Neural Networks: Design

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Machine Learning

Outline

1. **The Basics**
   - Example: Learning the XOR
2. **Training**
   - Back Propagation
3. **Neuron Design**
   - Cost Function & Output Neurons
   - Hidden Neurons
4. **Architecture Design**
   - Architecture Tuning

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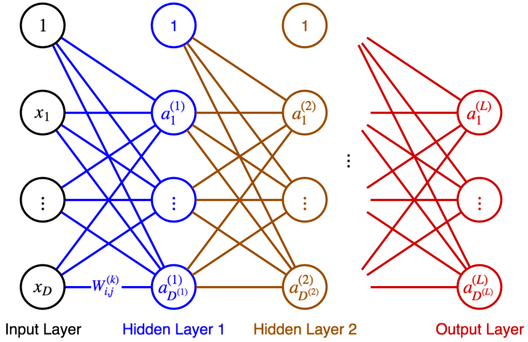
Model: a Composite Function I

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

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

that approximates the target function f^*



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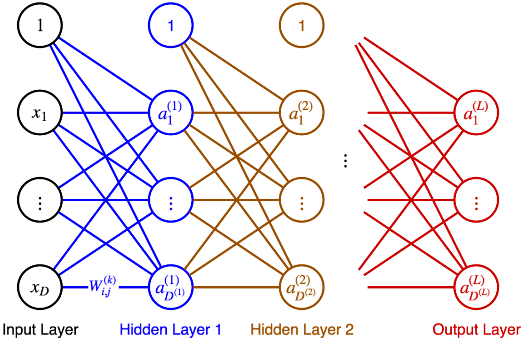

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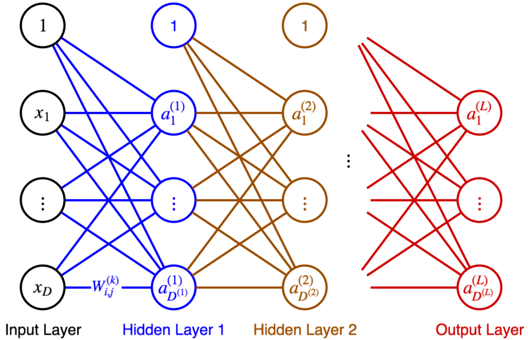
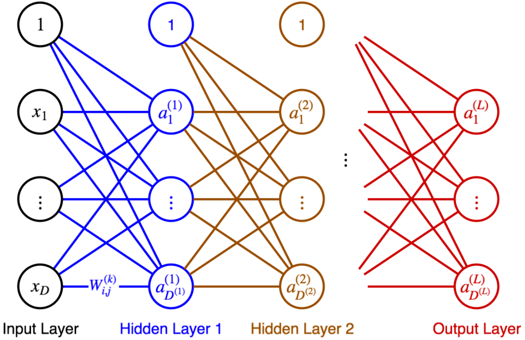
- "Feedforward" because information flows from input to output



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
$$\boldsymbol{a}^{(k)} = \mathrm{act}^{(k)}(\boldsymbol{W}^{(k)\top}\boldsymbol{a}^{(k-1)} + \boldsymbol{b}^{(k)})$$
    - $\mathrm{act}^{(\mathrm{i})}(\cdot):\mathbb{R}\to\mathbb{R}$ is an ***activation function*** applied elementwisely



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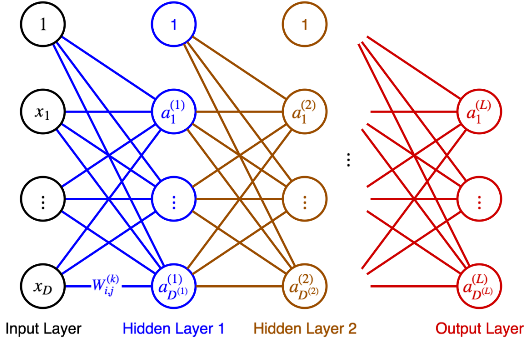
- Shorthand: $\boldsymbol{a}^{(k)} = \text{act}^{(k)}(\boldsymbol{W}^{(k)\top}\boldsymbol{a}^{(k-1)})$
  - $\boldsymbol{a}^{(k-1)} \in \mathbb{R}^{D^{(k-1)}+1}$, $a_0^{(k-1)} = 1$, and $\boldsymbol{W}^{(k)} \in \mathbb{R}^{(D^{(k-1)}+1)\times D^{(k)}}$



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

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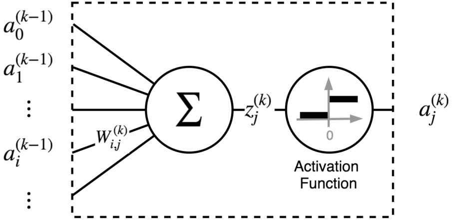

