Lecture 19: 07 April, 2022

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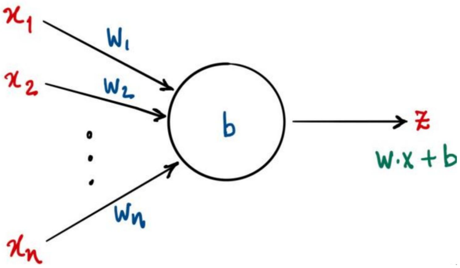
Data Mining and Machine Learning
January–May 2022

Linear separators and Perceptrons

- Perceptrons define linear separators $w \cdot x + b$
  - $w \cdot x + b > 0$, classify Yes $(+1)$
  - $w \cdot x + b < 0$, classify No (-1)



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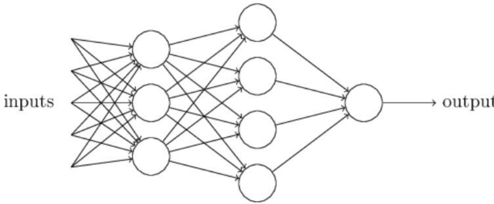

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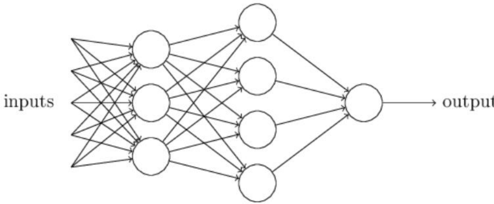

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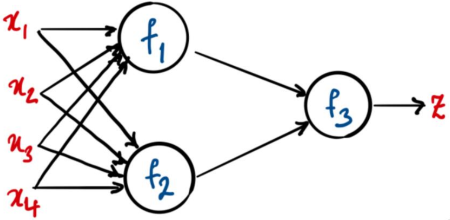

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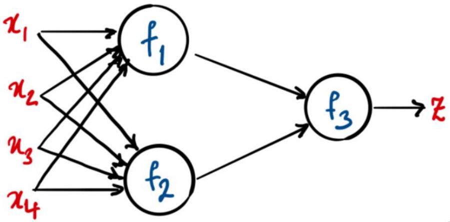

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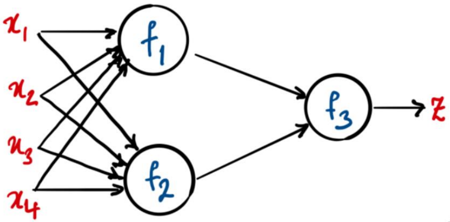

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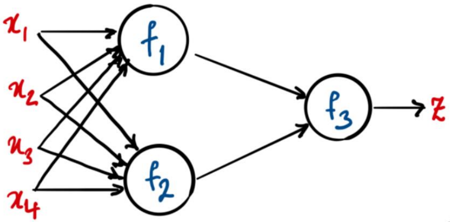
  - $f_3 = \sum_{i=1}^{4} (w_{3_1} w_{1_i} + w_{3_2} w_{2_i}) \cdot x_i$ $+(w_{3_1} b_1 + w_{3_2} b_2 + b_3)$



Limits of linearity

- Cannot compute *exclusive-or* (XOR)
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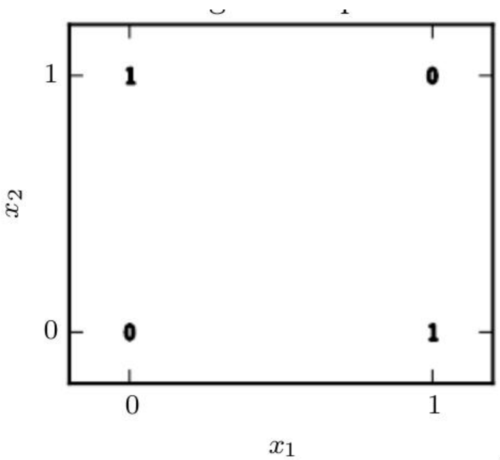

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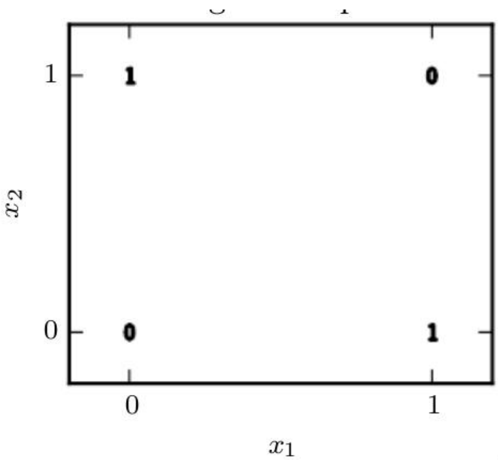

