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small evolutions : Patrick Reignier

Grenoble INP-Ensimag

2025-2026

Outline

About this class

- Deep learning
  - Very dynamic field of research
    - Increased computational power
    - Increased data availability

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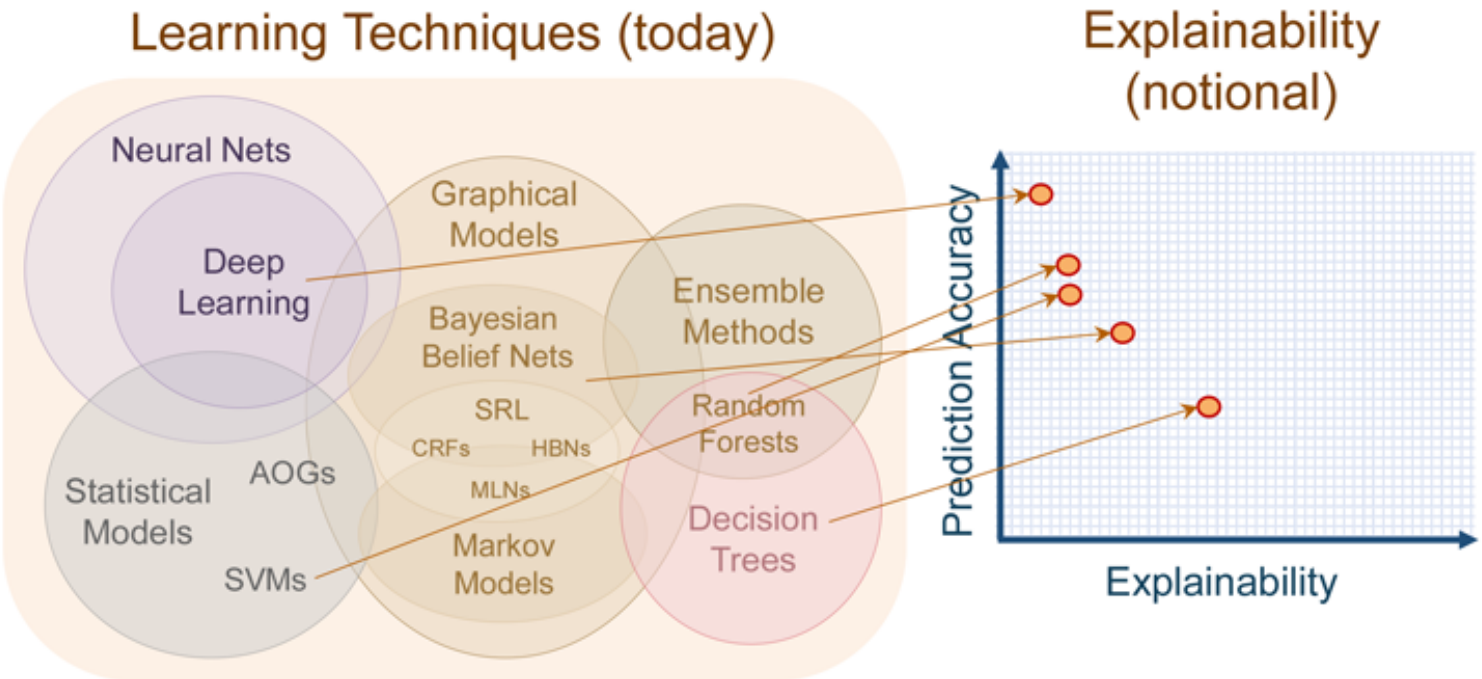
  - **Nb:** you may feel lost at the beginning of the hands-on labs but everything will fall into place with time

Prediction Accuracy vs Explainability



"Bornstein, Aaron M. "Is Artificial Intelligence Permanently Inscrutable?". Nautilus , no. (2016)."

Main outline

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

Timetable

1. Introduction, multilayer perceptrons, forward propagation
   - Hands-on: forward propagation
2. Gradient descents, backpropagation
   - Hands-on: backpropagation for stochastic gradient descent
3. Mini-batch gradient descent, gradient descent optimization
   - Hands-on: mini-batch gradient descent
4. Hands-on: mini-batch, Momentum
5. Regularization
   - Hands-on: L2 regularization
6. Feature preprocessing, batch normalization
   - Pricing project
7. Energy considerations
   - Pricing project
8. Pricing project

Some resources

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

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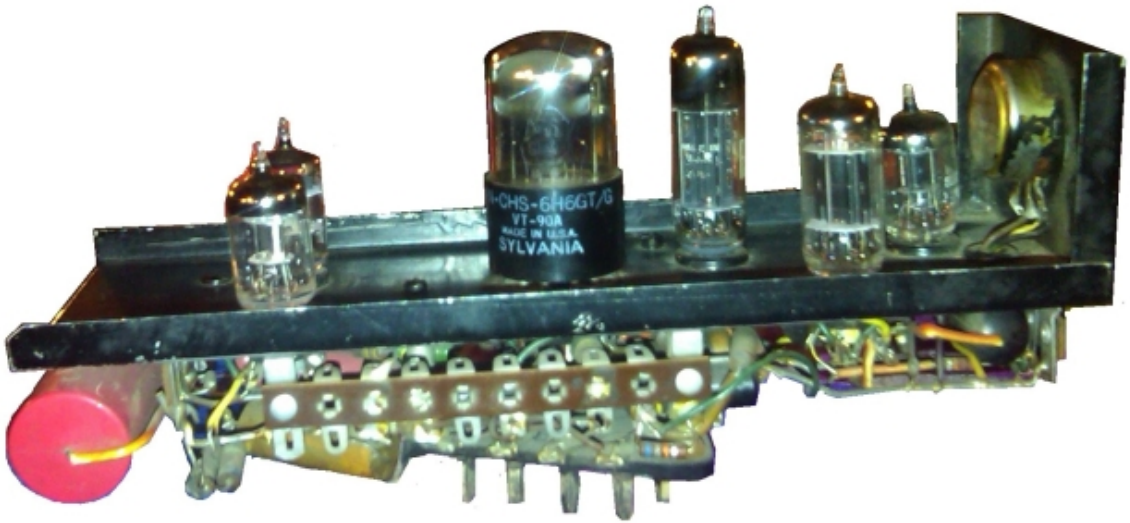
1951 M. Minsky and D. Edmonds: Stochastic Neural Analog Reinforcement Calculator (SNARC)

- First neural network machine

SNARC



- Image : `https://cyberneticzoo.com/mazesolvers/1951-maze-solver-minsky-edmonds-american/`
- Learning through trial and error (kind of reinforcement learning)
  - Feedback provided by the operator
- 40 neurons
- Simulate the behavior of a rat in a maze searching for food

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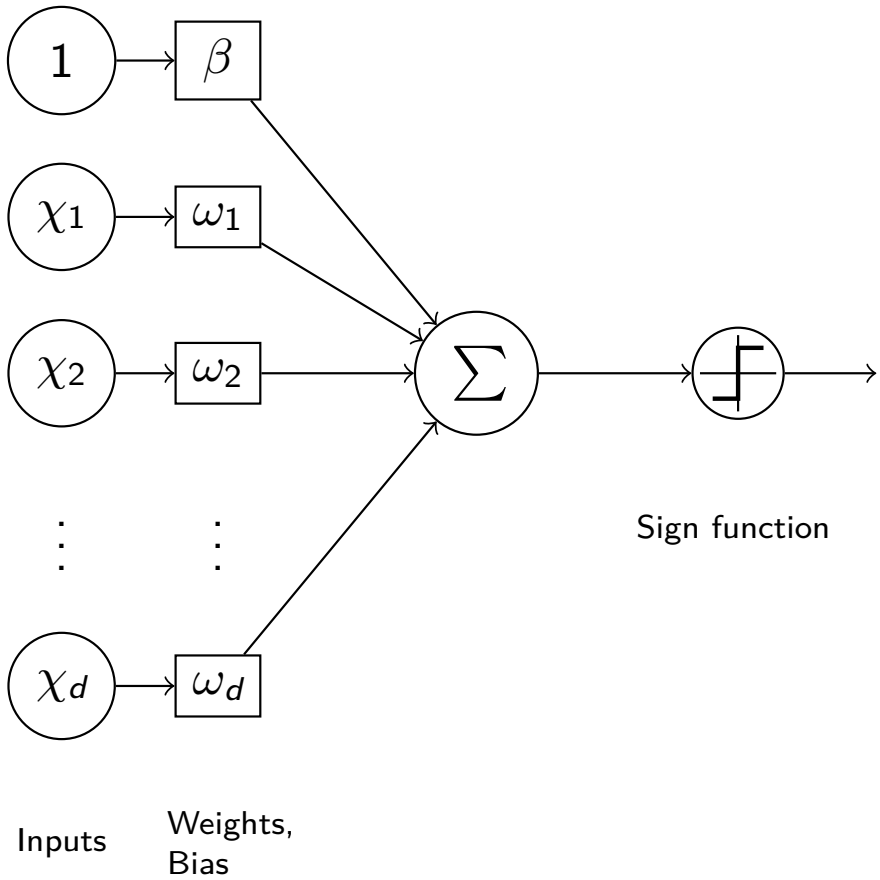

