Neural Networks: Design

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Machine Learning

Outline

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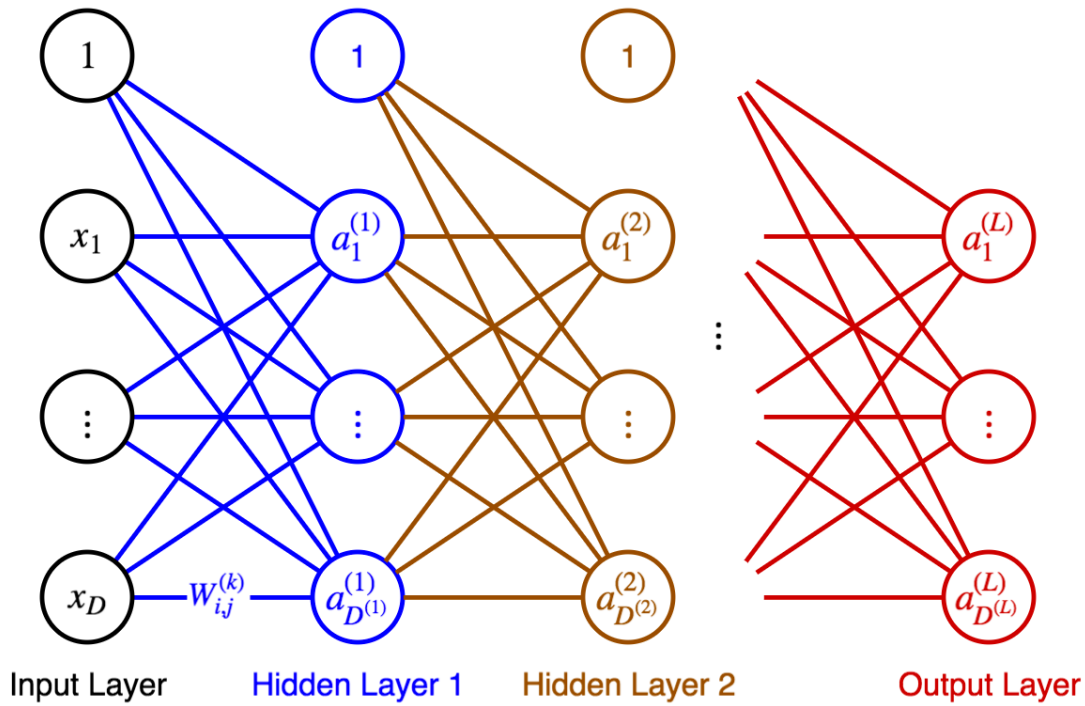
Model: a Composite Function I

- A ***feedforward neural networks***, or ***multilayer perceptron***, defines a function composition

$$\hat{y} = f^{(L)}(\cdots f^{(2)}(f^{(1)}(x;\theta^{(1)});\theta^{(2)});\theta^{(L)})$$

that approximates the target function f^*



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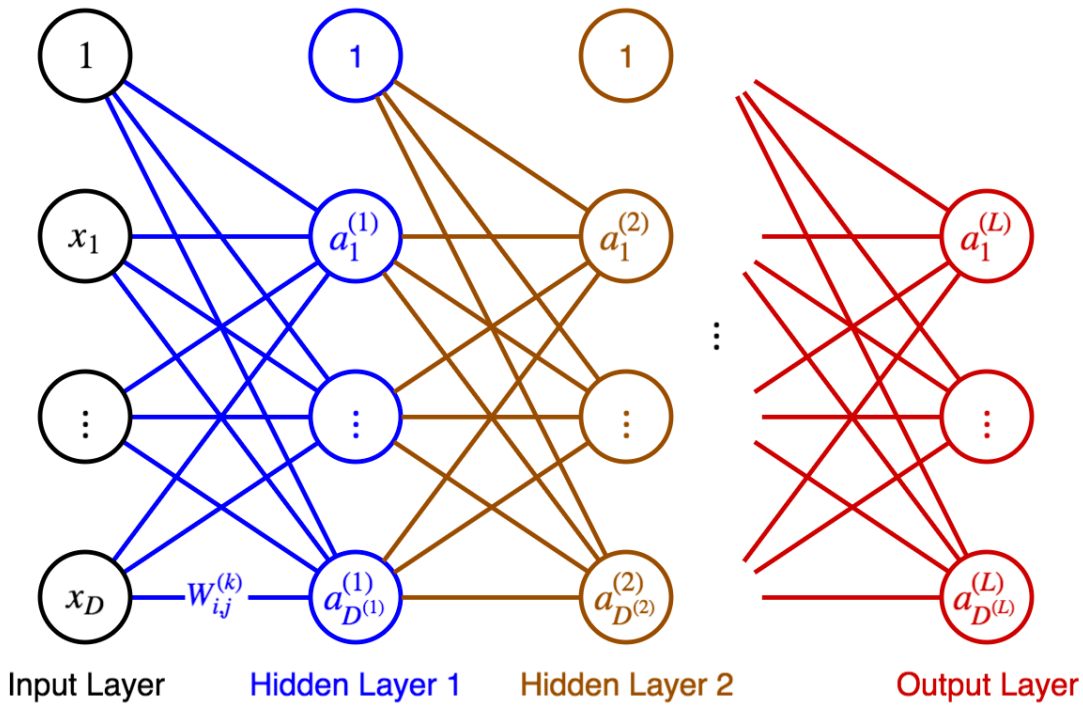

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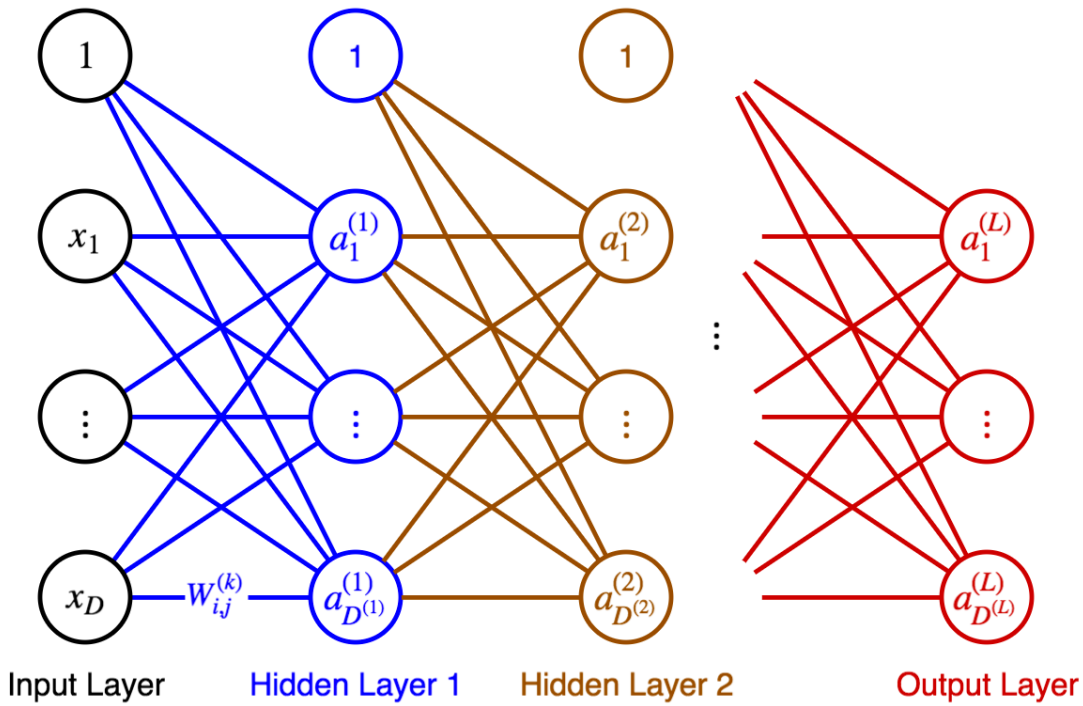
  that approximates the target function f^*
- Parameters $\theta^{(1)}, \cdots, \theta^{(L)}$ learned from training set $\mathbb{X}$
- "Feedforward" because information flows from input to output



Model: a Composite Function II

- At each layer k, the function $f^{(k)}(\cdot\,; \boldsymbol{W}^{(k)}, \boldsymbol{b}^{(k)})$ is ***nonlinear*** and outputs value $\boldsymbol{a}^{(k)} \in \mathbb{R}^{D^{(k)}}$, where

$$\boldsymbol{a}^{(k)} = \text{act}^{(k)}(\boldsymbol{W}^{(k)\top} \boldsymbol{a}^{(k-1)} + \boldsymbol{b}^{(k)})$$

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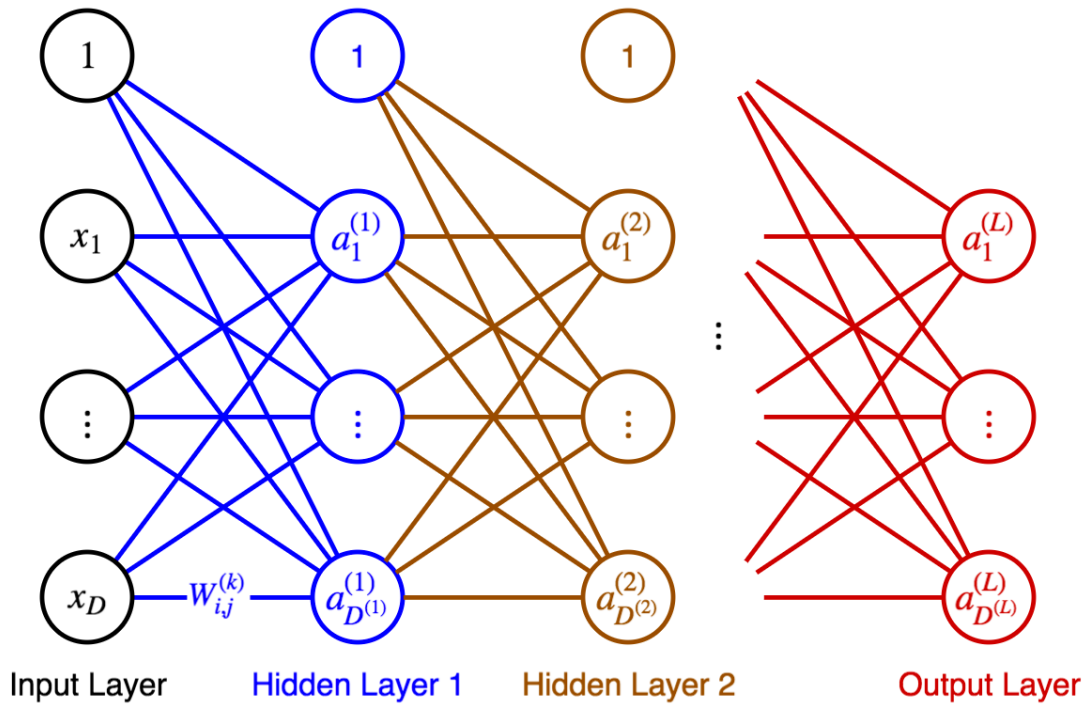