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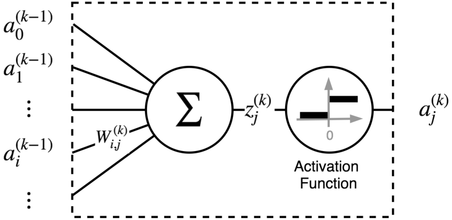
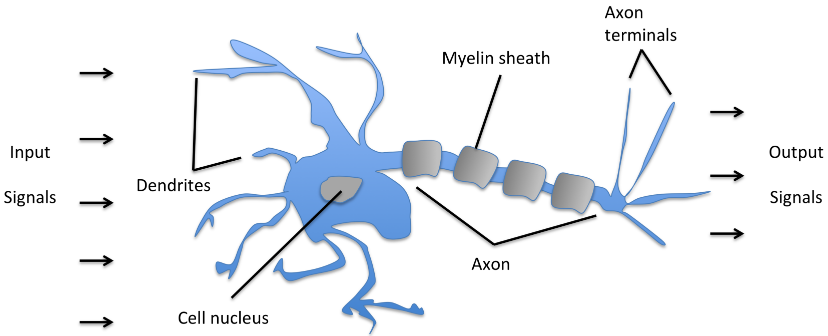
- Loosely guided by neuroscience





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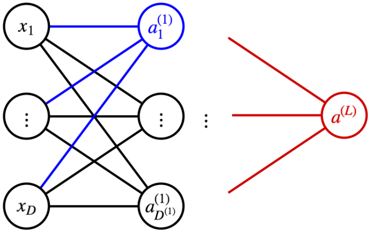
- Modern NN design is mainly guided by mathematical and engineering disciplines. Consider a binary classifier where $y \in \{0, 1\}$:



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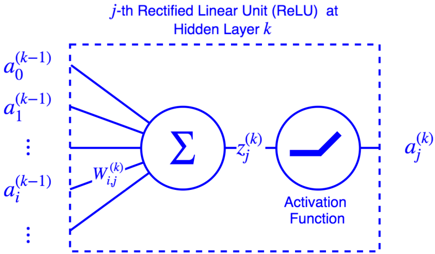

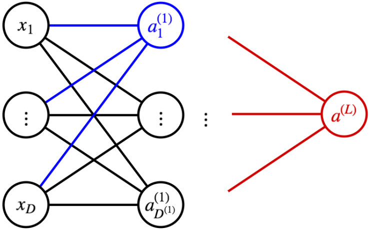

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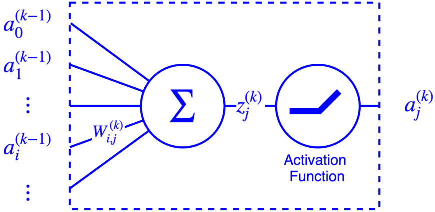
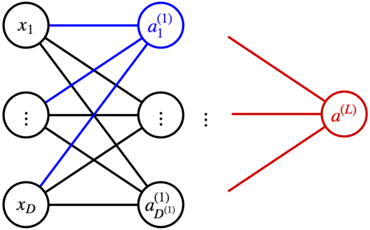
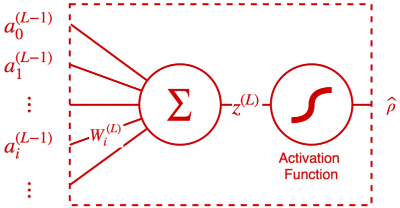
j-th Rectified Linear Unit (ReLU) at Hidden Layer k





Sigmoid Unit for Bernoulli $P(y \mid x; \rho)$



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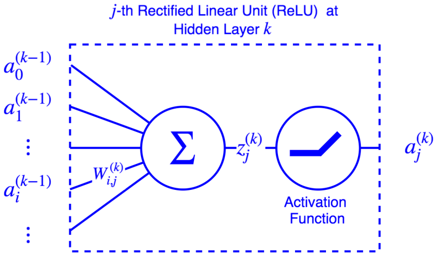
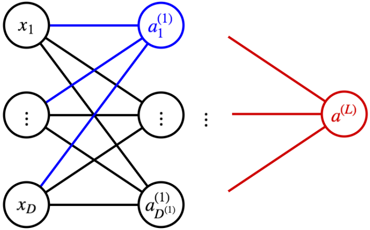
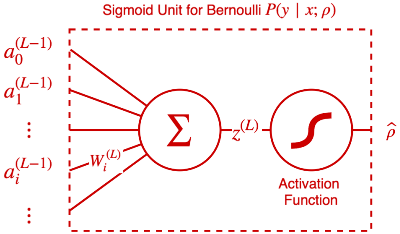
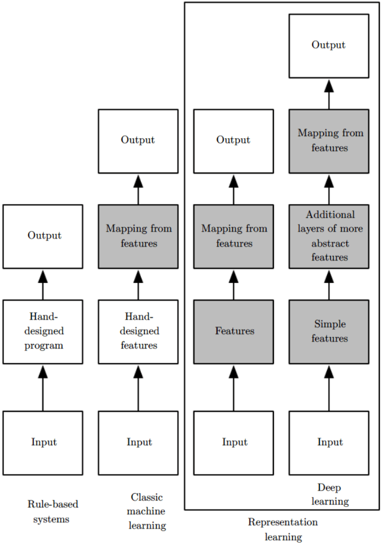
  - A logistic regressor with input $\boldsymbol{a}^{(L-1)}$