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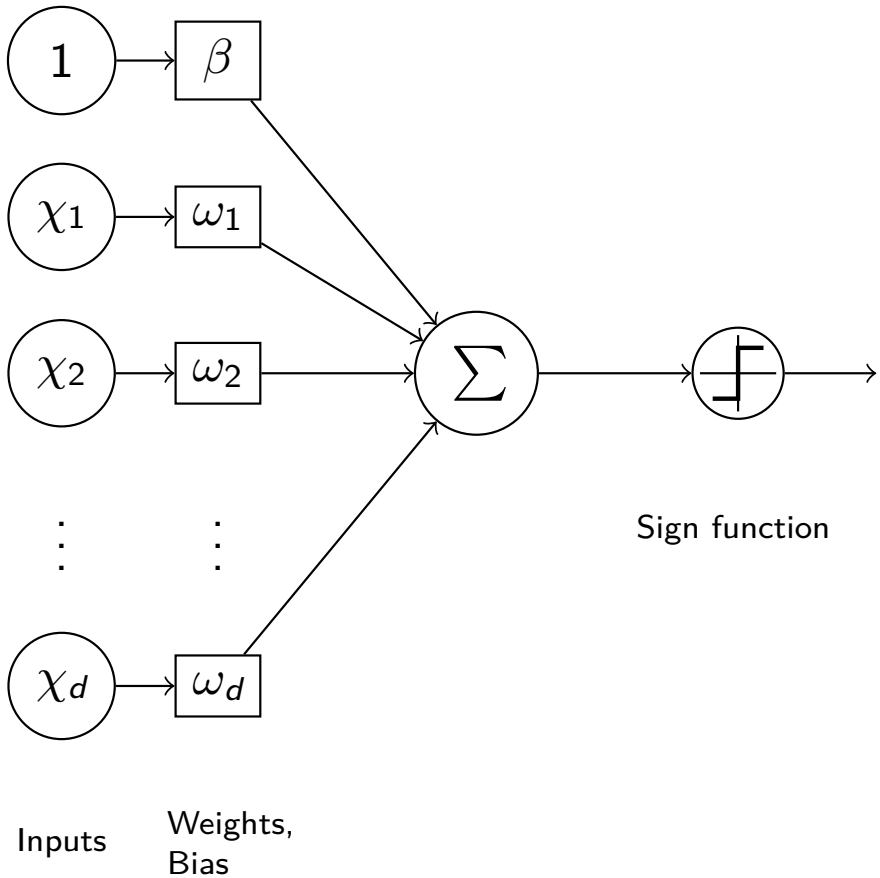

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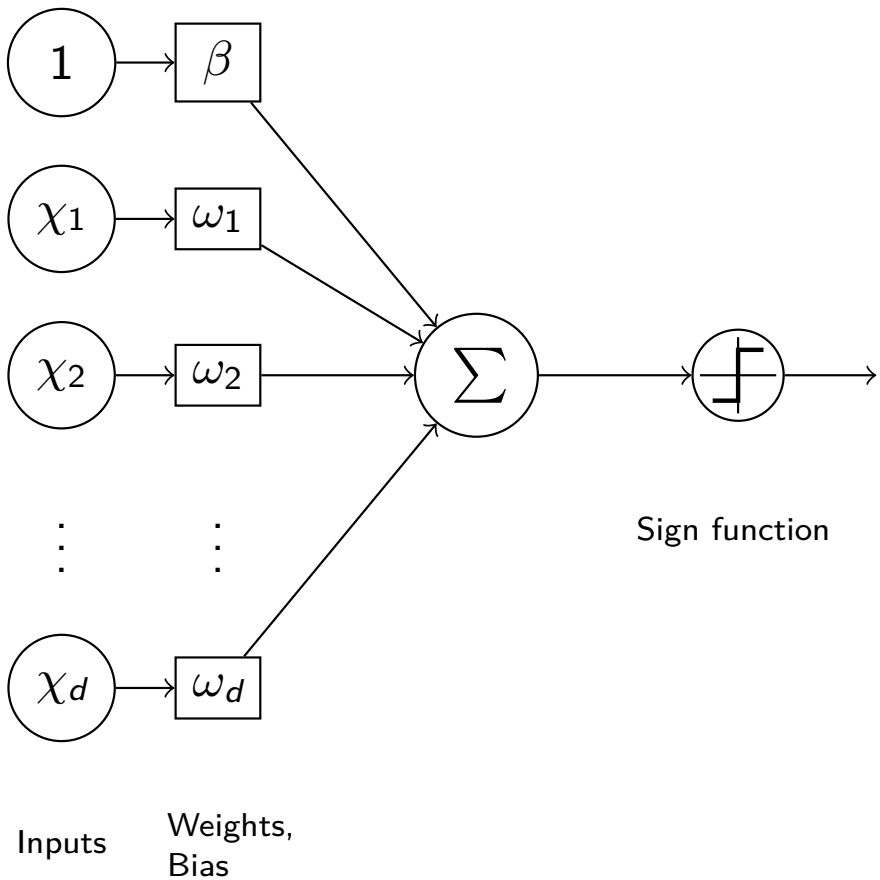

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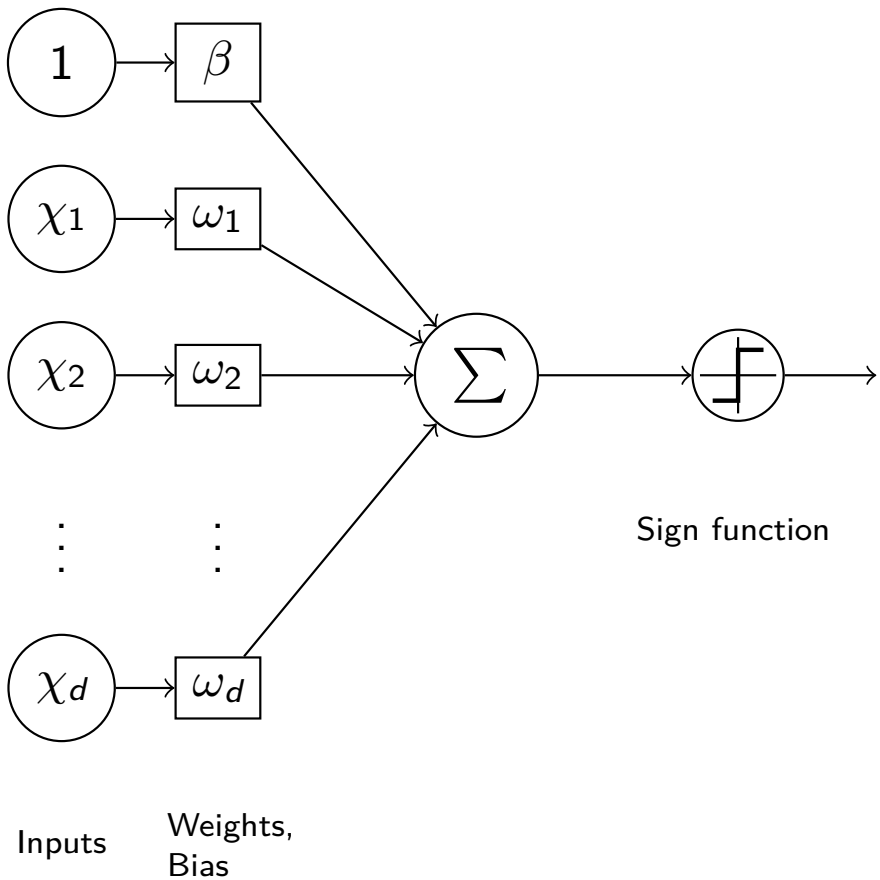
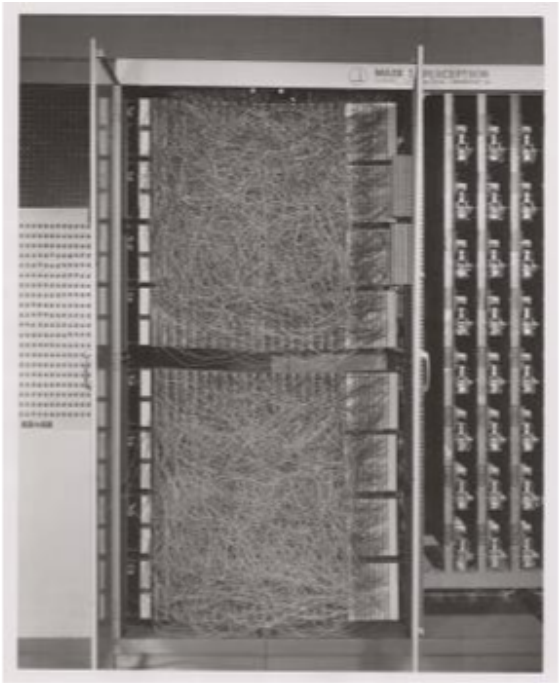
- Reformulation: find ω, β such that $\forall i = 1, \ldots, N$, $\rho_{(i)} \cdot (\omega^{\mathrm{T}}\chi_{(i)} + \beta) > 0$