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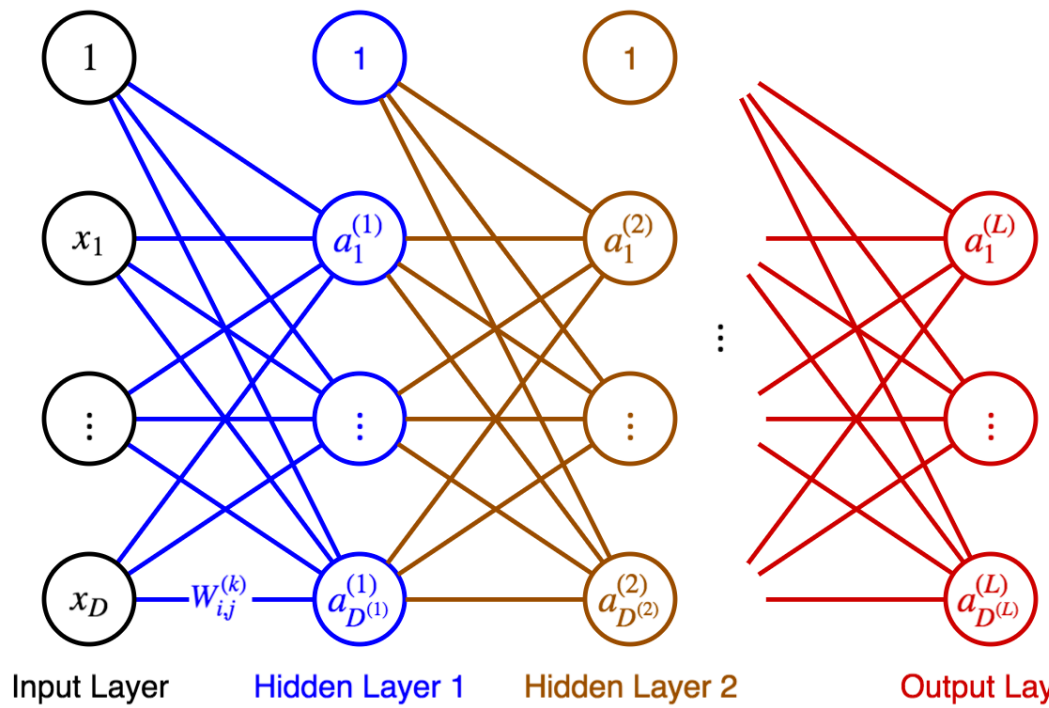
  - $\boldsymbol{a}^{(k-1)} \in \mathbb{R}^{D^{(k-1)}+1}$, $a_0^{(k-1)} = 1$, and $\boldsymbol{W}^{(k)} \in \mathbb{R}^{(D^{(k-1)}+1) \times D^{(k)}}$



Neurons I

- Each $f_j^{(k)} = \text{act}^{(k)}(\boldsymbol{W}_{:,j}^{(k)\top} \boldsymbol{a}^{(k-1)}) = \text{act}^{(k)}(z_j^{(k)})$ is a ***unit*** (or ***neuron***)

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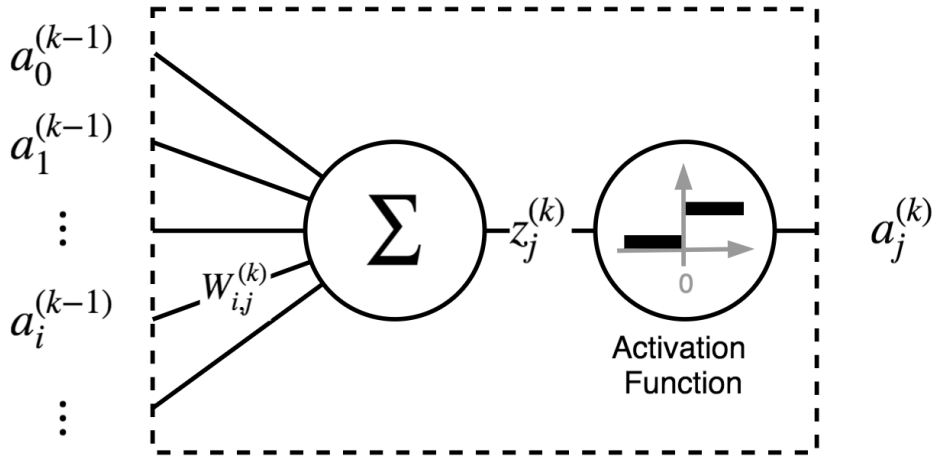

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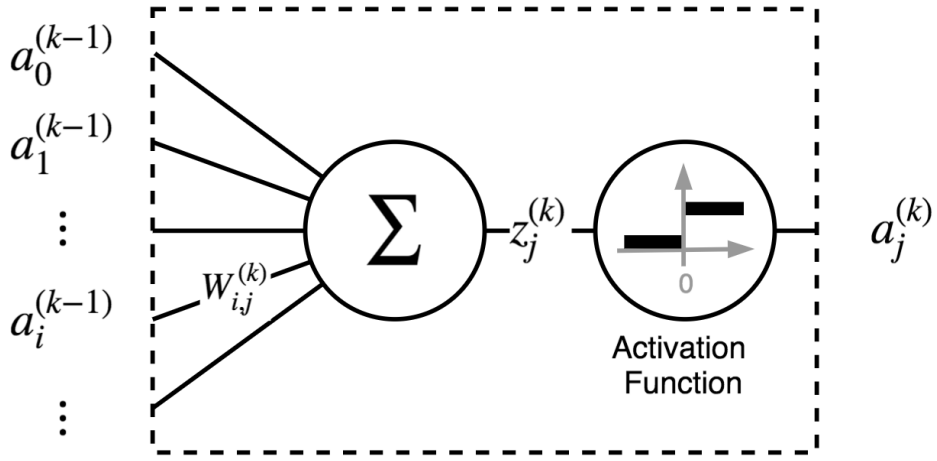
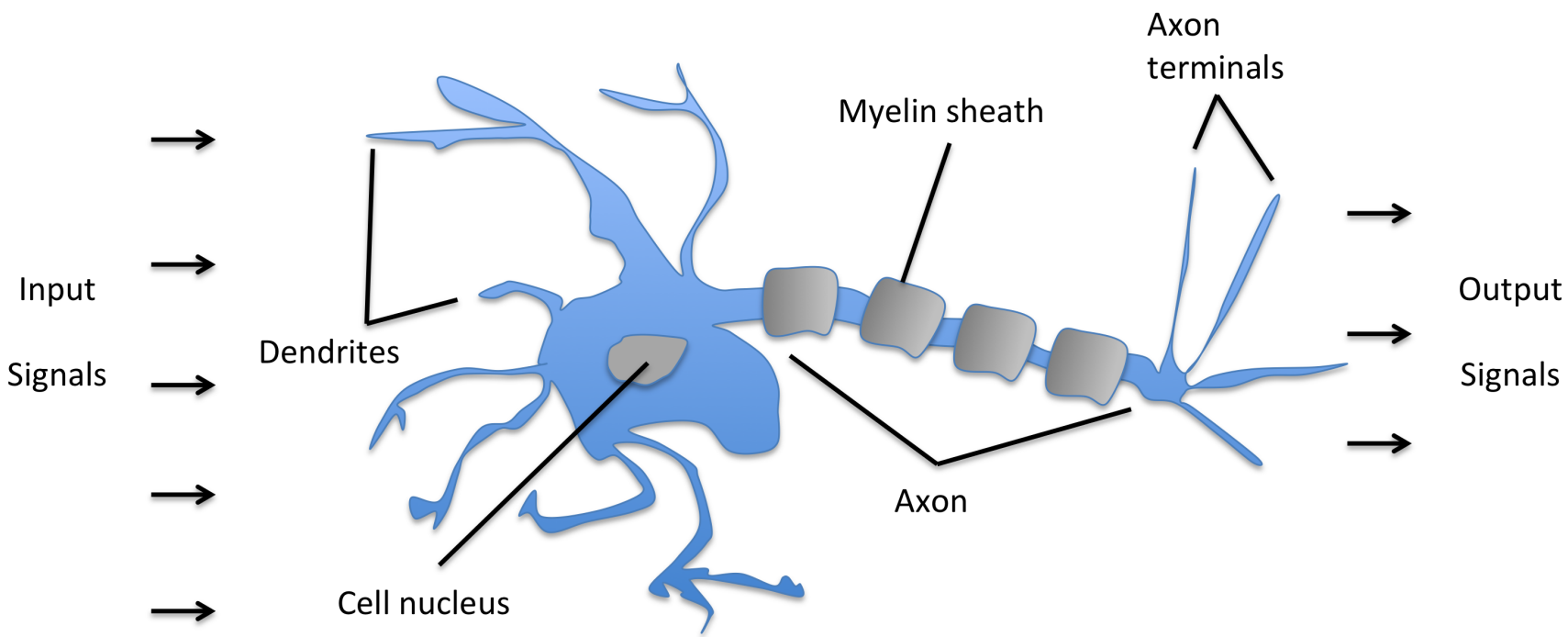
- Loosely guided by neuroscience





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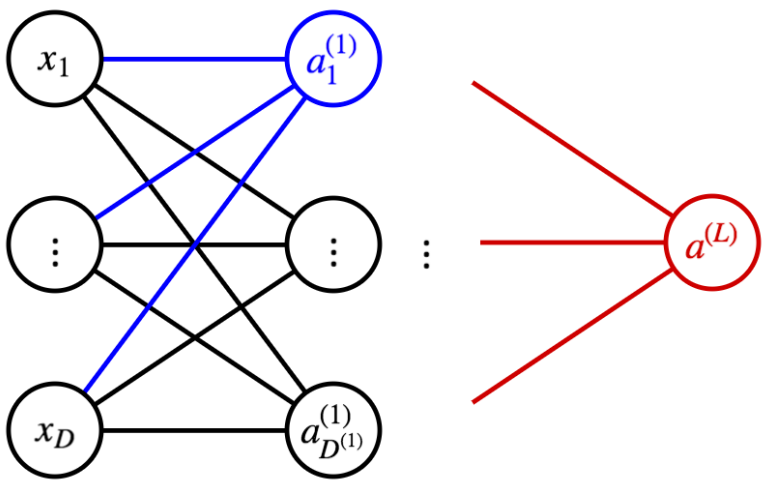

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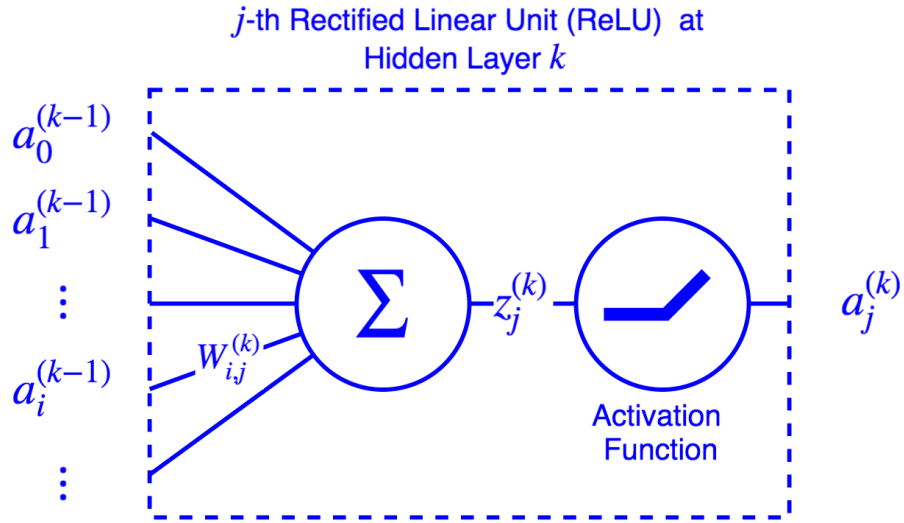

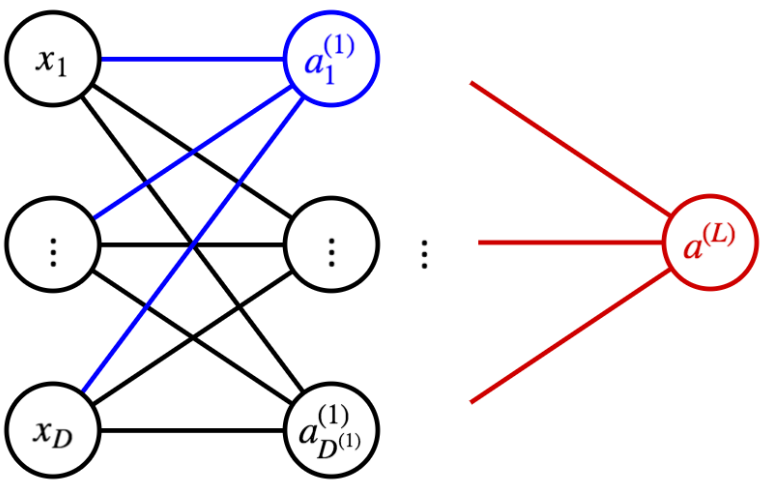

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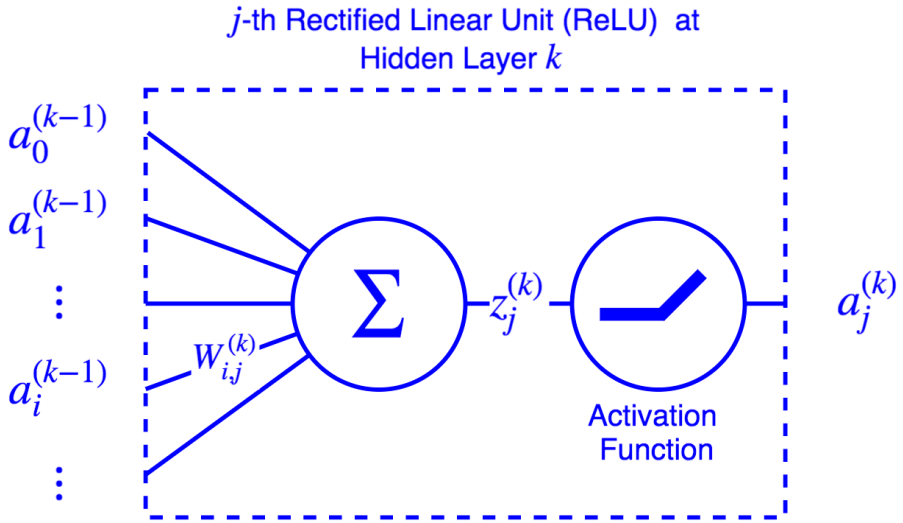