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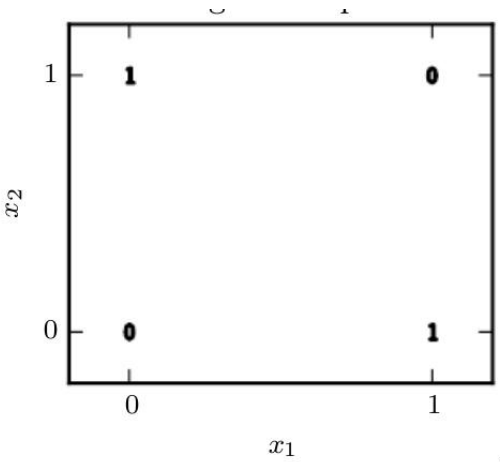

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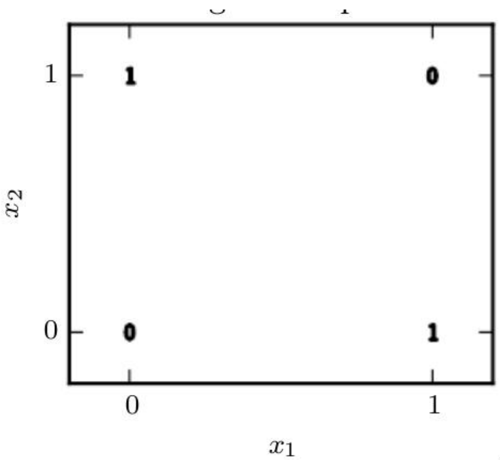

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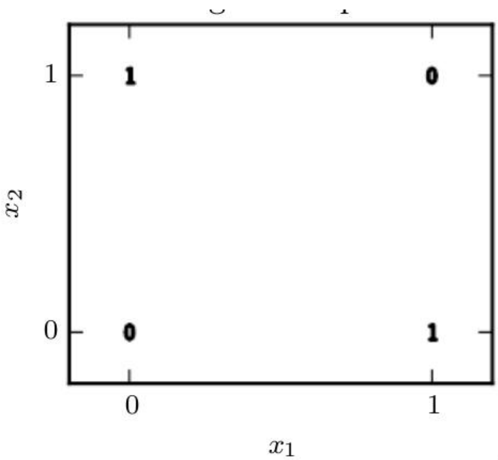
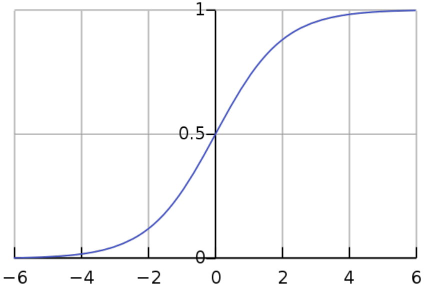
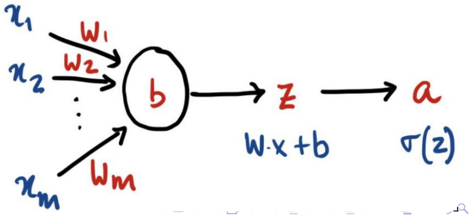
- Observed by Minsky and Papert, 1969, first "AI Winter"



Non-linear activation

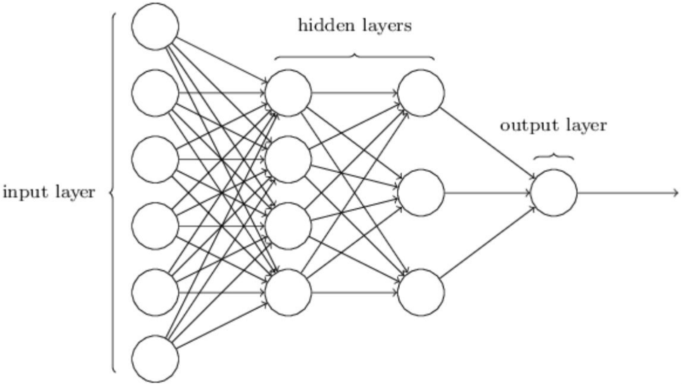
- Transform linear output z through a non-linear activation function
- Sigmoid function $\frac{1}{1+e^{-z}}$