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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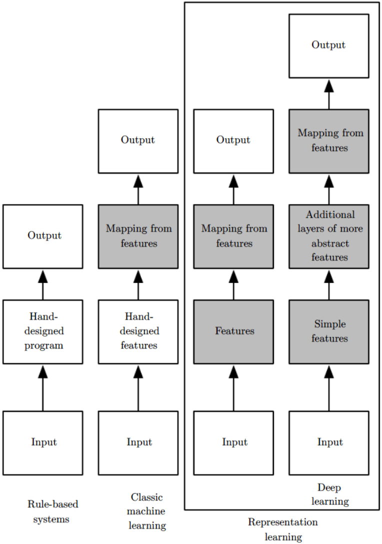

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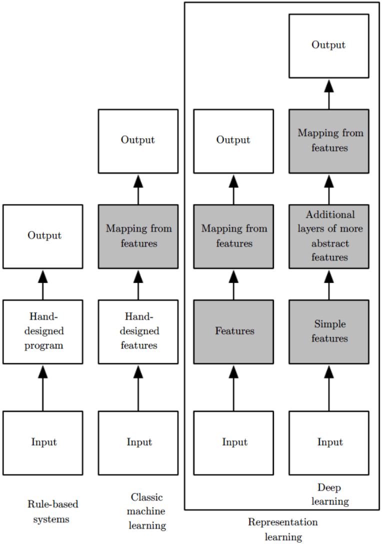

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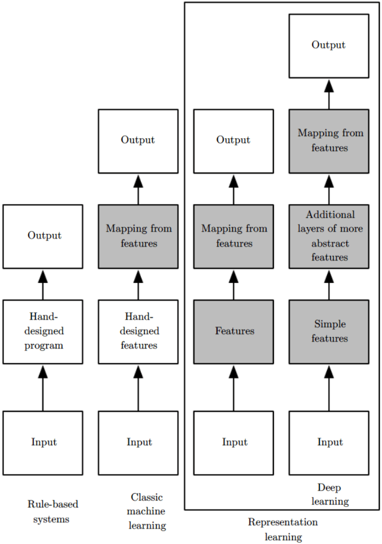

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  - $\mathrm{act}^{(L)}(\cdot)$ just "normalizes" $\boldsymbol{z}^{(L)}$ to give $\hat{\rho} \in (0,1)$

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Learning the XOR I

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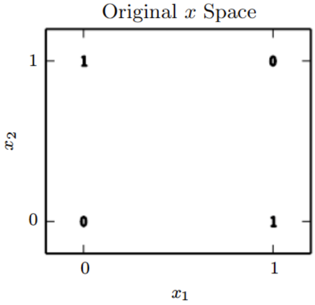

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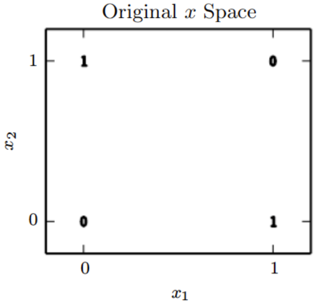

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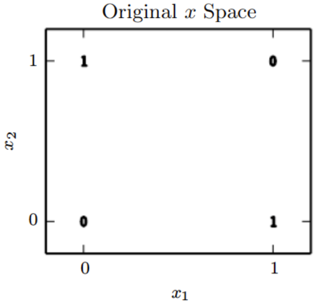

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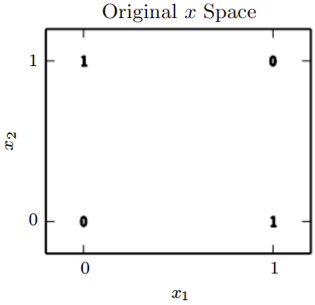