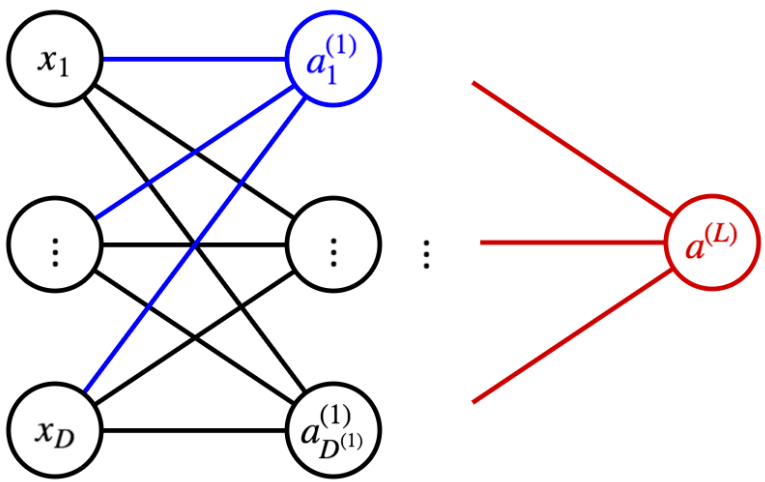

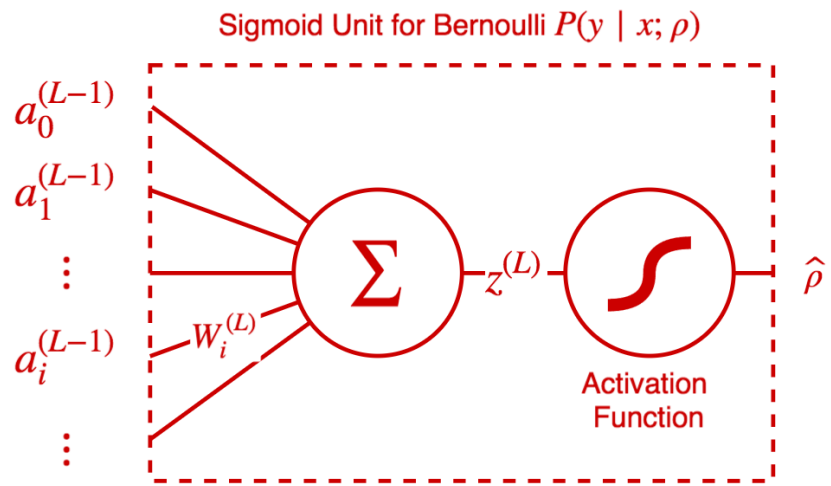

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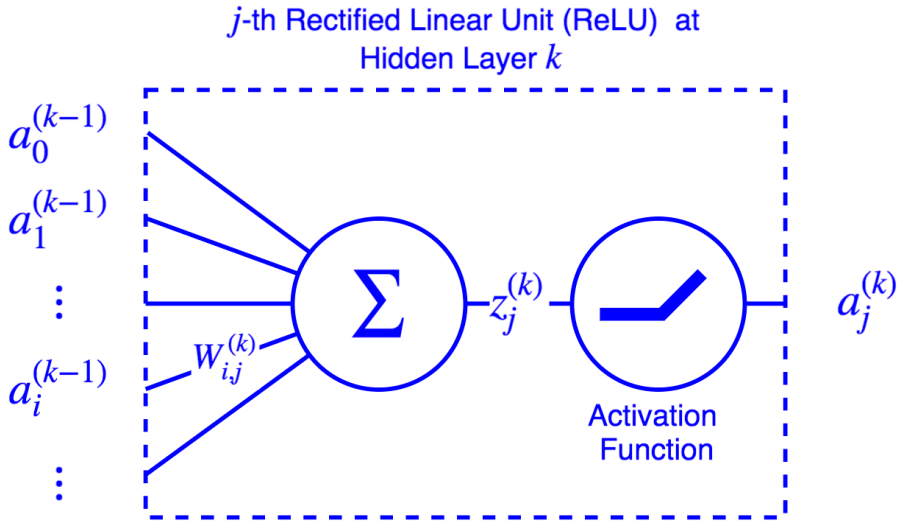
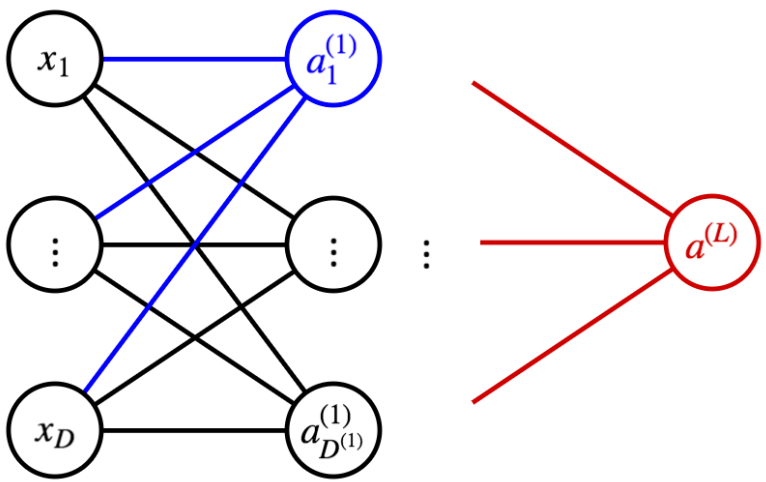
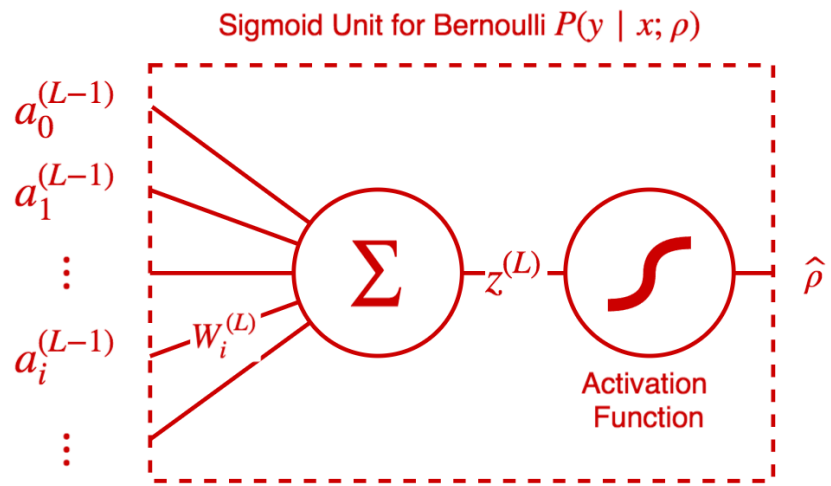
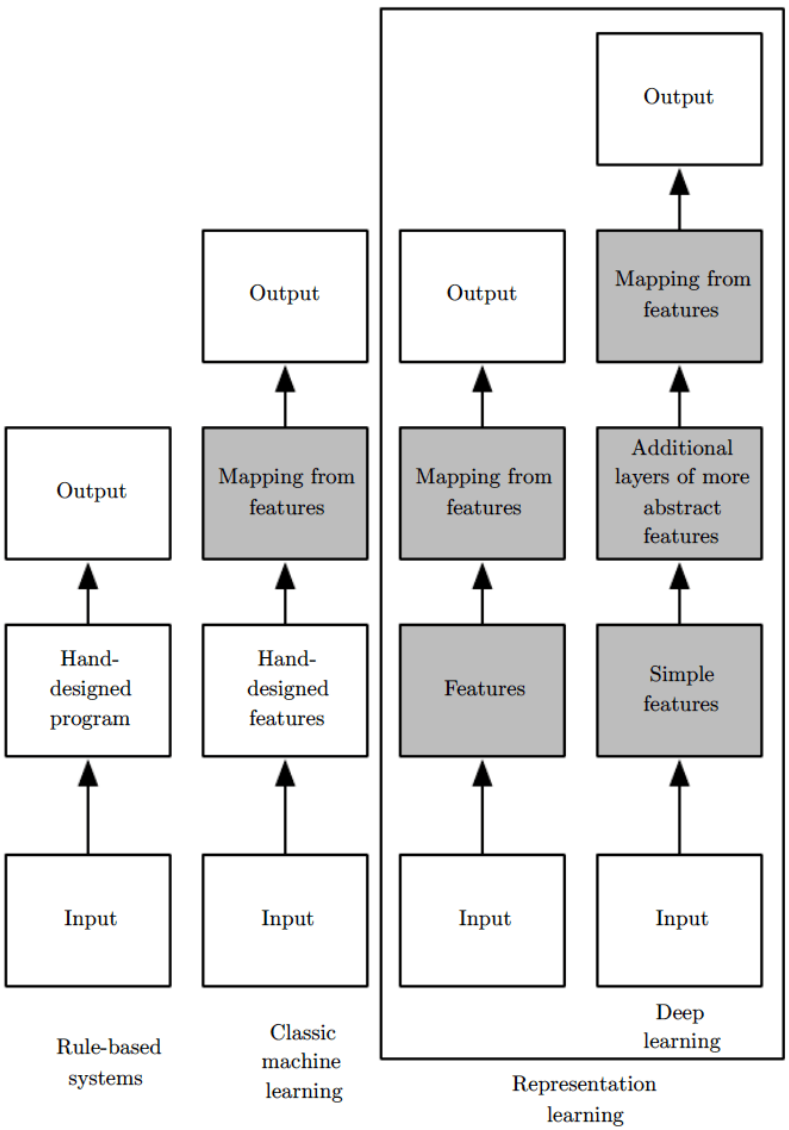
  - A logistic regressor with input $\boldsymbol{a}^{(L-1)}$