Structure of a neural network

- Acyclic
- Input layer, hidden layers, output layer



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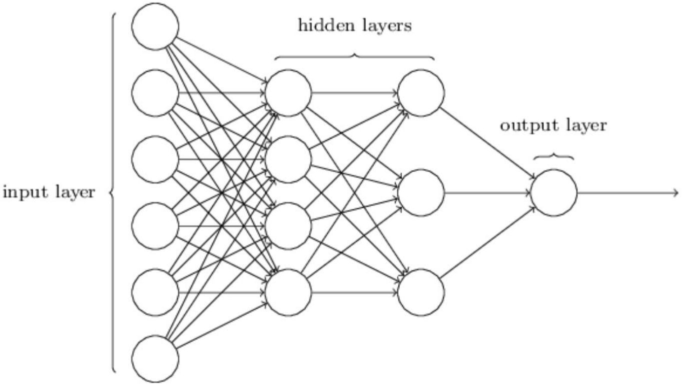

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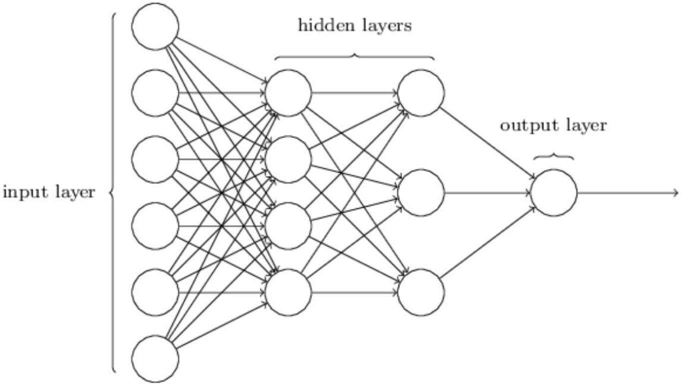

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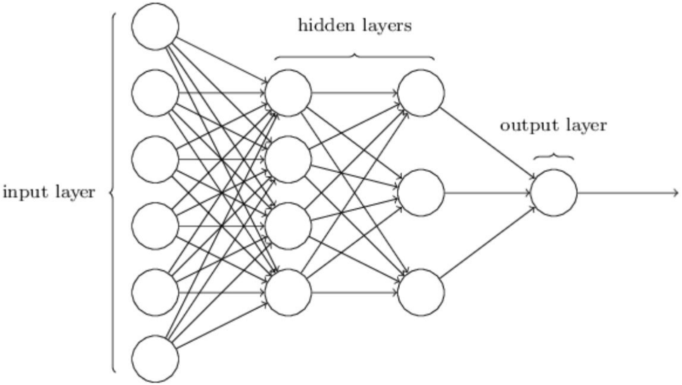

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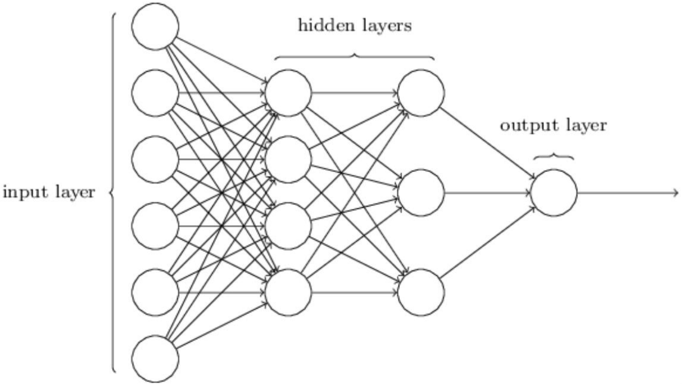

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- Transform linear output z through a non-linear activation function
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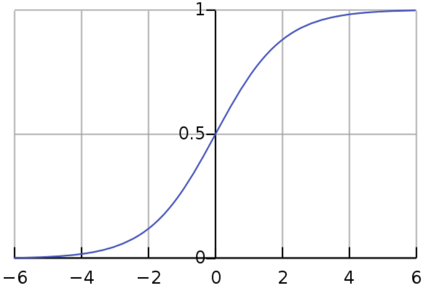
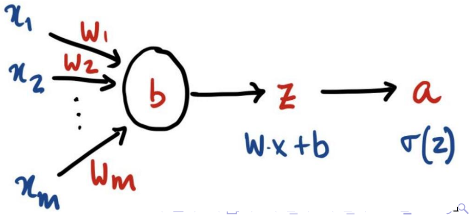
- Step is at $z = 0$
  - $z = wx + b$, so step is at $x = -b/w$
  - Increasing w makes step steeper