Mark1 - Perceptron



By Source (WP:NFCC#4), Fair use,
https://en.wikipedia.org/w/index.php?curid=47541432

Parameter update algorithm

We define:

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

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

$\theta \leftarrow (0, \ldots, 0)^{\mathrm{T}}$;
while $\exists j \in \{1, \ldots N\}$ *such that* $\rho_{(j)} \cdot \mathrm{sign}(\theta^{\mathrm{T}} \overline{\chi_{(j)}}) < 0$ **do**
  $\theta \leftarrow \theta + \rho_{(j)} \overline{\chi_{(j)}}$
end
return θ

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- We have (See, e.g., `http://www.cs.columbia.edu/~mcollins/courses/6998-2012/notes/perc.converge.pdf`):

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

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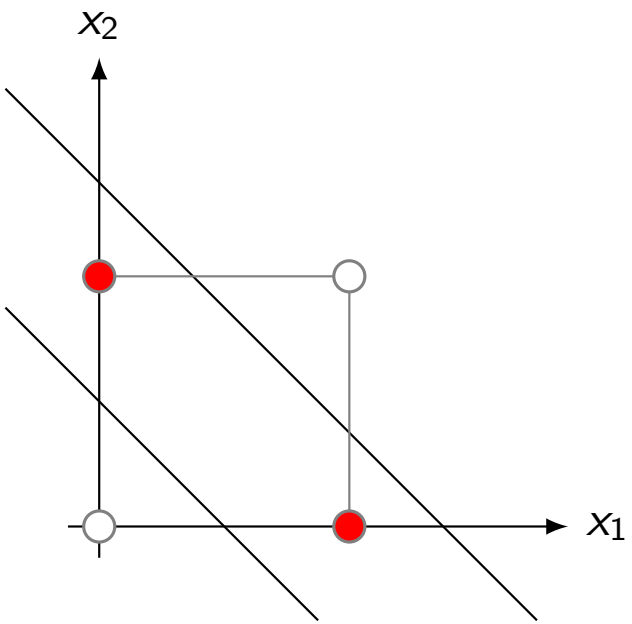

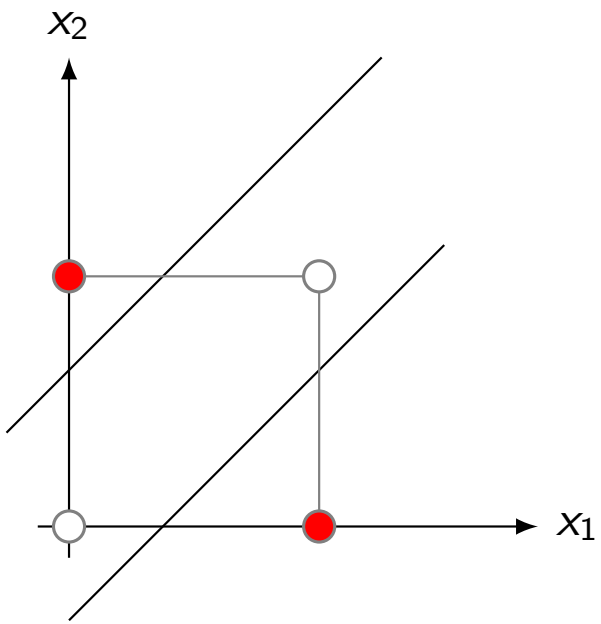

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- Minsky & Papert: there are simple functions that cannot be learned
  - This negative result slowed research on neural networks for a long time
- Question: what happens if we generalize the perceptron by
  - Interconnecting several neurons together
  - Allowing activation functions other than the sign function?

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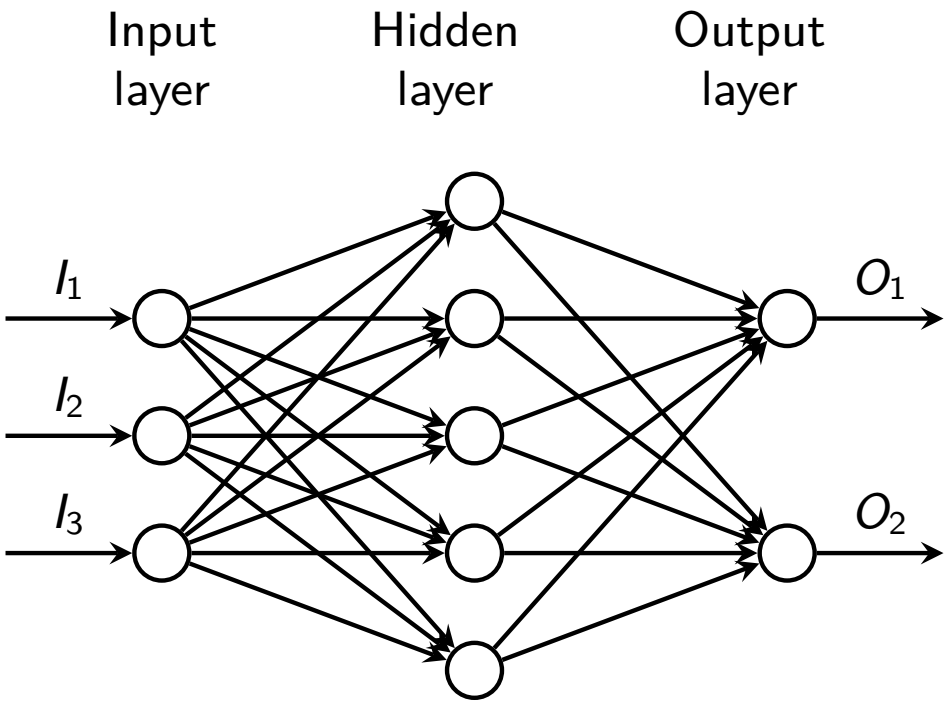
- Computations are performed in the hidden and output layers.