Representation Learning



- The outputs $\boldsymbol{a}^{(1)}, \boldsymbol{a}^{(2)}, \cdots, \boldsymbol{a}^{(L-1)}$ of hidden layers $\boldsymbol{f}^{(1)}, \boldsymbol{f}^{(2)}, \cdots, \boldsymbol{f}^{(L-1)}$ are ***distributed representation*** of $\boldsymbol{x}$
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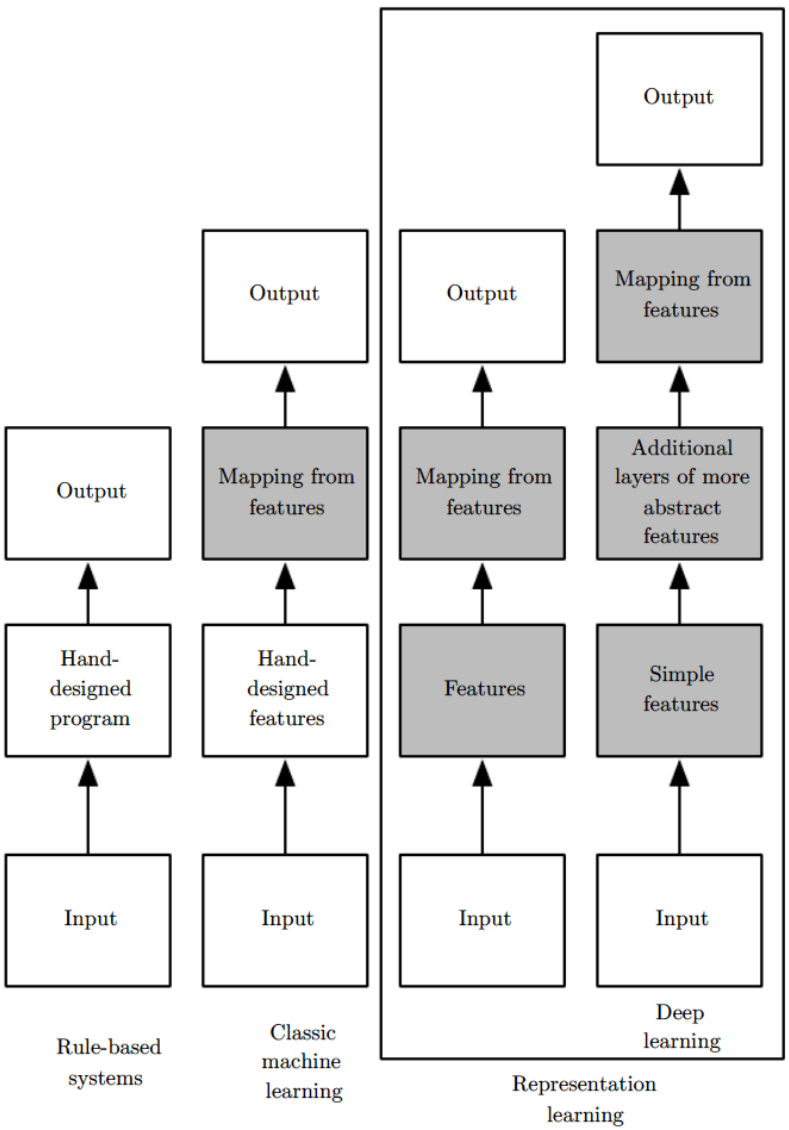

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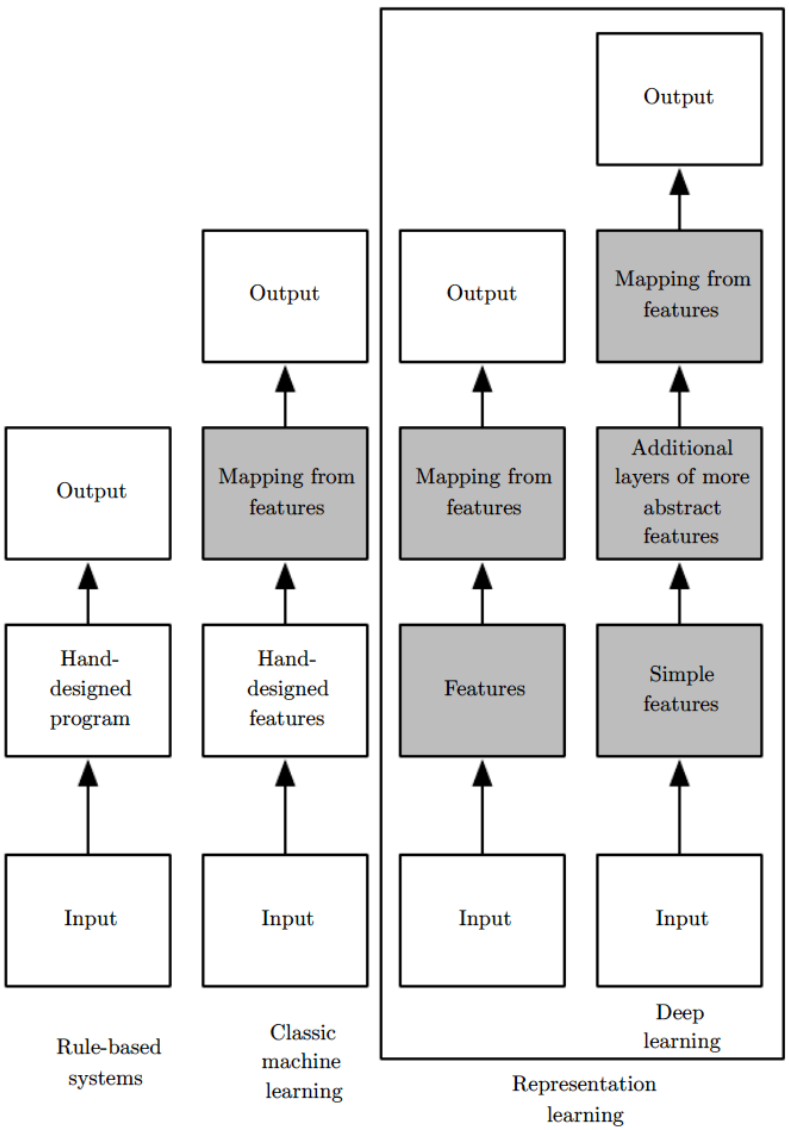

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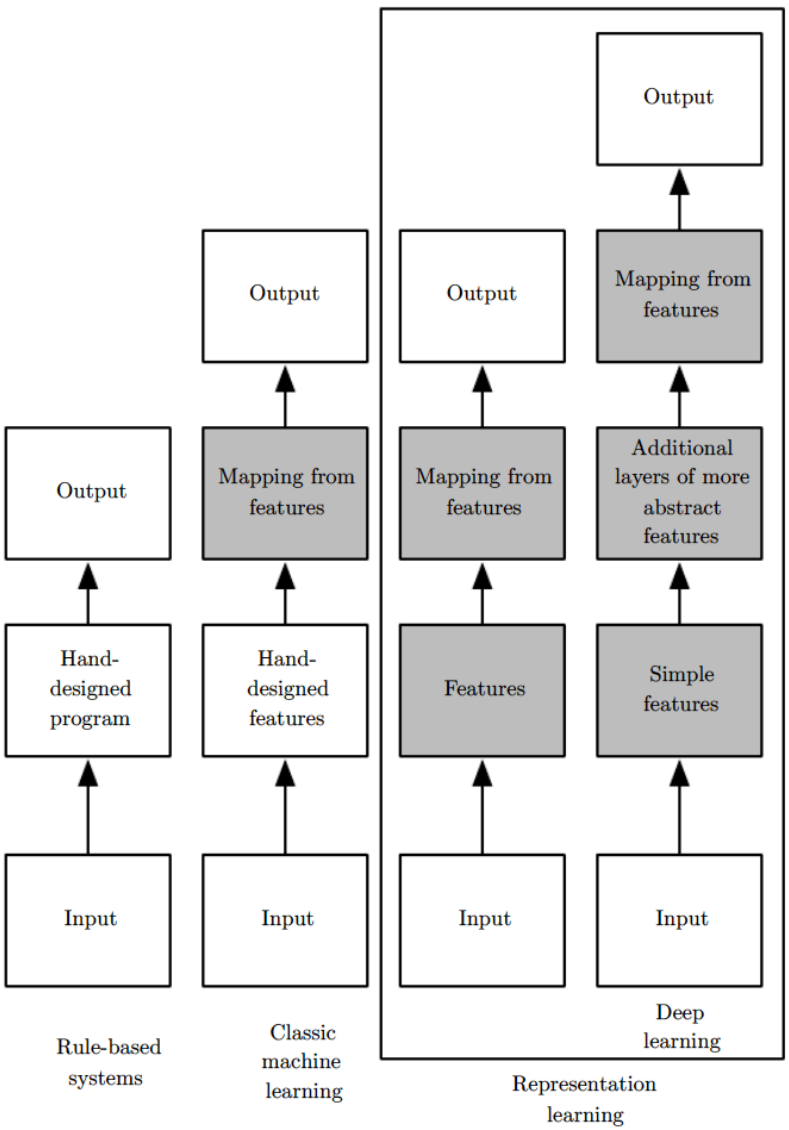

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  - $\text{act}^{(L)}(\cdot)$ just "normalizes" $\boldsymbol{z}^{(L)}$ to give $\hat{\rho} \in (0, 1)$

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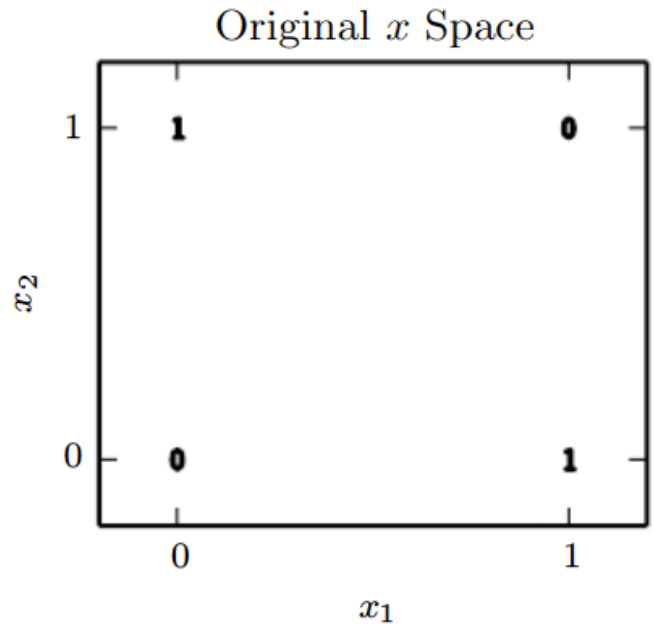
- Why ReLUs learn nonlinear (and better) representation?



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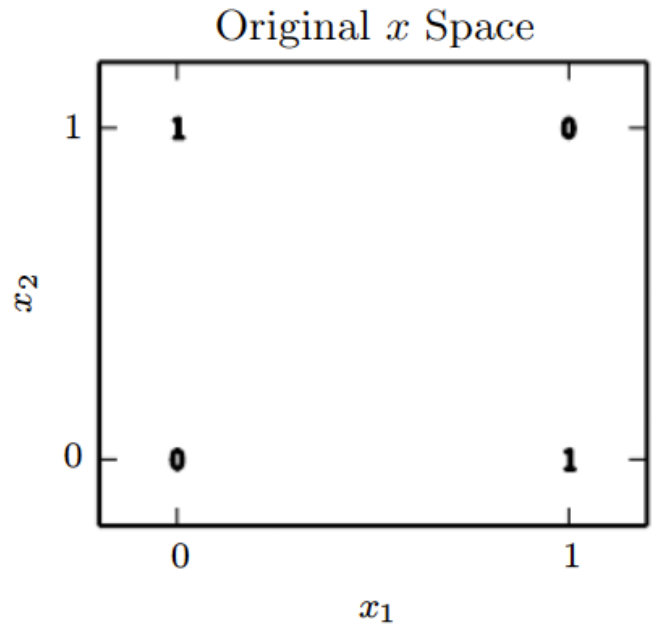

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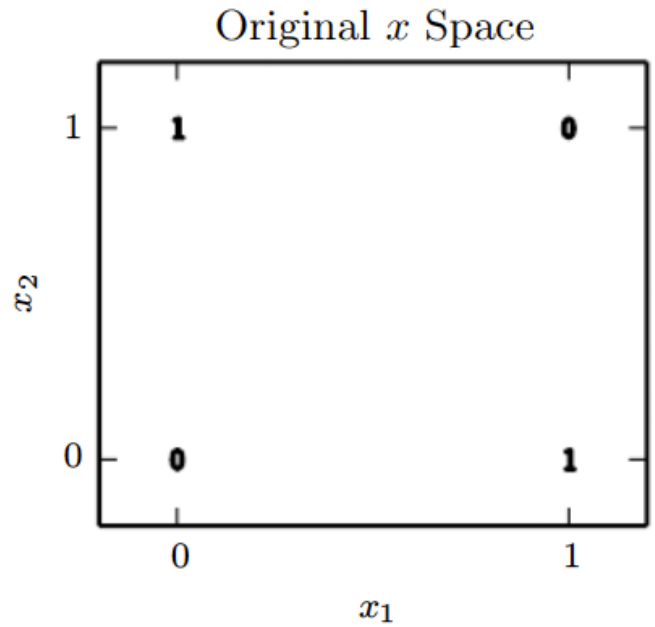