Universality

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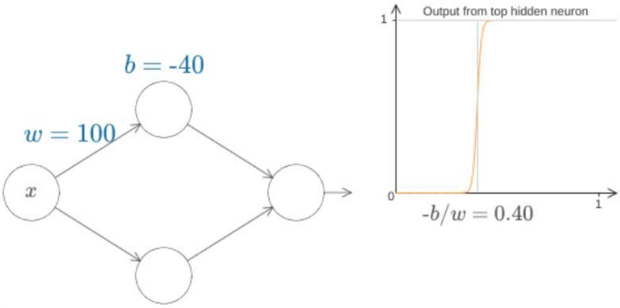

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- Create a step at $x = -b/w$
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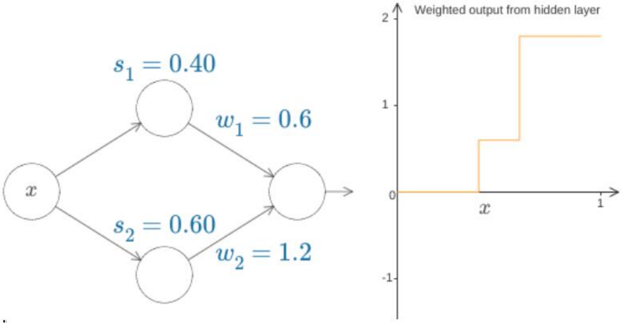

Universality

- Create a step at $x = -b/w$
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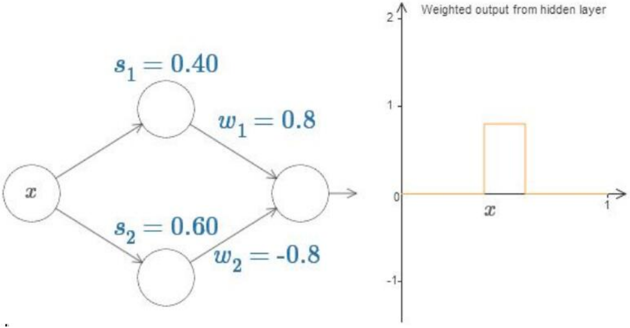

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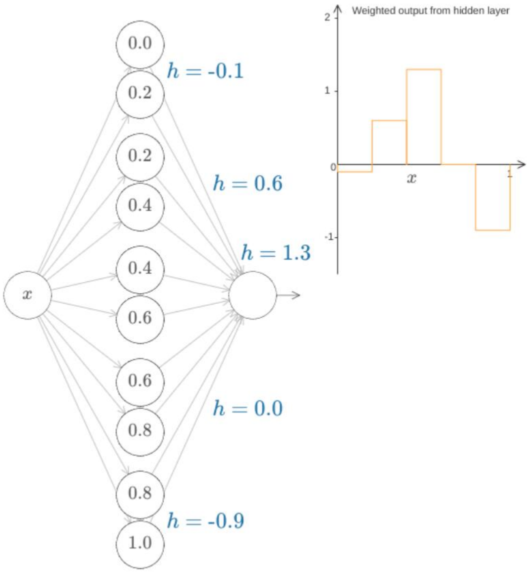

Universality

- Create a step at $x = -b/w$
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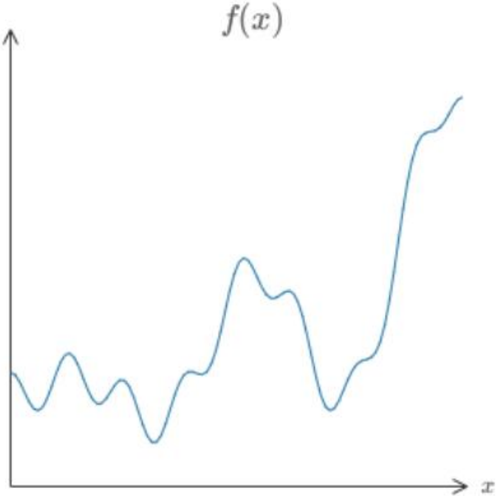
- Approximate any function