Fully connected multilayer perceptron (3 layers)



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

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

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- The activation function of ν_k^i is Φ, so that $\alpha_k^i = \Phi(\zeta_k^i)$
  - Unless stated otherwise (e.g., **Dropout**), we assume it is the same for all neurons

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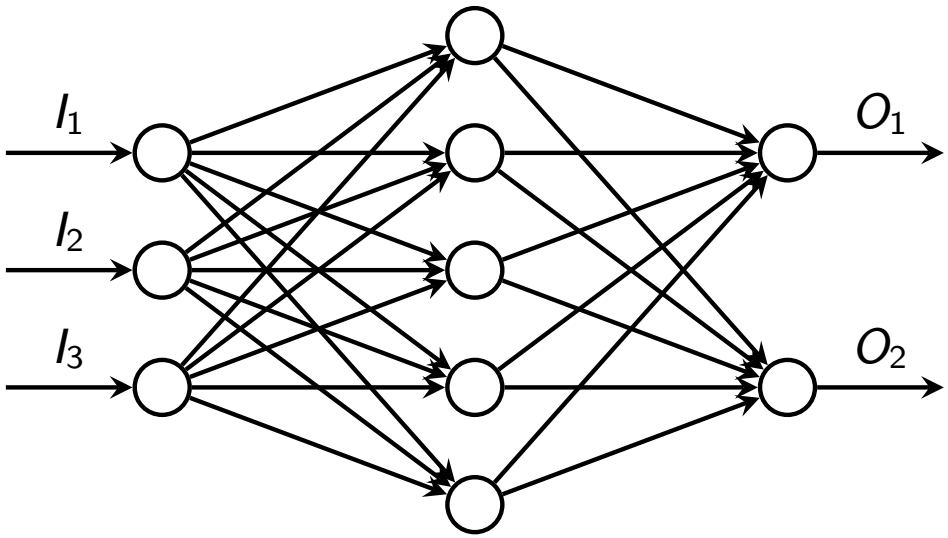
- The **activation** of ν_k^i is denoted by α_k^i
- The activation function of ν_k^i is Φ, so that $\alpha_k^i = \Phi(\zeta_k^i)$
  - Unless stated otherwise (e.g., **Dropout**), we assume it is the same for all neurons

Assumption

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

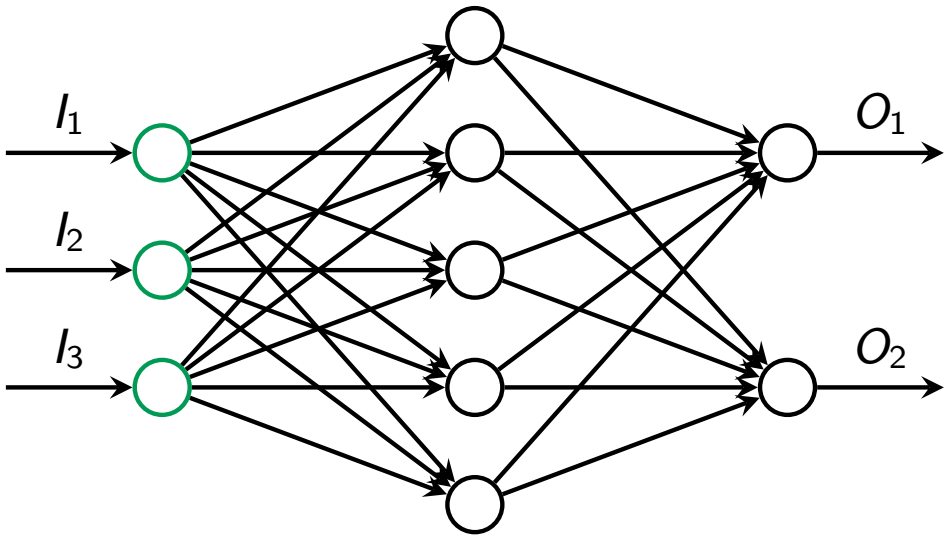
Forward propagation: an illustration



Forward propagation: an illustration

Neuron ν_1^1:

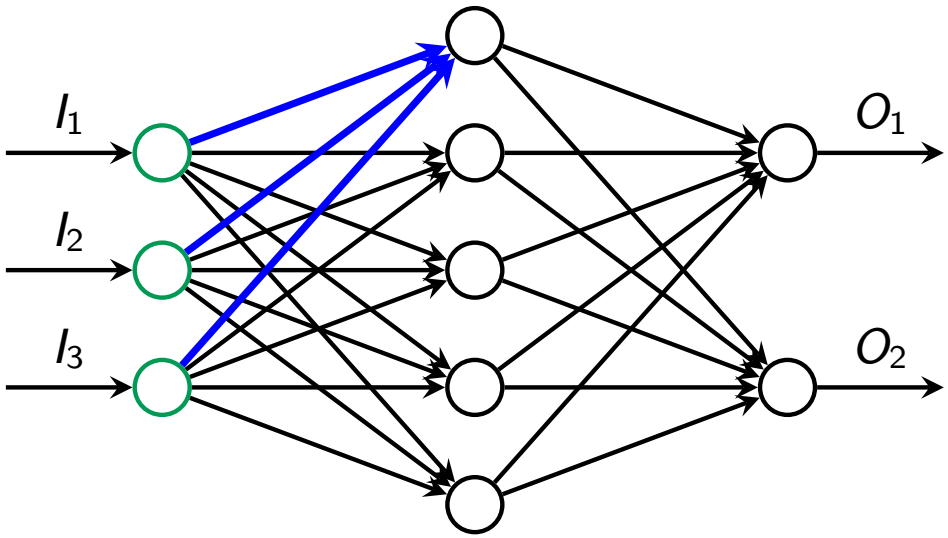
- Input: $\alpha_1^0, \alpha_2^0, \alpha_3^0$



Forward propagation: an illustration

Neuron ν_1^1:

- Input: $\alpha_1^0, \alpha_2^0, \alpha_3^0$
- Weights: $\omega_{1,1}^1$, $\omega_{2,1}^1$, $\omega_{3,1}^1$
- Bias: β_1^1



Forward propagation: an illustration

Neuron ν_1^1:

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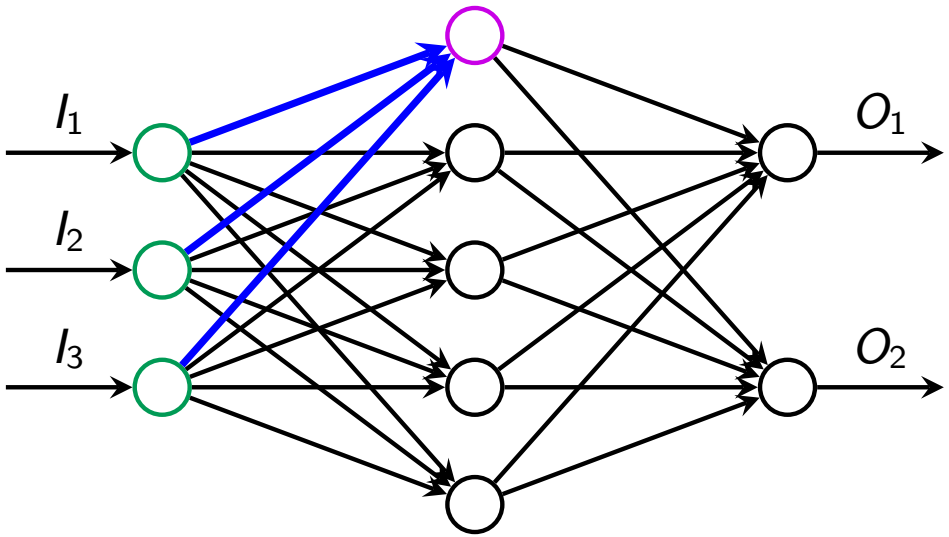
- Weights: $\omega_{1,1}^1$, $\omega_{2,1}^1$, $\omega_{3,1}^1$
- Bias: β_1^1
- Net input: $\zeta_1^1 = \omega_{1,1}^1 \cdot \alpha_1^0 + \omega_{2,1}^1 \cdot \alpha_2^0 + \omega_{3,1}^1 \cdot \alpha_3^0 + \beta_1^1$