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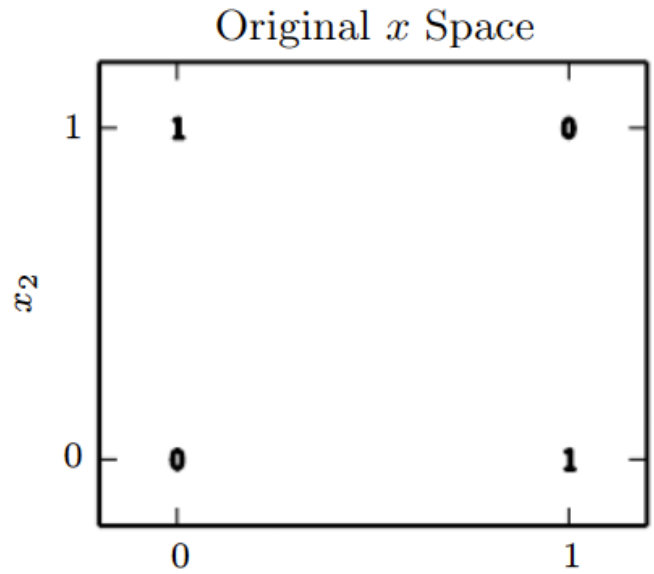

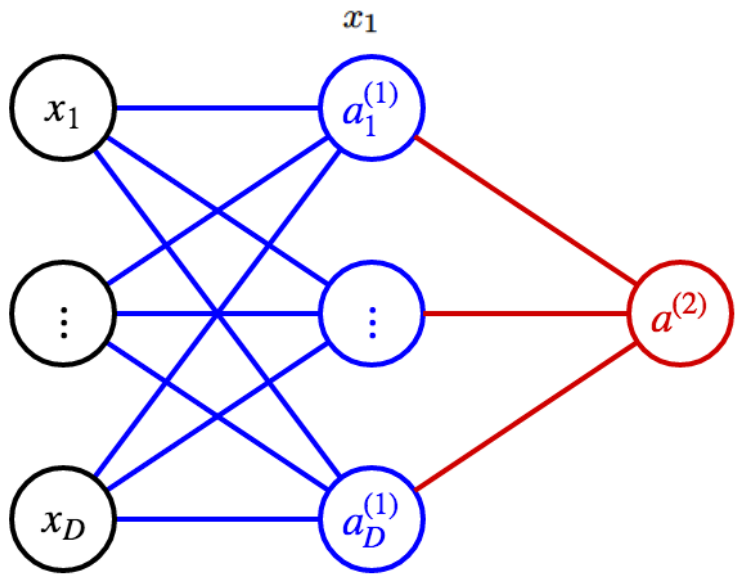

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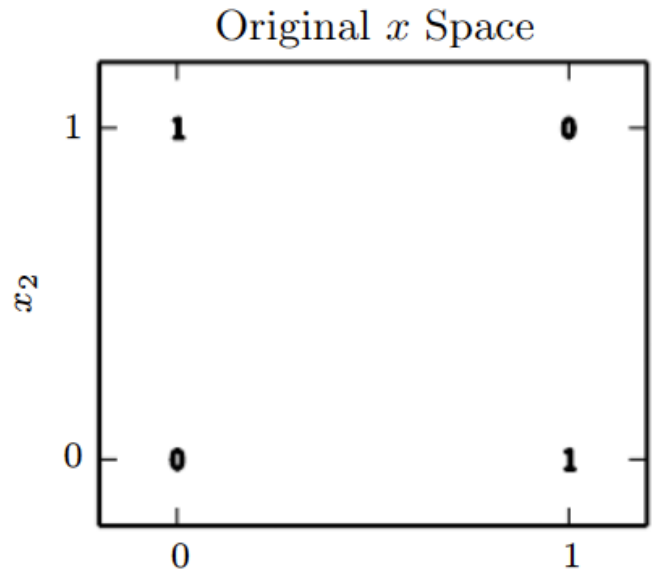
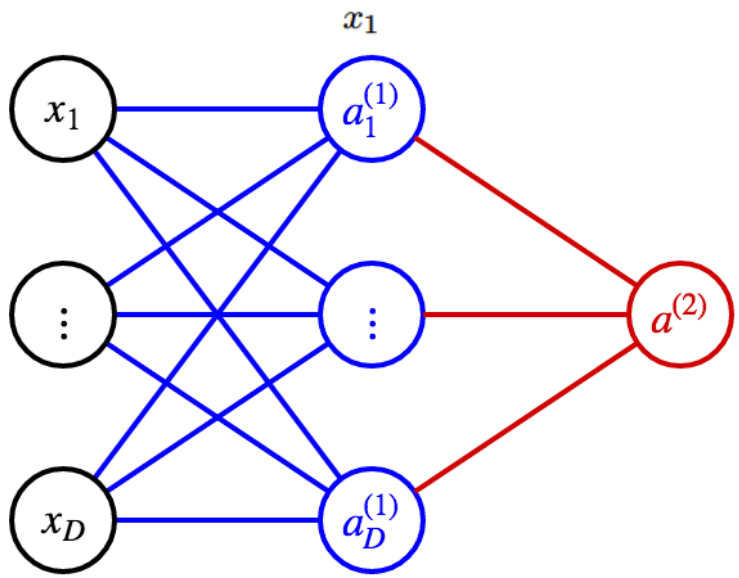
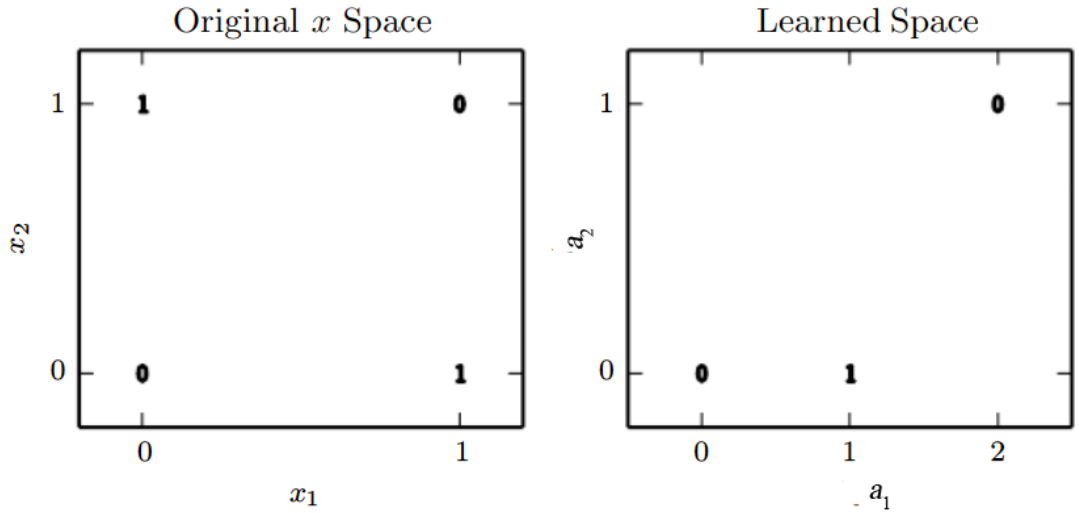
- Learns XOR by "merging" data points first



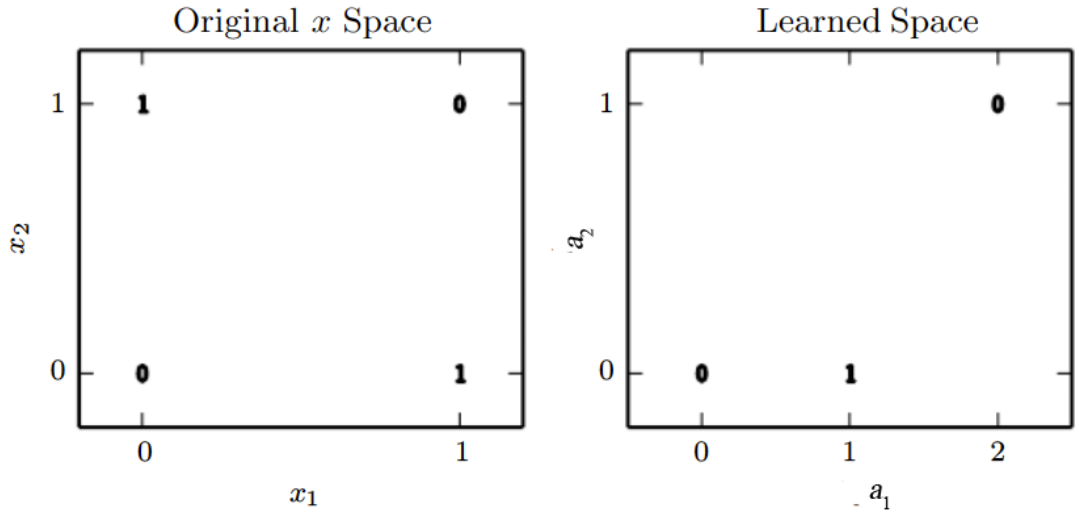


Learning the XOR II



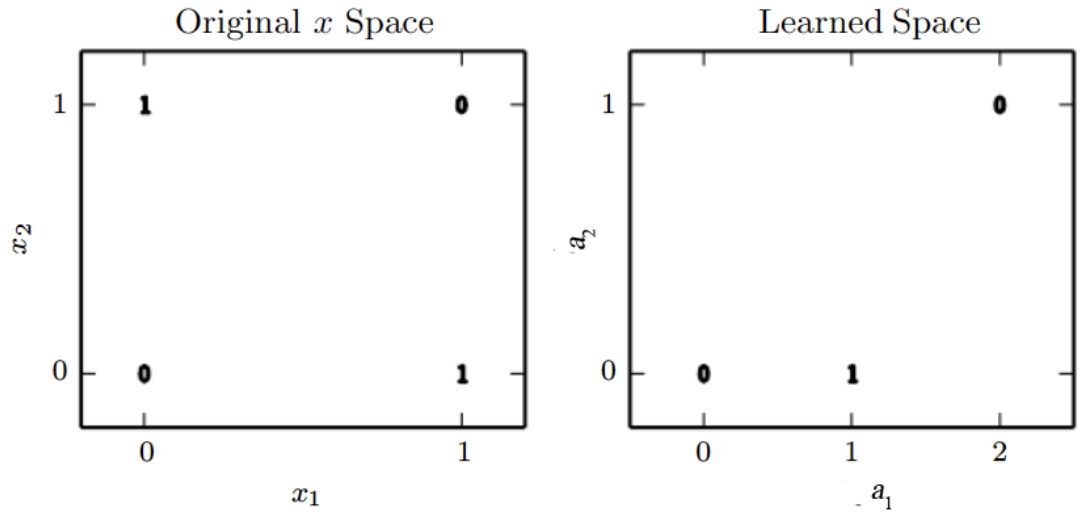
- $\boldsymbol{X} = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \\ 1 & 1 & 1 \end{bmatrix} \in \mathbb{R}^{N \times (1+D)}$, $\boldsymbol{W}^{(1)} = \begin{bmatrix} 1 & 1 \\ 1 & 1 \\ 0 & -1 \end{bmatrix}$, $\boldsymbol{w}^{(2)} = \begin{bmatrix} -1 \\ 2 \\ -4 \end{bmatrix}$
- $\hat{\boldsymbol{y}} = \begin{bmatrix} 0 \\ 1 \\ 1 \\ 0 \end{bmatrix} = 1(\sigma([\ 1 \quad \max(0, \boldsymbol{X}\boldsymbol{W}^{(1)})\ ]\boldsymbol{w}^{(2)}) > 0.5)$