Universality

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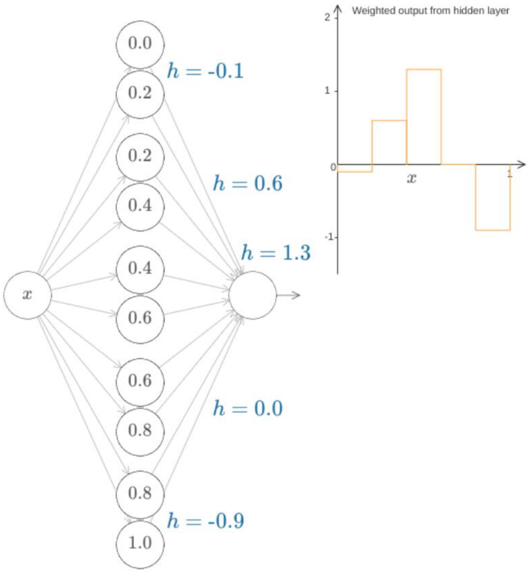
- Approximate any function
- Need only one hidden layer!



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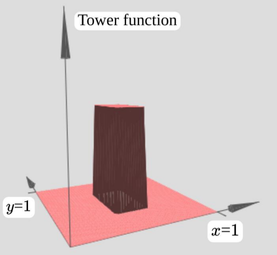
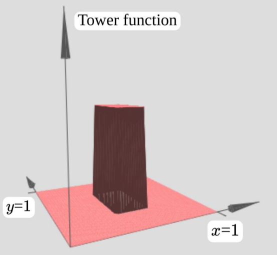
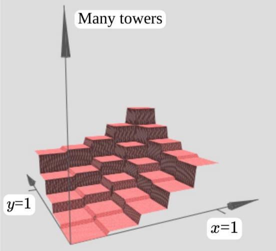


Non-linear activation

- With non-linear activation, network of neurons can approximate any function
  - Can build "rectangular" blocks
  - Combine blocks to capture any classification boundary





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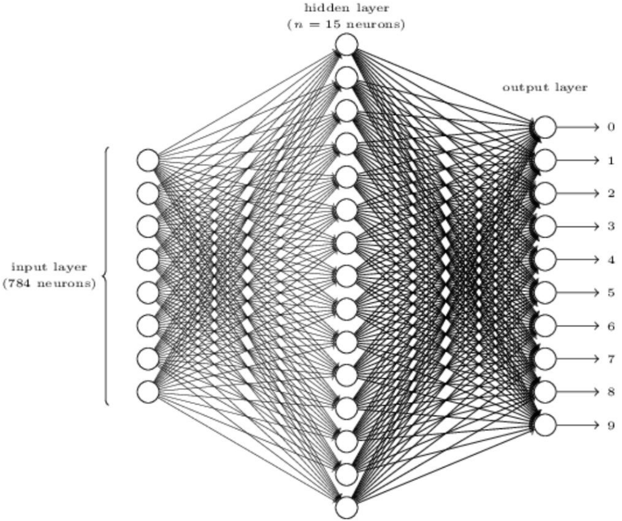
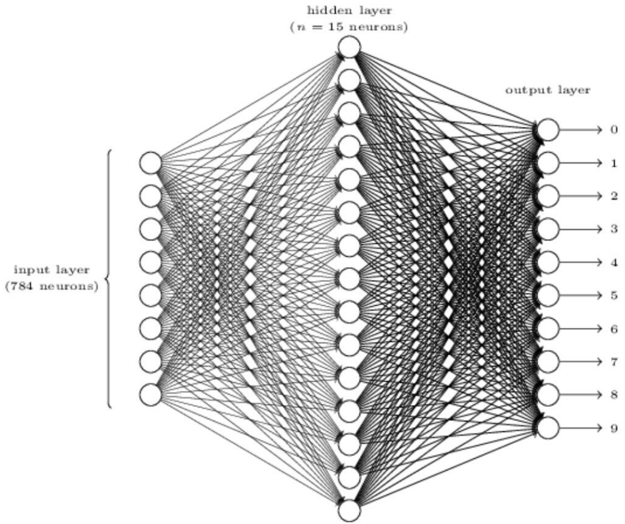
- Input $x = (x_1, x_2, \ldots, x_{784})$

