
Deep Learning

And besides innovations in **Architecture**, **Regularization**, **and Optimization** ...

- Tremendous improvement of computational capacity
- Availability of huge datasets

Why does it work ?

→ Deep learning is especially relevant for complex inputs like *images*, natural language, because it is especially good at learning **better data representation**.



From *Automatic fish species classification in underwater videos* (Siddiqui et al, 2016)

DL: a kind of representation learning

Various (tied !) ideas explaining the success of deep learning:

- It makes great use of *distributed representations*, allowing **generalization** (through shared features and **smoothness**) : the deep network is able to compactly represent complicated structures using a small number of features automatically !
- Learning to accomplish a task on some data will organize the hidden representation of this data to be easy to process for the task (discovering *explanatory factors*)
- Exponential gain through **depth**: features learned can be organized and re-used **hierarchicaly**, with more abstract representations on the top.
- All of these ideas are especially relevant when working in very high dimensions ....

Deep Learning

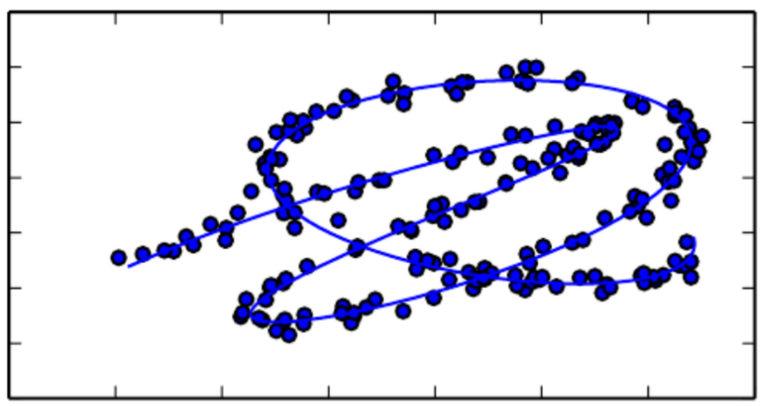
From *Deep Learning* (Ian Goodfellow, Yoshua Bengio and Aaron Courville, 2016)

$\rightarrow$ As the number of dimension increases, the number of possible relevant configurations increases **exponentially**, and the number of training examples to learn about them increases too !

Deep Learning

From *Deep Learning* (Ian Goodfellow, Yoshua Bengio and Aaron Courville, 2016)

$\rightarrow$ As the number of dimension increases, the number of possible relevant configurations increases **exponentially**, and the number of training examples to learn about them increases too !



$\rightarrow$ Learning incrementally abstract representations may help us discover the underlying **manifold**

Acknowledgements & References

From the slides by **Florence d'Alché-Buc** and by **Alexandre Allauzen**

Some references:

- *The Deep Learning Book*, Chapters 5, 6, 7, 8, 11, 14 and 15 !
- Hugo Larochelle's class.
- Y. Bengio et al (2007). *Greedy Layer-Wise Training of Deep Networks* - NIPS
- X. Glorot et al (2011). *Deep Sparse Rectifier Neural Networks* - JMLR
- N. Srivastava et al (2014). *Dropout: a simple way to prevent neural networks from overfitting* - JMLR
- Duchi, J., Hazan, E., & Singer, Y. (2011). *Adaptive Subgradient Methods for Online Learning and Stochastic Optimization* - JMLR
- Zeiler, M. D. (2012). *ADADELTA: An Adaptive Learning Rate Method*
- Kingma, D. P., & Ba, J. L. (2015). *Adam: a Method for Stochastic Optimization* - ICLR