Forward propagation: an illustration

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- Input: $\alpha_1^0, \alpha_2^0, \alpha_3^0$
- Weights: $\omega_{1,1}^1$, $\omega_{2,1}^1$, $\omega_{3,1}^1$
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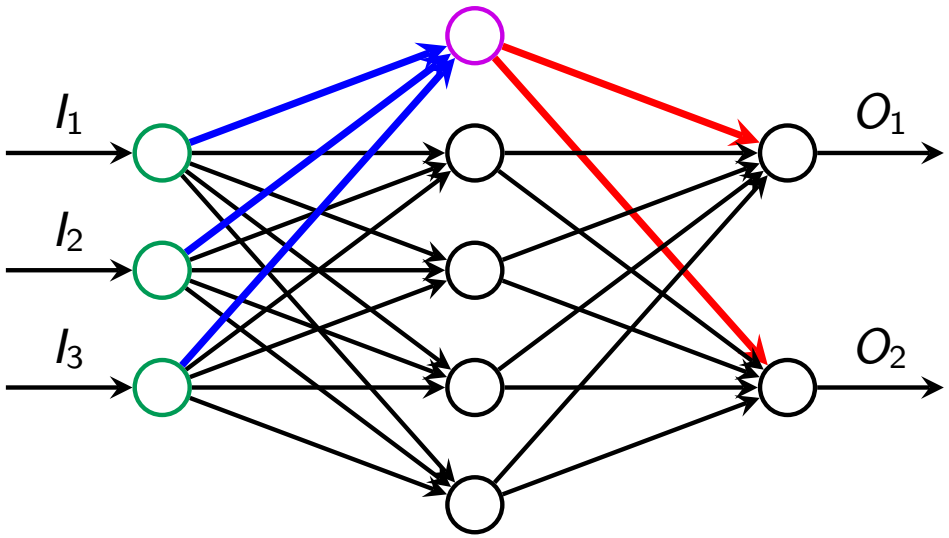
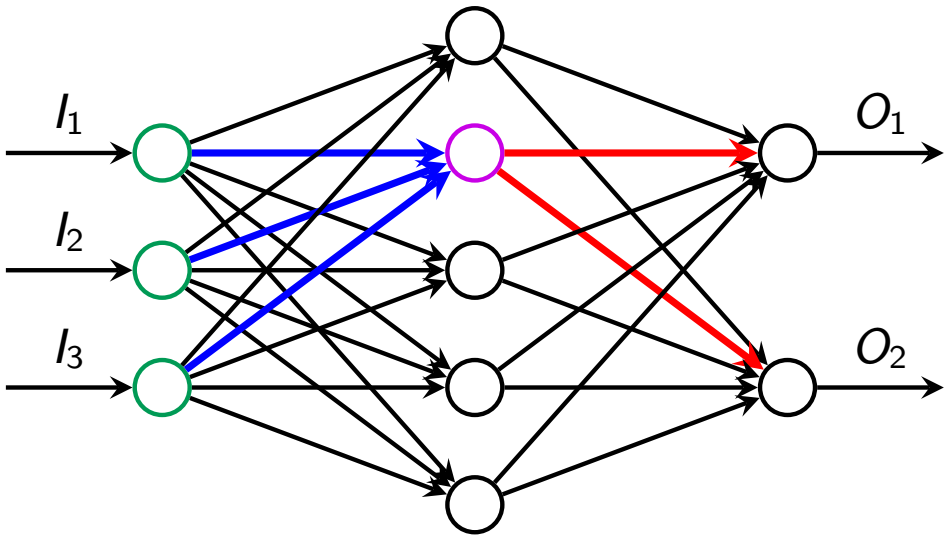
- Activation: $\alpha_1^1 = \Phi(\zeta_1^1)$



Forward propagation: an illustration

Neuron ν_1^1:

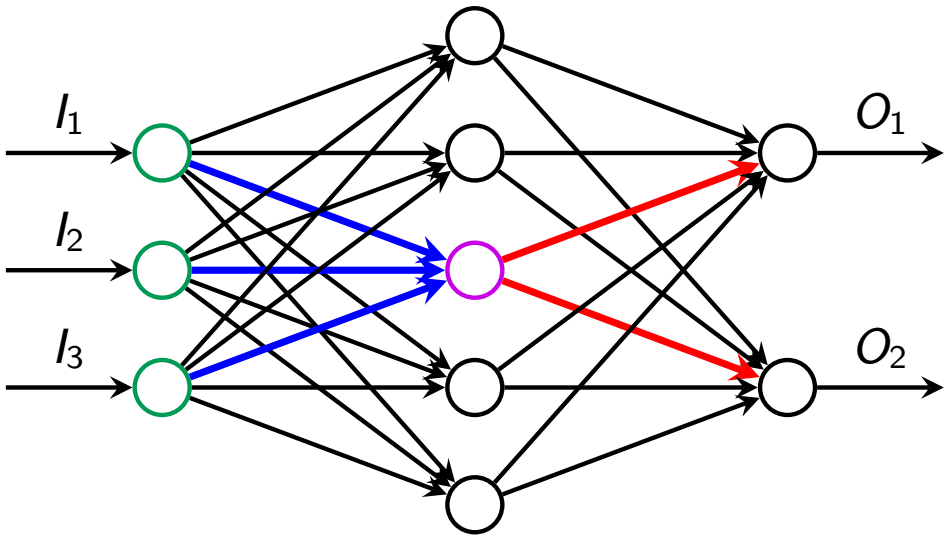
- Input: $\alpha_1^0, \alpha_2^0, \alpha_3^0$
- Weights: $\omega_{1,2}^1$, $\omega_{2,2}^1$, $\omega_{3,2}^1$
- Bias: β_2^1
- Net input: $\zeta_1^1 = \omega_{1,2}^1 \cdot \alpha_1^0 + \omega_{2,2}^1 \cdot \alpha_2^0 + \omega_{3,2}^1 \cdot \alpha_3^0 + \beta_2^1$
- Activation: $\alpha_2^1 = \Phi(\zeta_2^1)$



Forward propagation: an illustration

Neuron ν_1^1:

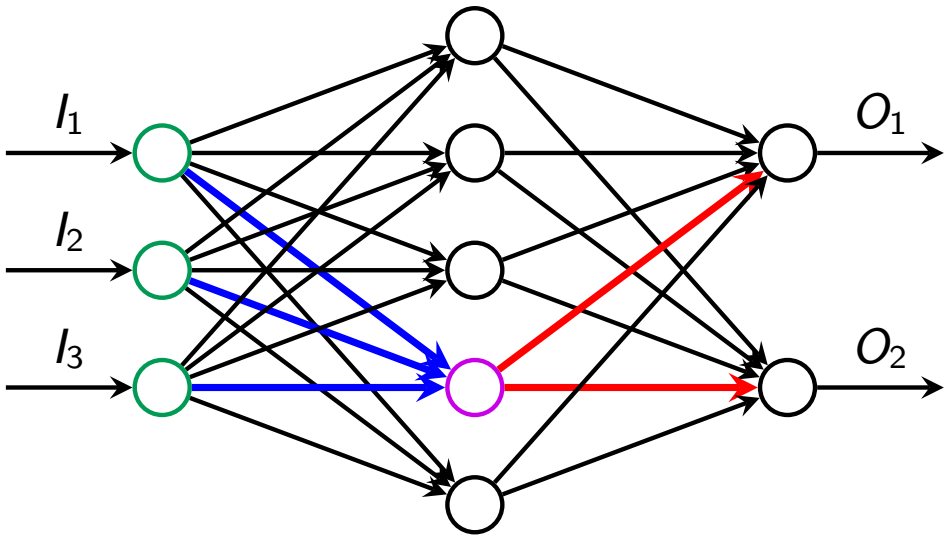
- Input: $\alpha_1^0, \alpha_2^0, \alpha_3^0$
- Weights: $\omega_{1,3}^1$, $\omega_{2,3}^1$, $\omega_{3,3}^1$
- Bias: β_3^1
- Net input: $\zeta_1^1 = \omega_{1,2}^1 \cdot \alpha_1^0 + \omega_{2,3}^1 \cdot \alpha_2^0 + \omega_{3,3}^1 \cdot \alpha_3^0 + \beta_3^1$
- Activation: $\alpha_3^1 = \Phi(\zeta_3^1)$



Forward propagation: an illustration

Neuron ν_1^1:

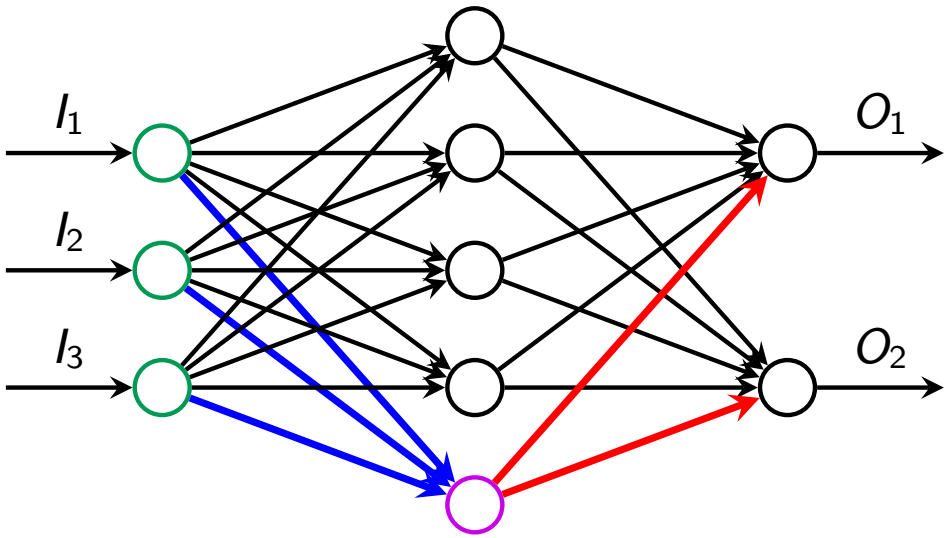
- Input: $\alpha_1^0, \alpha_2^0, \alpha_3^0$
- Weights: $\omega_{1,4}^1$, $\omega_{2,4}^1$, $\omega_{3,4}^1$
- Bias: β_4^1
- Net input: $\zeta_1^1 = \omega_{1,2}^1 \cdot \alpha_1^0 + \omega_{2,4}^1 \cdot \alpha_2^0 + \omega_{3,4}^1 \cdot \alpha_3^0 + \beta_4^1$
- Activation: $\alpha_4^1 = \Phi(\zeta_4^1)$



Forward propagation: an illustration

Neuron ν_1^1:

- Input: $\alpha_1^0, \alpha_2^0, \alpha_3^0$
- Weights: $\omega_{1,5}^1$, $\omega_{2,5}^1$, $\omega_{3,5}^1$
- Bias: β_5^1
- Net input: $\zeta_1^1 = \omega_{1,2}^1 \cdot \alpha_1^0 + \omega_{2,5}^1 \cdot \alpha_2^0 + \omega_{3,5}^1 \cdot \alpha_3^0 + \beta_5^1$
- Activation: $\alpha_5^1 = \Phi(\zeta_5^1)$



A basic forward propagation algorithm

Input: A network with L layers
Input: $\alpha^0 \stackrel{\text{def}}{=} (\alpha_1^0, \ldots, \alpha_{n_0}^0)^{\mathrm{T}}$
for $i \leftarrow 1$ **to** L **do**
  for $k \leftarrow 1$ **to** n_i **do**
    $\zeta_k^i \leftarrow \left(\sum_{j=1}^{n_{i-1}} \omega_{j,k}^i \alpha_j^{i-1} \right) + \beta_k^i$;
    $\alpha_k^i \leftarrow \Phi(\zeta_k^i)$;
  end
end

Algorithm 1: Forward propagation, basic version

Matrix representation

Matrix representation

- The weights at layer i are stored in a matrix $\Omega^i \in \mathbb{R}^{n_{i-1} \times n_i}$, where $(\Omega^i)_{j,k} = \omega^i_{j,k}$

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- The net inputs at layer i are stored in a vector $\zeta^i \stackrel{\text{def}}{=} (\zeta^i_1, \ldots, \zeta^i_{n_i})^{\mathrm{T}}$
- The activation function is extended to vectors: if $u = (u_1, \ldots, u_n)^{\mathrm{T}}$, then $\Phi(u) = (\Phi(u_1), \ldots, \Phi(u_n))^{\mathrm{T}}$

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- The activations of layer i are stored in a vector $\alpha^i \stackrel{\text{def}}{=} (\alpha^i_1, \ldots, \alpha^i_{n_i})^{\mathrm{T}}$

For all $i = 1, \ldots, L$, we have $\zeta^i = \left[\Omega^i\right]^{\mathrm{T}} \cdot \alpha^{i-1} + \beta^i$

Forward propagation algorithms

Input: A network with L layers
Input: $\alpha^0 \stackrel{\text{def}}{=} (\alpha_1^0, \ldots, \alpha_{n_0}^0)^{\mathrm{T}}$
for $i \leftarrow 1$ **to** L **do**
  for $k \leftarrow 1$ **to** n_i **do**
    $\zeta_k^i \leftarrow \left(\sum_{j=1}^{n_{i-1}} \omega_{j,k}^i \alpha_j^{i-1}\right) + \beta_k^i$;
    $\alpha_k^i \leftarrow \Phi(\zeta_k^i)$;
  end
end

Algorithm 2: Forward propagation, basic version

Forward propagation algorithms

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

Input: A network with L layers
Input: α^0
1 **for** $i \leftarrow 1$ **to** L **do**
2 $\zeta^i \leftarrow \left[\Omega^i\right]^{\mathrm{T}} \cdot \alpha^{i-1} + \beta^i$;
3 $\alpha^i \leftarrow \Phi(\zeta^i)$;
4 **end**
Algorithm 5: Forward propagation, vectorized version

Outline

Identity activation function

What happens if the activation function is the identity?

Identity activation function

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

Identity activation function

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- $\alpha^i = \zeta^i = \left[\Omega^i\right]^{\mathrm{T}} \alpha^{i-1} + \beta^i$
- Induction: there exists Γ^i, λ^i such that $\alpha^i = \left[\Gamma^i\right]^{\mathrm{T}} \alpha^0 + \lambda^i$:

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

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- Induction: there exists Γ^i, λ^i such that $\alpha^i = \left[\Gamma^i\right]^{\mathrm{T}} \alpha^0 + \lambda^i$:

$$\begin{aligned} \alpha^i &= \left[\Omega^i\right]^{\mathrm{T}} \alpha^{i-1} + \beta^i \\ &= \left[\Omega^i\right]^{\mathrm{T}} \left(\left[\Gamma^{i-1}\right]^{\mathrm{T}} \alpha^0 + \lambda^{i-1}\right) + \beta^i \end{aligned}$$

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  - We let $\Gamma^i \stackrel{\text{def}}{=} \Gamma^{i-1}\Omega^i$ and $\lambda^i \stackrel{\text{def}}{=} \left[\Omega^i\right]^{\mathrm{T}} \lambda^{i-1} + \beta^i$

Identity activation function

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  - We let $\Gamma^i \stackrel{\text{def}}{=} \Gamma^{i-1}\Omega^i$ and $\lambda^i \stackrel{\text{def}}{=} \left[\Omega^i\right]^{\mathrm{T}} \lambda^{i-1} + \beta^i$
- At the last layer, we have $\alpha^L = \left[\Gamma^L\right]^{\mathrm{T}} \alpha^0 + \lambda^L$
  - This is the perceptron without the step activation function

Linear activation function

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

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

- Let $\overline{\mu} \overset{\text{def}}{=} \mu \cdot \mathbf{Id}$ and $\overline{\lambda} \overset{\text{def}}{=} (\lambda, \ldots, \lambda)^{\mathrm{T}}$

Linear activation function

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

- Let $\overline{\mu} \overset{\text{def}}{=} \mu \cdot \mathbf{Id}$ and $\overline{\lambda} \overset{\text{def}}{=} (\lambda, \ldots, \lambda)^{\mathrm{T}}$
- At layer i we have $\alpha^i = \overline{\mu}\zeta^i + \overline{\lambda} = \overline{\mu}\left[\Omega^i\right]^{\mathrm{T}} \alpha^{i-1} + \overline{\mu}\beta^i + \overline{\lambda}$

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  - By letting $\underline{\Omega^i} \overset{\text{def}}{=} \Omega^i \left[\overline{\mu}\right]^{\mathrm{T}}$ and $\underline{\beta^i} \overset{\text{def}}{=} \overline{\mu}\beta^i + \overline{\lambda}$ we have $\alpha^i = \left[\underline{\Omega^i}\right]^{\mathrm{T}} \alpha^{i-1} + \underline{\beta^i}$