- Input layer $(x_1, x_2, \ldots, x_{784})$



Example: Network structure

- Input layer $(x_1, x_2, \ldots, x_{784})$
- Single hidden layer, 15 nodes



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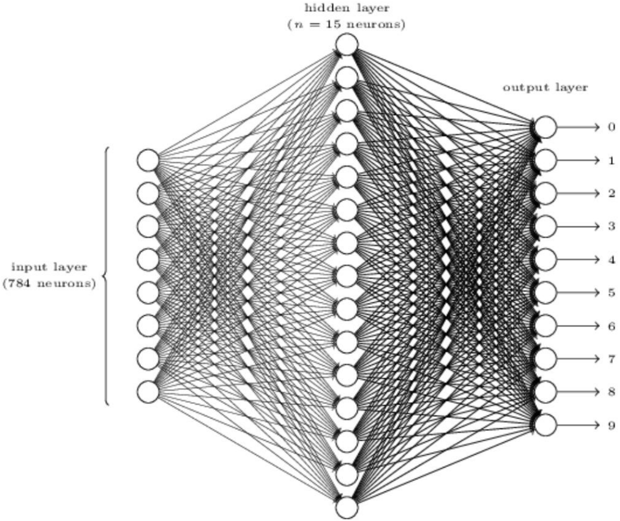

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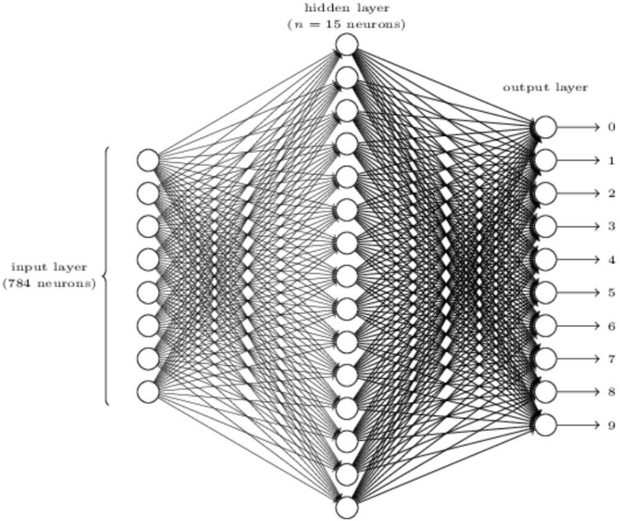

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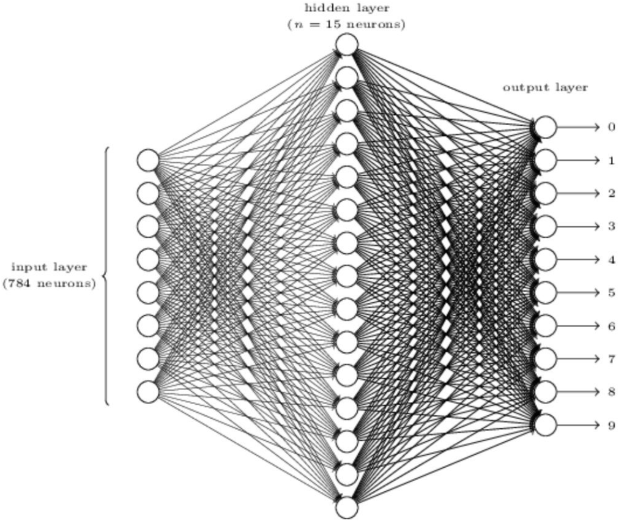

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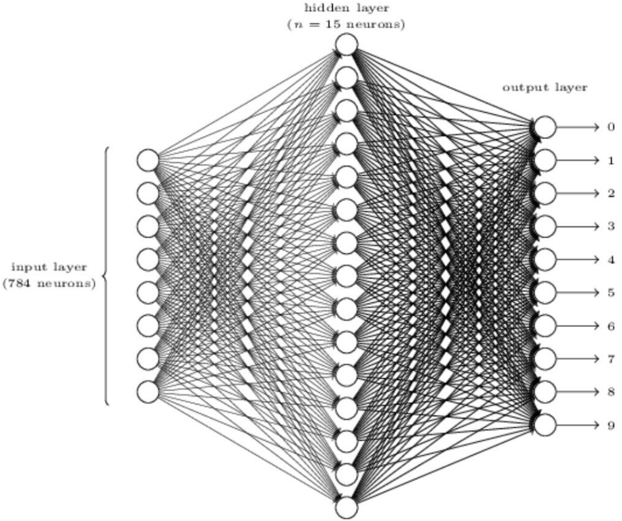
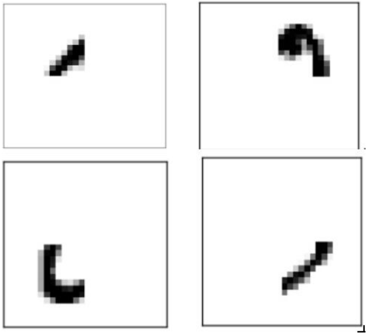
  - Softmax, $\arg\max_j \frac{e^{a_j}}{\sum_j e^{a_j}}$
    - "Smooth" version of $\arg\max$