Latent Representation $A^{(1)}$



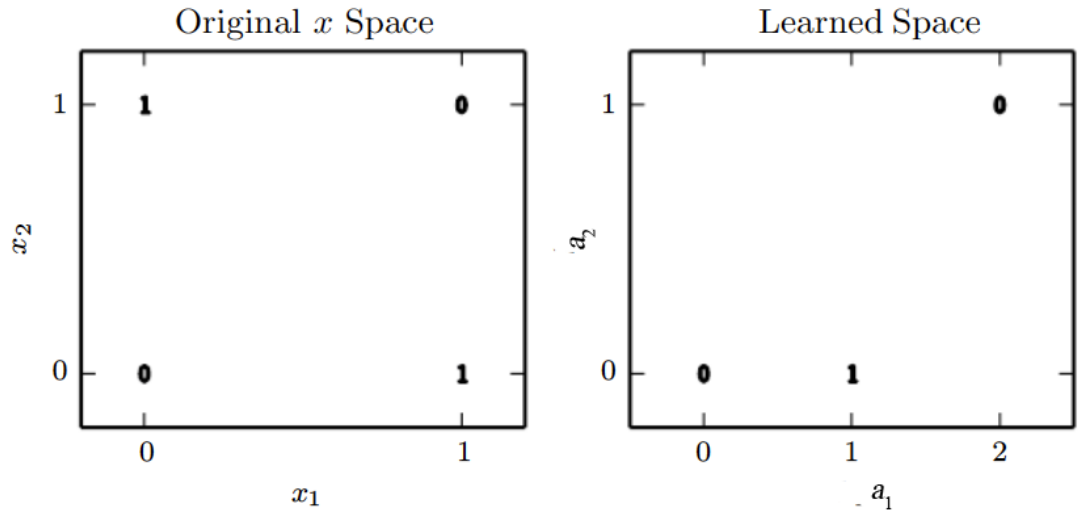
- $\boldsymbol{XW}^{(1)} = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \\ 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 0 & -1 \\ 1 & 1 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \\ 1 & 0 \\ 2 & 1 \end{bmatrix}$
- $\boldsymbol{A}^{(1)} = \begin{bmatrix} 1 & \max(0, \boldsymbol{XW}^{(1)}) \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 2 & 1 \end{bmatrix}$

Output Distribution $a^{(2)}$



- $\boldsymbol{a}^{(2)} = \sigma(\boldsymbol{A}^{(1)}\boldsymbol{w}^{(2)}) = \sigma\left(\begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 2 & 1 \end{bmatrix} \begin{bmatrix} -1 \\ 2 \\ -4 \end{bmatrix}\right) = \sigma\left(\begin{bmatrix} -1 \\ 1 \\ 1 \\ -1 \end{bmatrix}\right)$
- $\hat{\boldsymbol{y}} = 1(\boldsymbol{a}^{(2)} > 0.5) = \begin{bmatrix} 0 \\ 1 \\ 1 \\ 0 \end{bmatrix}$

Output Distribution $a^{(2)}$



- $\boldsymbol{a}^{(2)} = \sigma(\boldsymbol{A}^{(1)}\boldsymbol{w}^{(2)}) = \sigma\left(\begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 2 & 1 \end{bmatrix} \begin{bmatrix} -1 \\ 2 \\ -4 \end{bmatrix}\right) = \sigma\left(\begin{bmatrix} -1 \\ 1 \\ 1 \\ -1 \end{bmatrix}\right)$
- $\hat{\boldsymbol{y}} = 1(\boldsymbol{a}^{(2)} > 0.5) = \begin{bmatrix} 0 \\ 1 \\ 1 \\ 0 \end{bmatrix}$
- But how to train $\boldsymbol{W}^{(1)}$ and $\boldsymbol{w}^{(2)}$ from examples?

Outline

Training an NN

- Given examples: $\mathbb{X} = \{(\boldsymbol{x}^{(i)}, \boldsymbol{y}^{(i)})\}_{i=1}^{N}$
- How to learn parameters $\Theta = \{\boldsymbol{W}^{(1)}, \cdots, \boldsymbol{W}^{(L)}\}$?

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- The minimizer $\hat{\Theta}$ is an unbiased estimator of "true" Θ^*
  - Good for large N

Example: Binary Classification

- $\Pr(\mathrm{y} = 1 \,|\, \boldsymbol{x}) \sim \mathrm{Bernoulli}(\rho)$, where $\boldsymbol{x} \in \mathbb{R}^D$ and $y \in \{0, 1\}$
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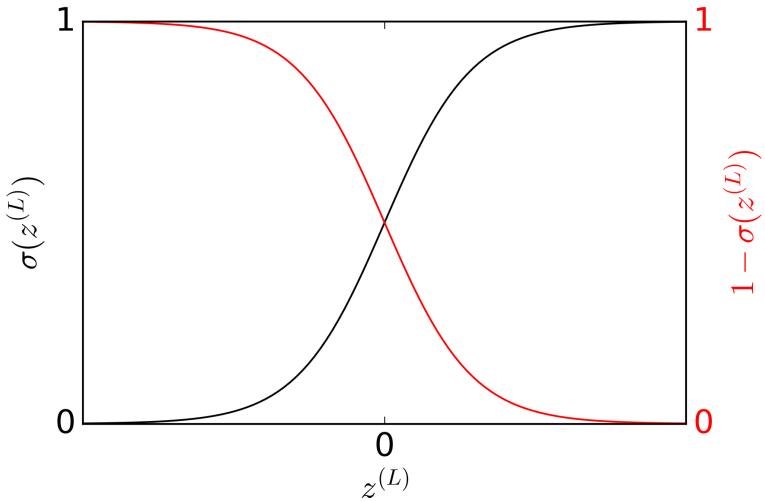

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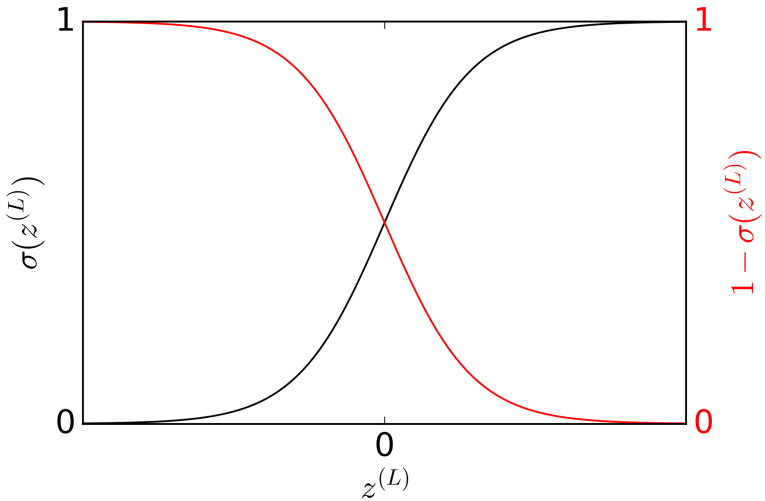

  - $\zeta(\cdot)$ is the softplus function

Optimization Algorithm

- Most NNs use ***SGD*** to solve the problem $\arg\min_{\Theta} \sum_i C^{(i)}(\Theta)$

(Mini-Batched) Stochastic Gradient Descent (SGD)

Initialize $\Theta^{(0)}$ randomly;
Repeat until convergence {
  Randomly partition the training set $\mathbb{X}$ into ***minibatches*** of size M;
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- How to compute $\nabla_\Theta \sum_i C^{(i)}(\Theta^{(t)})$ efficiently?
  - There could be a huge number of $W_{i,j}^{(k)}$'s in Θ

Outline

Back Propagation

$$\Theta^{(t+1)} \leftarrow \Theta^{(t)} - \eta \nabla_{\Theta} \sum_{n=1}^{M} C^{(n)}(\Theta^{(t)})$$

- We have $\nabla_{\Theta} \sum_n C^{(n)}(\Theta^{(t)}) = \sum_n \nabla_{\Theta} C^{(n)}(\Theta^{(t)})$

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- By the chain rule, we have

$$\frac{\partial c^{(n)}}{\partial W_{i,j}^{(k)}} = \frac{\partial c^{(n)}}{\partial z_j^{(k)}} \cdot \frac{\partial z_j^{(k)}}{\partial W_{i,j}^{(k)}}$$

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- We can get the second terms of all $\frac{\partial c^{(n)}}{\partial W_{i,j}^{(k)}}$'s starting from the ***most shallow*** layer

Backward Pass I

- Conversely, we can get the first terms of all $\frac{\partial C^{(n)}}{\partial W_{i,j}^{(k)}}$'s starting from the ***deepest*** layer

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- E.g., in binary classification, we have:

$$\delta^{(L)} = \frac{\partial c^{(n)}}{\partial z^{(L)}} = \frac{\partial \zeta((1-2y^{(n)})z^{(L)})}{\partial z^{(L)}} = \sigma((1-2y^{(n)})z^{(L)}) \cdot (1-2y^{(n)})$$

Backward Pass II

- When $k < L$, we have

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Theorem (Chain Rule)

Let $\boldsymbol{g} : \mathbb{R} \to \mathbb{R}^d$ and $f : \mathbb{R}^d \to \mathbb{R}$, then f

$$(f \circ \boldsymbol{g})'(x) = f'(\boldsymbol{g}(x))\boldsymbol{g}'(x) = \nabla f(\boldsymbol{g}(x))^\top \begin{bmatrix} g_1'(x) \\ \vdots \\ g_n'(x) \end{bmatrix}.$$

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$$\delta_j^{(k)} = \left(\sum_s \delta_s^{(k+1)} \cdot W_{j,s}^{(k+1)} \right) \text{act}'(z_j^{(k)})$$

- We can evaluate all $\delta_j^{(k)}$'s starting from the deepest layer

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- The information propagate along a new kind of feedforward network:

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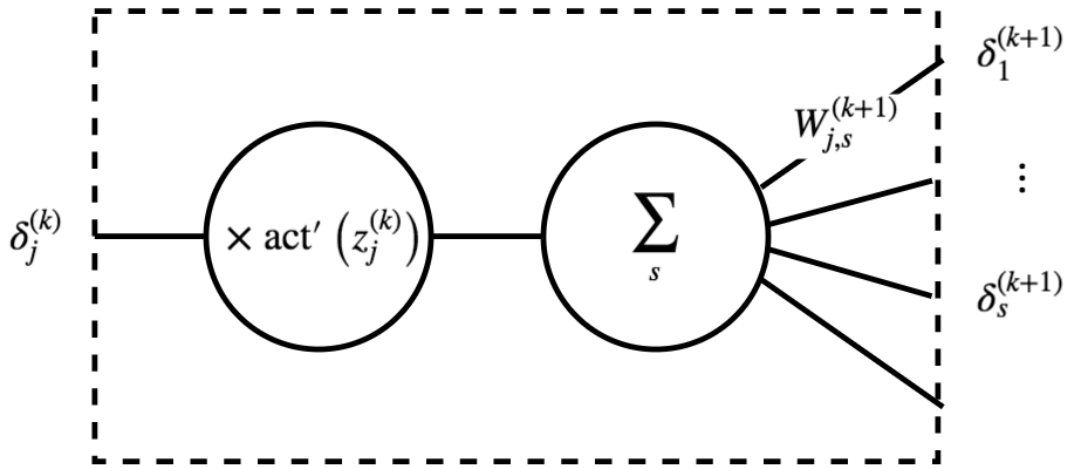

Backprop Algorithm (Minibatch Size $M = 1$)

Input: $(\boldsymbol{x}^{(n)}, \boldsymbol{y}^{(n)})$ and $\Theta^{(t)}$

Forward pass:

$\boldsymbol{a}^{(0)} \leftarrow \begin{bmatrix} 1 & \boldsymbol{x}^{(n)} \end{bmatrix}^\top$;

for $k \leftarrow 1$ *to* L **do**

$\quad \boldsymbol{z}^{(k)} \leftarrow \boldsymbol{W}^{(k)\top} \boldsymbol{a}^{(k-1)}$;

$\quad \boldsymbol{a}^{(k)} \leftarrow \text{act}(\boldsymbol{z}^{(k)})$;

end

Backward pass:

Compute error signal $\delta^{(L)}$ (e.g., $(1-2y^{(n)})\sigma((1-2y^{(n)})z^{(L)})$ in binary classification)

for $k \leftarrow L-1$ *to* 1 **do**

$\quad \boldsymbol{\delta}^{(k)} \leftarrow \text{act}'(\boldsymbol{z}^{(k)}) \odot (\boldsymbol{W}^{(k+1)} \boldsymbol{\delta}^{(k+1)})$;

end

Return $\frac{\partial c^{(n)}}{\partial \boldsymbol{W}^{(k)}} = \boldsymbol{a}^{(k-1)} \otimes \boldsymbol{\delta}^{(k)}$ for all k