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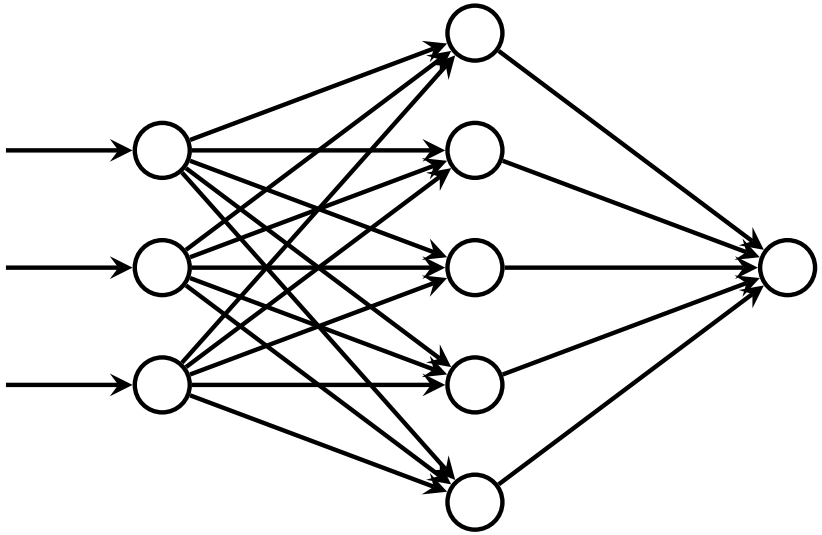
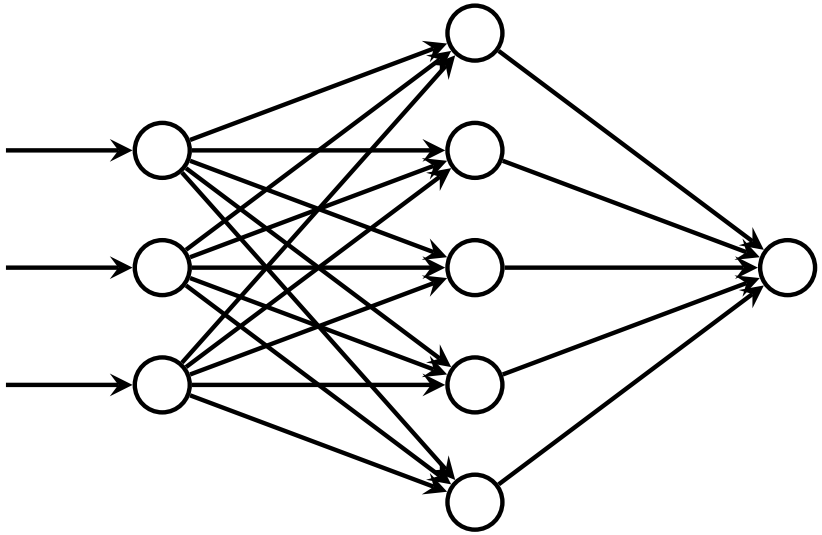
- This is the same as having an identity activation function

A specific MLP

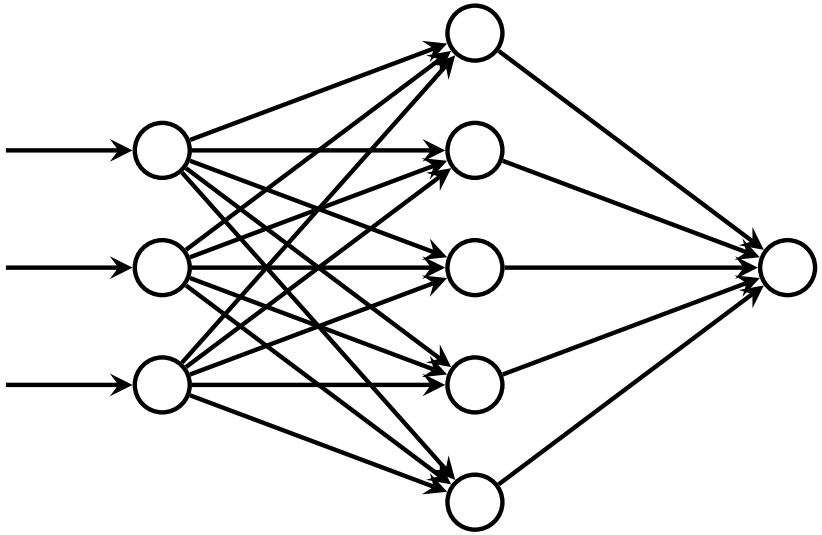


A specific MLP



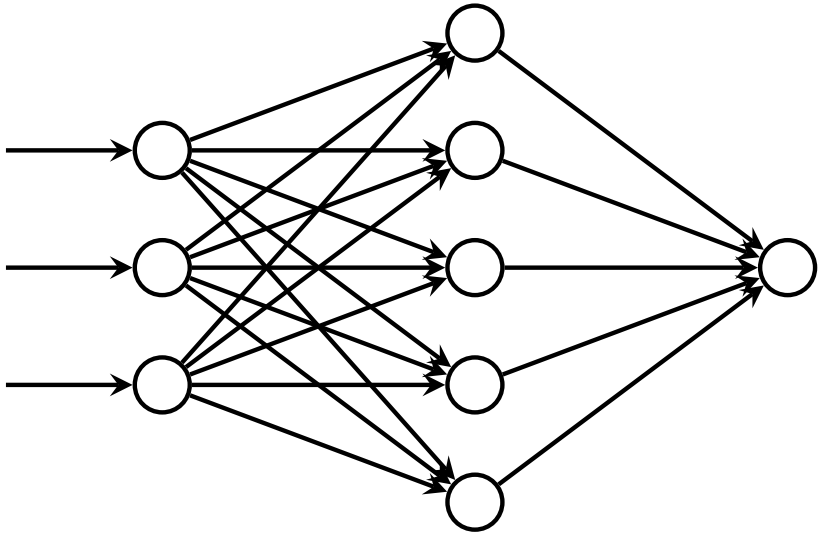
- Input layer of size d

A specific MLP



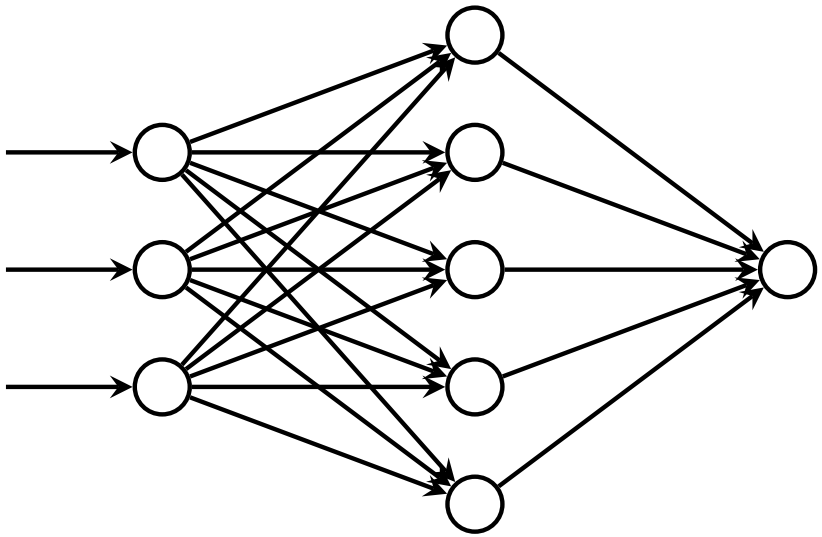
- Input layer of size d
- Single hidden layer of size K

A specific MLP



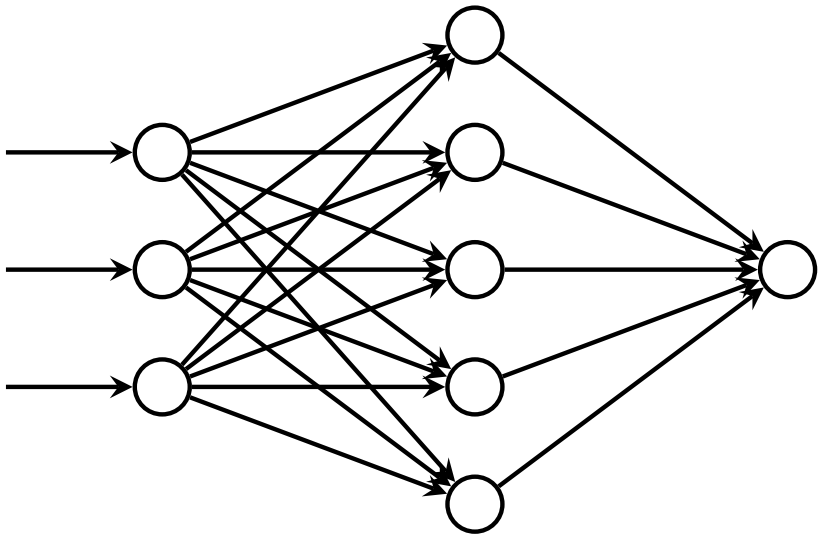
- Input layer of size d
- Single hidden layer of size K
- Single output neuron