Example: Extracting features

- Hidden layers extract features
  - For instance, patterns in different quadrants



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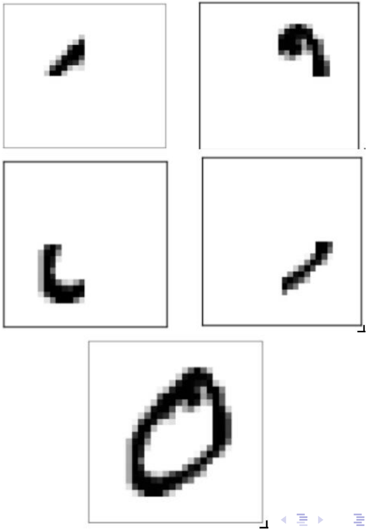

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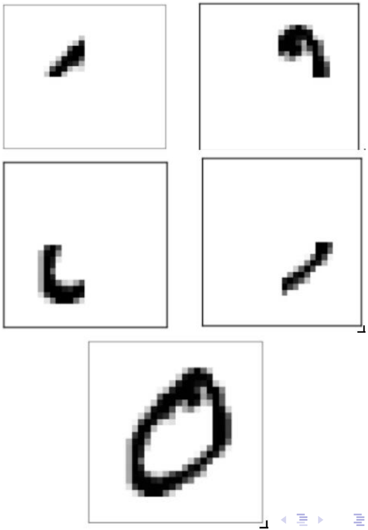

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- Hidden layers extract features
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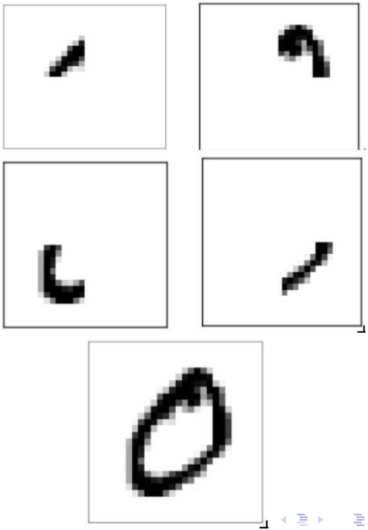
- Claim: Automatic identification of features is strength of the model
- Counter argument: implicitly extracted features are impossible to interpret
  - Explainability



Neural networks

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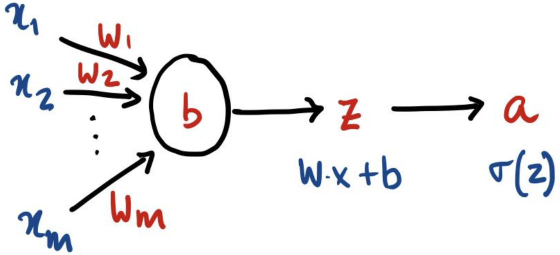
- Structure of an individual neuron
  - Input weights $w_1, \ldots, w_m$, bias b, output z, activation value a



Notation

- Layers $\ell \in \{1, 2, \ldots, L\}$
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  - Layer L is the output layer
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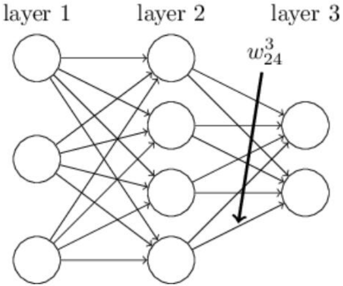
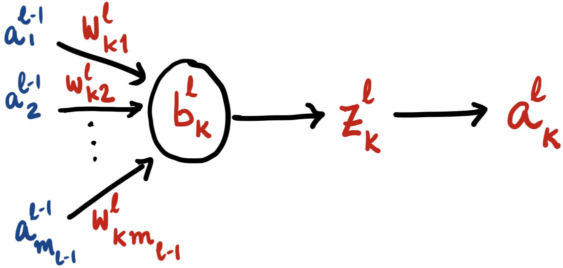
- Layer ℓ has m_ℓ nodes $1, 2, \ldots, m_\ell$
- Node k in layer ℓ has bias b_k^ℓ, output z_k^ℓ and activation value a_k^ℓ
- Weight on edge from node j in level $\ell-1$ to node k in level ℓ is w_{kj}^ℓ