Backprop Algorithm (Minibatch Size $M > 1$)

Input: $\{(\boldsymbol{x}^{(n)}, \boldsymbol{y}^{(n)})\}_{n=1}^{M}$ and $\Theta^{(t)}$

Forward pass:

$\boldsymbol{A}^{(0)} \leftarrow \left[\begin{array}{ccc} \boldsymbol{a}^{(0,1)} & \cdots & \boldsymbol{a}^{(0,M)} \end{array} \right]^\top$;

for $k \leftarrow 1$ *to* L **do**

$\boldsymbol{Z}^{(k)} \leftarrow \boldsymbol{A}^{(k-1)} \boldsymbol{W}^{(k)}$;

$\boldsymbol{A}^{(k)} \leftarrow \text{act}(\boldsymbol{Z}^{(k)})$;

end

Backward pass:

Compute error signals

$\Delta^{(L)} = \left[\begin{array}{ccc} \delta^{(L,0)} & \cdots & \delta^{(L,M)} \end{array} \right]^\top$

for $k \leftarrow L-1$ *to* 1 **do**

$\Delta^{(k)} \leftarrow \text{act}'(\boldsymbol{Z}^{(k)}) \odot (\Delta^{(k+1)} \boldsymbol{W}^{(k+1)\top})$;

end

Return $\frac{\partial c^{(n)}}{\partial \boldsymbol{W}^{(k)}} = \sum_{n=1}^{M} \boldsymbol{a}^{(k-1,n)} \otimes \delta^{(k,n)}$ for all k

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end

Backward pass:

Compute error signals

$\Delta^{(L)} = \left[\begin{array}{ccc} \delta^{(L,0)} & \cdots & \delta^{(L,M)} \end{array} \right]^{\top}$

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Backprop Algorithm (Minibatch Size $M > 1$)

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  - During SGD, the gradient

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  should be sufficiently large before we get a satisfactory NN

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- Provides a consistent way to define output units

Sigmoid Units for Bernoulli Output Distributions

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- In practice, the two versions make little difference

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- Linear units do not saturate, so they pose little difficulty for gradient based optimization

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- Why not, for example, use Sigmoid as hidden units?

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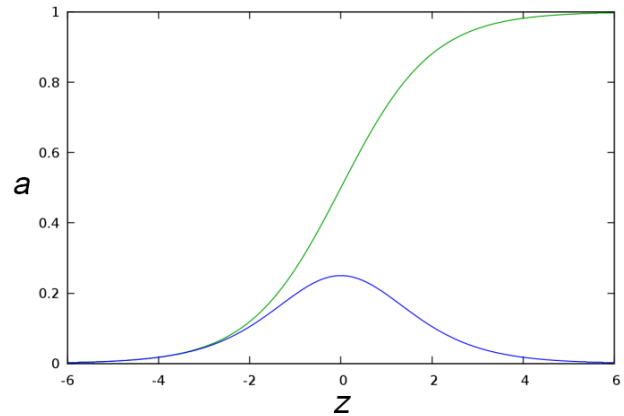

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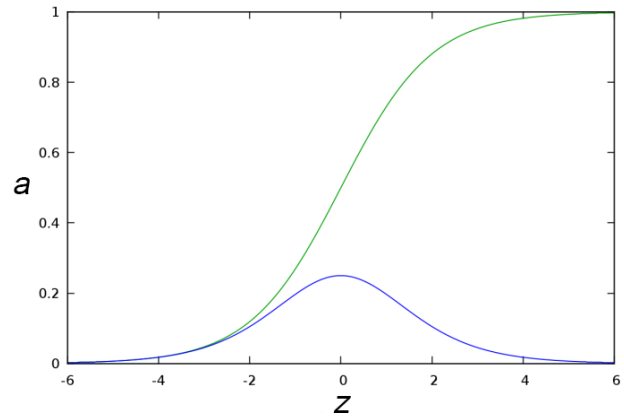

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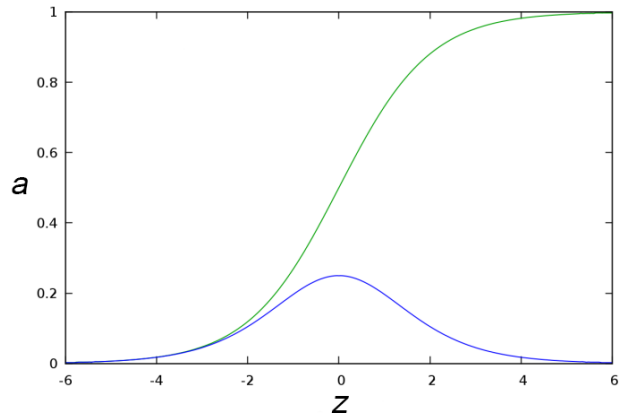

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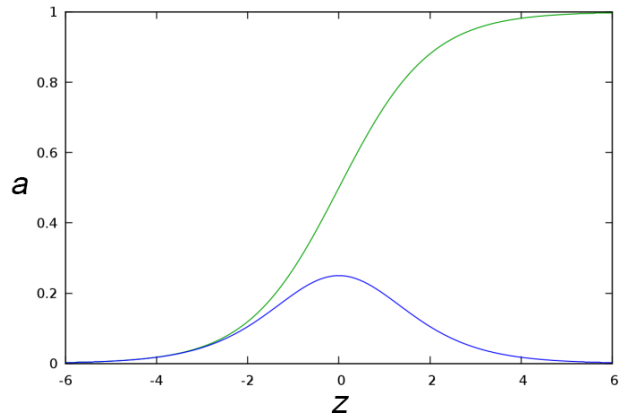

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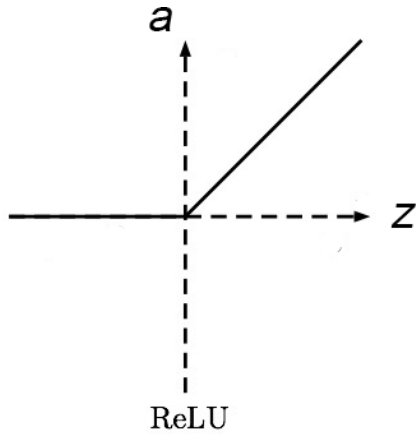

$$\text{act}'(z^{(k)}) = \begin{cases} 1, & \text{if } z^{(k)} > 0 \\ 0, & \text{otherwise} \end{cases}$$

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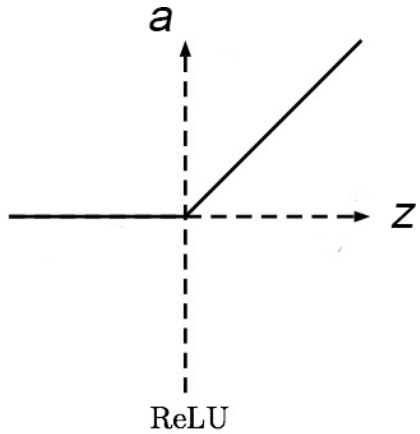

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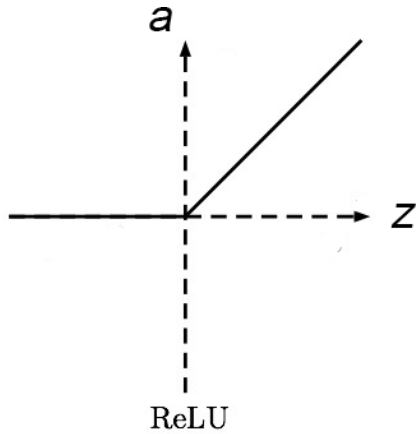

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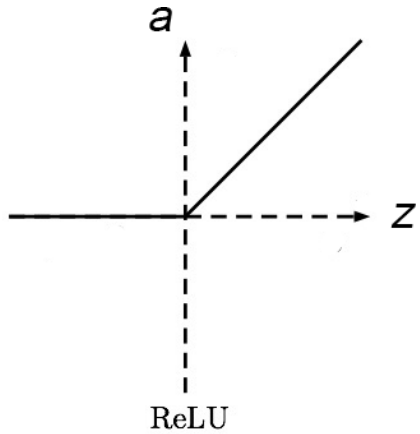

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- What if $z^{(k)} = 0$?
- In practice, we usually assign 1 or 0 randomly
  - Floating points are not precise anyway

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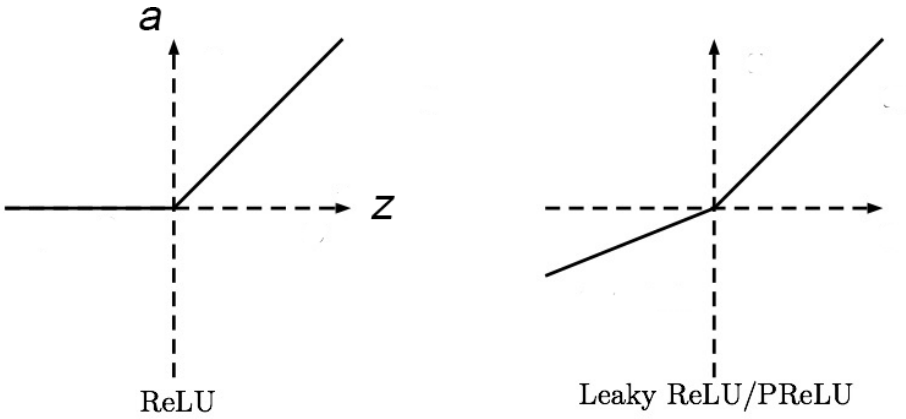
- The second derivative $\mathrm{ReLU}''(\cdot)$ is 0 everywhere
  - Eliminates the second-order effects and makes the gradient-based optimization more useful (than, e.g., Newton methods)
- Problem: for neurons with $\delta_j^{(k)} = 0$, theirs weights $\boldsymbol{W}_{:,j}^{(k)}$ will ***not*** be updated

$$\frac{\partial c^{(n)}}{\partial W_{i,j}^{(k)}} = \boldsymbol{\delta}^{(k)} \frac{\partial z_j^{(k)}}{\partial W_{i,j}^{(k)}}$$

- Improvement?