A specific MLP



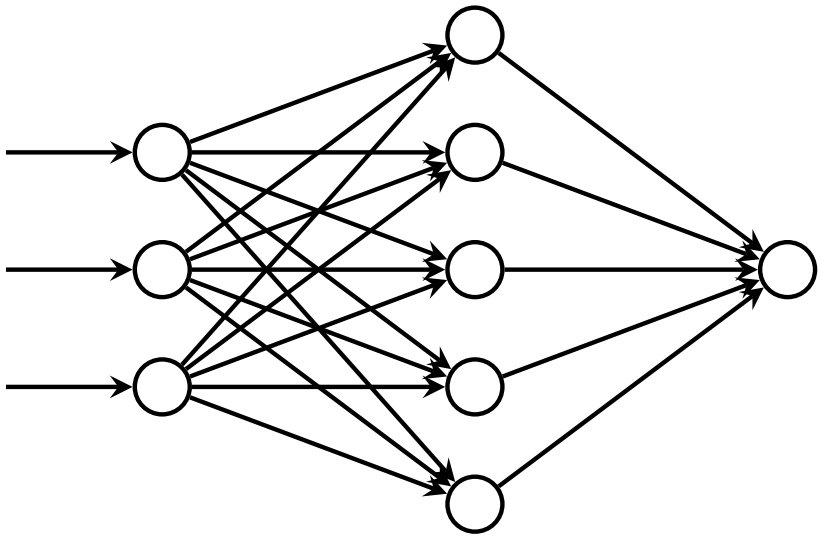
- Input layer of size d
- Single hidden layer of size K
- Single output neuron
- Activation function Φ only on hidden layer (identity on output)

A specific MLP



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

A specific MLP



- Input layer of size d
- Single hidden layer of size K
- Single output neuron
- Activation function Φ only on hidden layer (identity on output)
- No bias on output layer
- Activation of output neuron is $[\omega']^{\mathrm{T}} \cdot \Phi\left([\Omega]^{\mathrm{T}} \alpha^0 + \beta\right)$

A class of functions

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

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- For $\lambda \in \Lambda$, we define

$$\begin{array}{rccl} f_\lambda : & \mathbb{R}^d & \to & \mathbb{R} \\ & x & \mapsto & [\omega']^{\mathrm{T}} \cdot \Phi\left(\Omega^{\mathrm{T}} x + \beta\right) = \sum_{k=1}^{K} \omega'_k \Phi([\Omega_k]^{\mathrm{T}} x + \beta_k) \end{array}$$

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

A class of functions

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

$$\begin{array}{rccl} f_\lambda : & \mathbb{R}^d & \to & \mathbb{R} \\ & x & \mapsto & [\omega']^{\mathrm{T}} \cdot \Phi\left(\Omega^{\mathrm{T}} x + \beta\right) = \sum_{k=1}^{K} \omega'_k \Phi([\Omega_k]^{\mathrm{T}} x + \beta_k) \end{array}$$

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

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

The Universal Approximation Theorem

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

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A visual "proof" (or intuition):
`http://neuralnetworksanddeeplearning.com/chap4.html`

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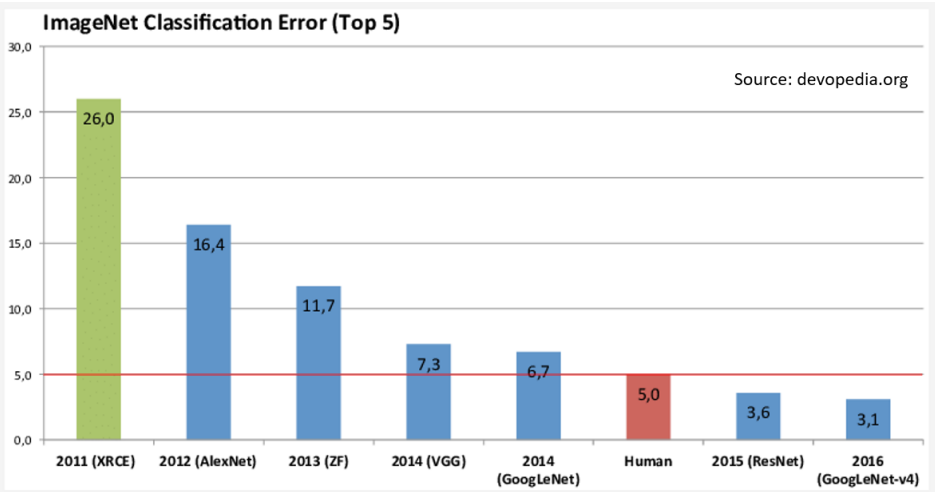

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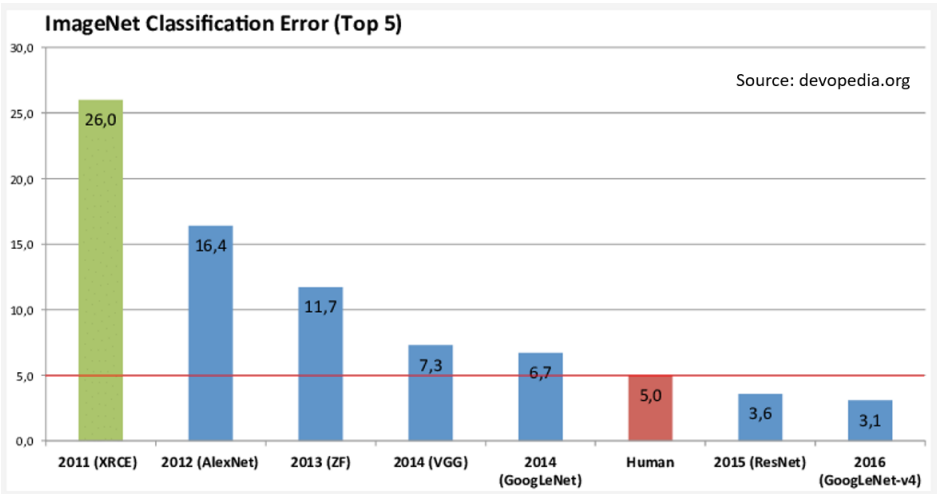

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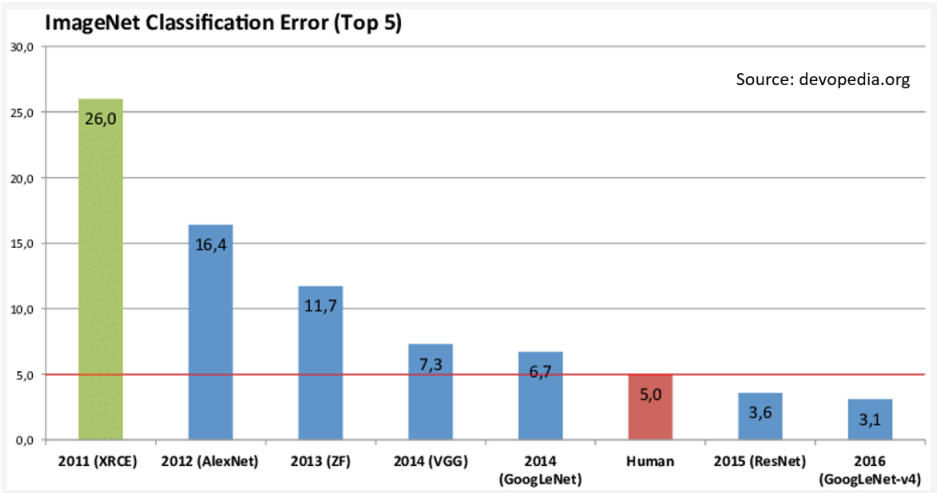

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  - For the time being, it is still not possible to formally explain why things work so well