Notation

- Why the inversion of indices in the subscript w_{kj}^{ℓ}?
  - $z_k^{\ell} = w_{k1}^{\ell} a_1^{\ell-1} + w_{k2}^{\ell} a_2^{\ell-1} + \cdots + w_{km_{\ell-1}}^{\ell} a_{m_{\ell-1}}^{\ell-1}$
  - Let $\overline{w}_k^{\ell} = (w_{k1}^{\ell}, w_{k2}^{\ell}, \ldots, w_{km_{\ell-1}}^{\ell})$
    and $\overline{a}^{\ell-1} = (a_1^{\ell-1}, a_2^{\ell-1}, \ldots, a_{m_{\ell-1}}^{\ell-1})$
  - Then $z_k^{\ell} = \overline{w}_k^{\ell} \cdot \overline{a}^{\ell-1}$

Notation

- Why the inversion of indices in the subscript w^{ℓ}_{kj}?
  - $z^{\ell}_k = w^{\ell}_{k1} a^{\ell-1}_1 + w^{\ell}_{k2} a^{\ell-1}_2 + \cdots + w^{\ell}_{km_{\ell-1}} a^{\ell-1}_{m_{\ell-1}}$
  - Let $\overline{w}^{\ell}_k = (w^{\ell}_{k1}, w^{\ell}_{k2}, \ldots, w^{\ell}_{km_{\ell-1}})$ and $\overline{a}^{\ell-1} = (a^{\ell-1}_1, a^{\ell-1}_2, \ldots, a^{\ell-1}_{m_{\ell-1}})$
  - Then $z^{\ell}_k = \overline{w}^{\ell}_k \cdot \overline{a}^{\ell-1}$
- Assume all layers have same number of nodes
  - Let $m = \max\limits_{\ell \in \{1.2,\ldots,L\}} m_\ell$
  - For any layer i, for $k > m_i$, we set all of $w^{\ell}_{kj}, b^{\ell}_k, z^{\ell}_k, a^{\ell}_k$ to 0
- Matrix formulation

$$\begin{bmatrix} \overline{z}^{\ell}_1 \\ \overline{z}^{\ell}_2 \\ \cdots \\ \overline{z}^{\ell}_m \end{bmatrix} = \begin{bmatrix} \overline{w}^{\ell}_1 \\ \overline{w}^{\ell}_2 \\ \cdots \\ \overline{w}^{\ell}_m \end{bmatrix} \begin{bmatrix} a^{\ell-1}_1 \\ a^{\ell-1}_2 \\ \cdots \\ a^{\ell-1}_m \end{bmatrix}$$

Learning the parameters

- Need to find optimum values for all weights w_{kj}^{ℓ}
- Use gradient descent
  - Cost function C, partial derivatives $\dfrac{\partial C}{\partial w_{kj}^{\ell}}, \dfrac{\partial C}{\partial b_{k}^{\ell}}$

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  1. For input $\mathbf{x}$, $C(\mathbf{x})$ is a function of only the output layer activation, a^L
     - For instance, for training input $(\mathbf{x}_i, y_i)$, sum-squared error is $(y_i - a_i^L)^2$
     - Note that $\mathbf{x}_i$, y_i are fixed values, only a_i^L is a variable

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  2. Total cost is average of individual input costs
     - Each input $\boldsymbol{x}_i$ incurs cost $C(\boldsymbol{x}_i)$, total cost is $\frac{1}{n}\sum_{i=1}^{n} C(\boldsymbol{x}_i)$
     - For instance, mean sum-squared error $\frac{1}{n}\sum_{i=1}^{n}(y_i - a^L_i)^2$

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- With these assumptions:
  - We can write $\dfrac{\partial C}{\partial w_{kj}^{\ell}}, \dfrac{\partial C}{\partial b_k^{\ell}}$ in terms of individual $\dfrac{\partial a_i^L}{\partial w_{kj}^{\ell}}, \dfrac{\partial a_i^L}{\partial b_k^{\ell}}$
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  - Can extrapolate change in individual cost $C(x)$ to change in overall cost C — stochastic gradient descent
- Complex dependency of C on w^ℓ_{kj}, b^ℓ_k
  - Many intermediate layers
  - Many paths through these layers
- Use chain rule to decompose into local dependencies
  - $y = g(f(x)) \Rightarrow \dfrac{\partial g}{\partial x} = \dfrac{\partial g}{\partial f}\dfrac{\partial f}{\partial x}$