Leaky/Parametric ReLU



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for some $\alpha \in \mathbb{R}$

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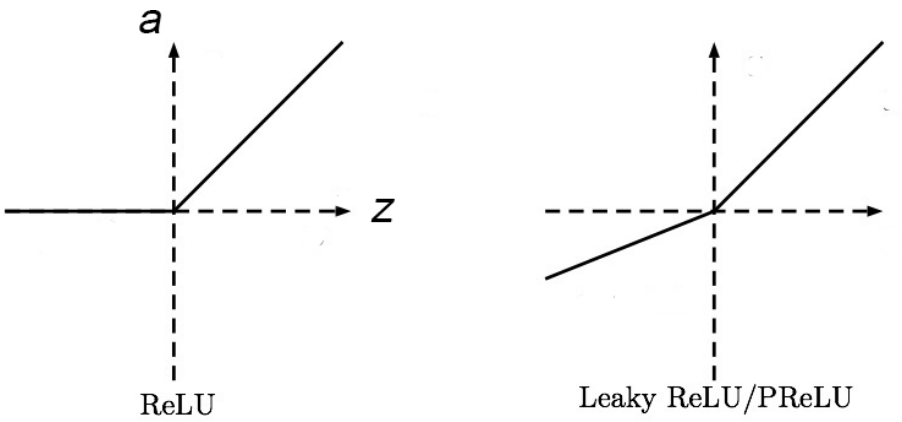

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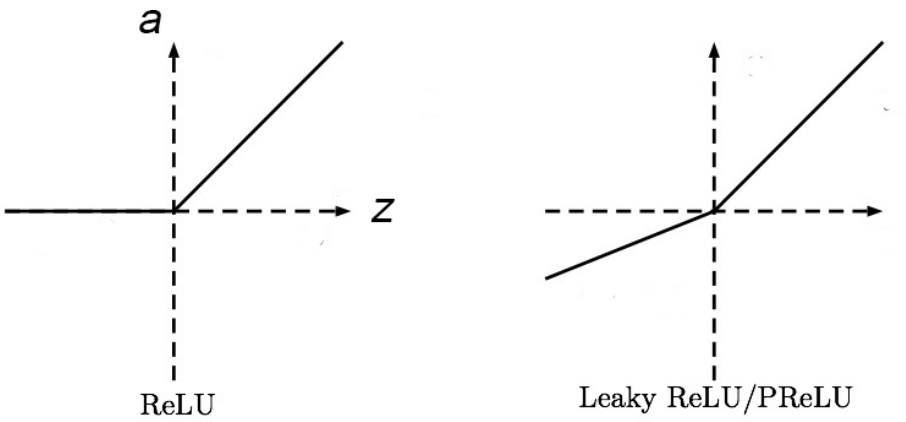

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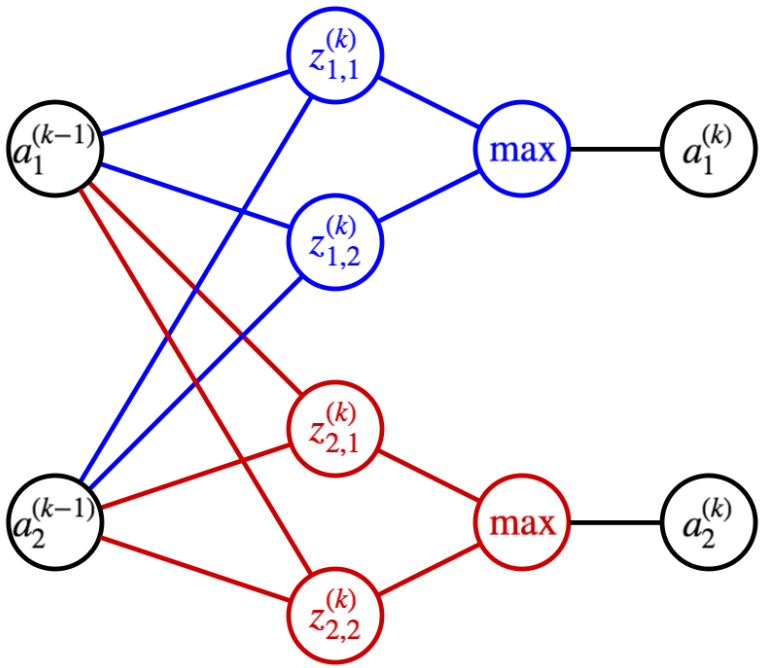
- ***Leaky ReLU***: α is set in advance (fixed during training)
  - Usually a small value
  - Or domain-specific
- Example: ***absolute value rectification*** $\alpha = -1$
  - Used for object recognition from images
  - Seek features that are invariant under a polarity reversal of the input illumination
- ***Parametric ReLU*** (PReLU): α learned automatically by gradient descent

Maxout Units I

- ***Maxout units*** generalize ReLU variants further:

$$\text{act}(\boldsymbol{z}^{(k)})_j = \max_s z_{j,s}$$

  - $\boldsymbol{a}^{(k-1)}$ is linearly mapped to multiple groups of $\boldsymbol{z}_{j,:}^{(k)}$'s



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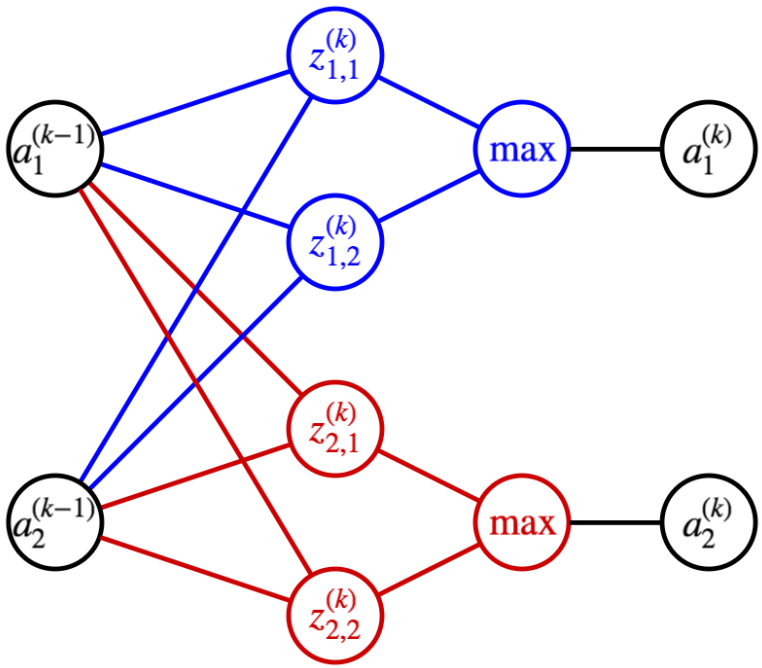
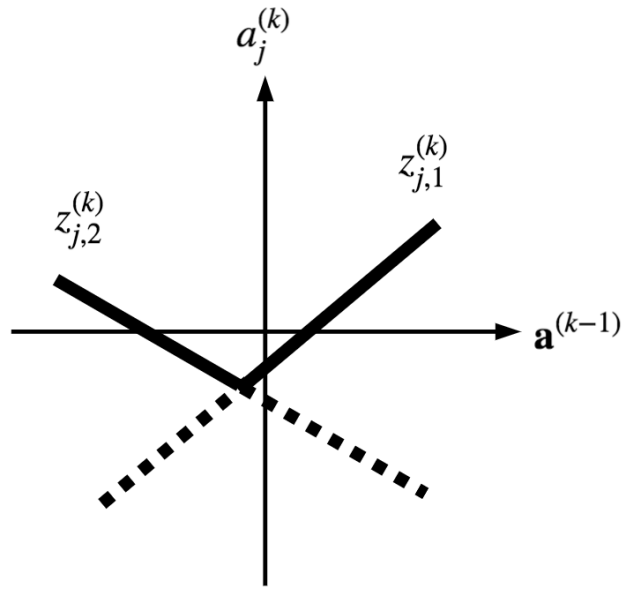
- Learns a piecewise linear, convex activation function automatically
  - Covers both leaky ReLU and PReLU





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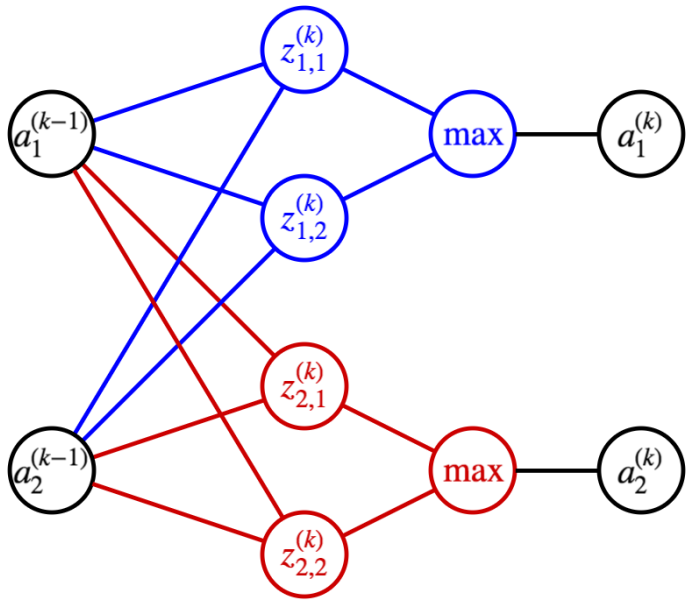

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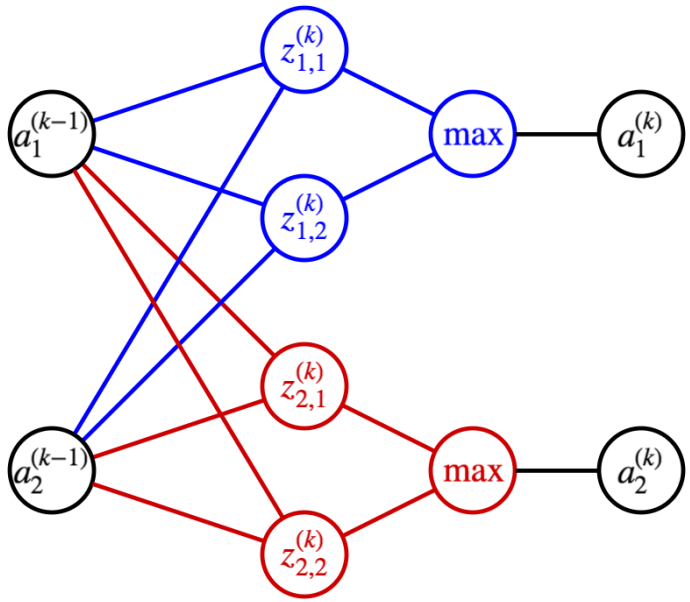

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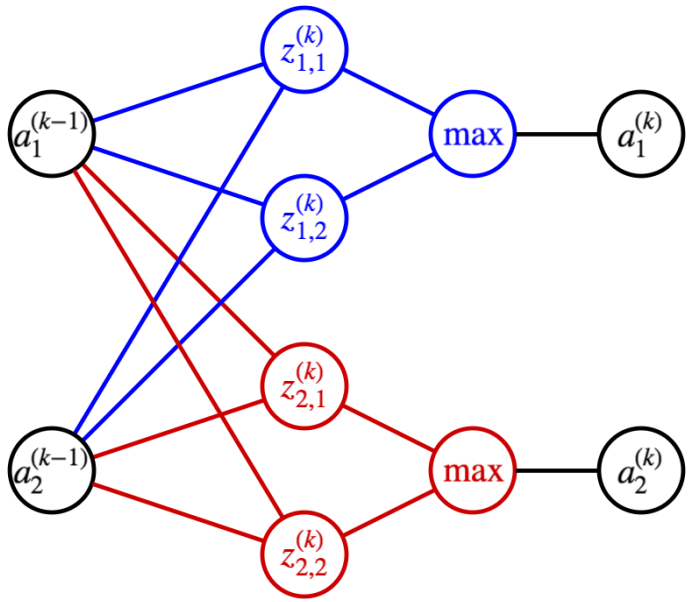

- Offers some "redundancy" that helps to resist the ***catastrophic forgetting*** phenomenon [2]
  - An NN may forget how to perform tasks that they were trained on in the past

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- Typically requires more training data
- Otherwise, regularization is needed

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A feedforward network with at least one hidden layer can approximate any continuous function (on a closed and bounded subset of $\mathbb{R}^D$) or any function mapping from a finite dimensional discrete space to another.

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- Why going deep?

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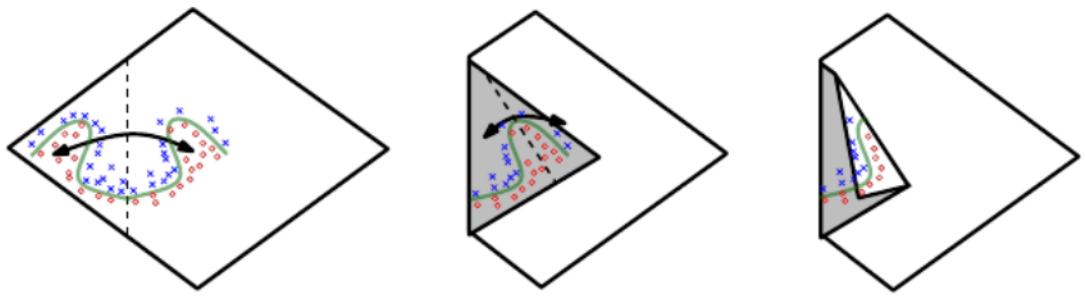
- Example: an NN with absolute value rectification units



- Each hidden unit specifies where to fold the input space in order to create mirror responses (on both sides of the absolute value)
- By composing these folding operations, we obtain an exponentially large number of piecewise linear regions which can capture all kinds of regular (e.g., repeating) patterns

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  - Intermediate outputs can be counters or pointers for internal processing

Outline

- width & depth

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