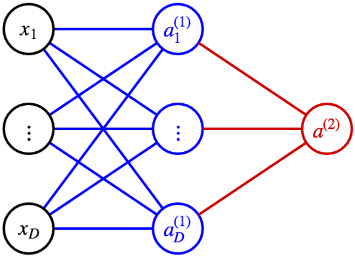

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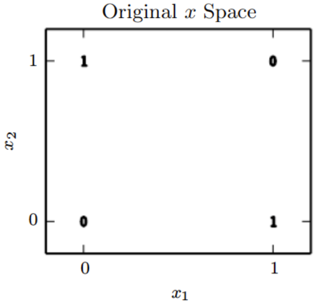
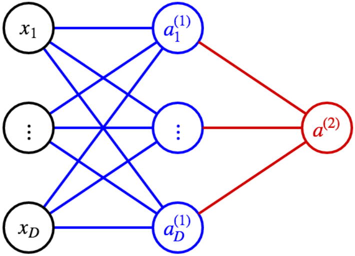
- Learns XOR by "merging" data points first





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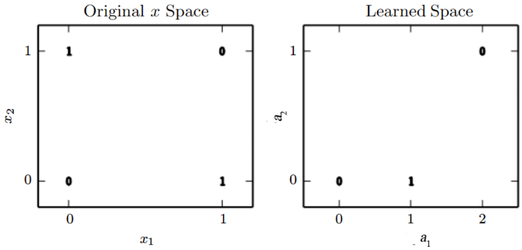
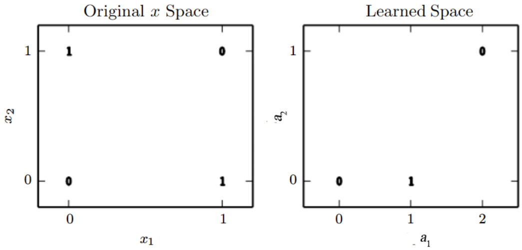


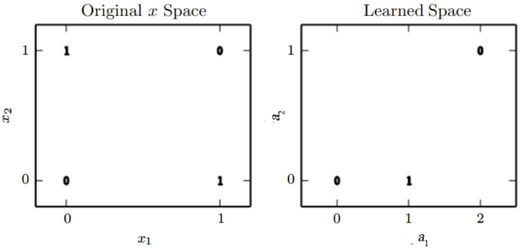
- $\boldsymbol{X} = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \\ 1 & 1 & 1 \end{bmatrix} \in \mathbb{R}^{N\times(1+D)}$, $\boldsymbol{W}^{(1)} = \begin{bmatrix} 1 & 1 \\ 1 & 1 \\ 0 & -1 \end{bmatrix}$, $\boldsymbol{w}^{(2)} = \begin{bmatrix} -1 \\ 2 \\ -4 \end{bmatrix}$
- $\hat{\boldsymbol{y}}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

Latent Representation $A^{(1)}$



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

Output Distribution $\boldsymbol{a}^{(2)}$



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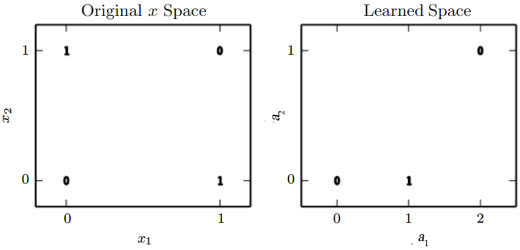

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- $\hat{\boldsymbol{y}} = 1(\boldsymbol{a}^{(2)} > 0.5) = \begin{bmatrix} 0 \\ 1 \\ 1 \\ 0 \end{bmatrix}$
- But how to train $\boldsymbol{W}^{(1)}$ and $\boldsymbol{w}^{(2)}$ from examples?

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Training an NN

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- How to learn parameters $\Theta = \{\boldsymbol{W}^{(1)}, \cdots, \boldsymbol{W}^{(L)}\}$?

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\end{aligned}
$$

Training an NN

- Given examples: $\mathbb{X} = \{(\boldsymbol{x}^{(i)}, \boldsymbol{y}^{(i)})\}_{i=1}^{N}$
- How to learn parameters $\Theta = \{\boldsymbol{W}^{(1)}, \cdots, \boldsymbol{W}^{(L)}\}$?
- Most NNs are trained using the ***maximum likelihood*** by default (assuming i.i.d examples):

$$\begin{aligned}
&\arg\max_{\Theta} \log \mathrm{P}(\mathbb{X} \mid \Theta) \\
&\quad = \arg\min_{\Theta} -\log \mathrm{P}(\mathbb{X} \mid \Theta) \\
&\quad = \arg\min_{\Theta} \sum_i -\log \mathrm{P}(\boldsymbol{x}^{(i)}, \boldsymbol{y}^{(i)} \mid \Theta) \\
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\end{aligned}$$

- 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 $y \in \{0, 1\}$
- $a^{(L)} = \hat{\rho} = \sigma(z^{(L)})$ the predicted distribution

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&C^{(i)}(\Theta) \\
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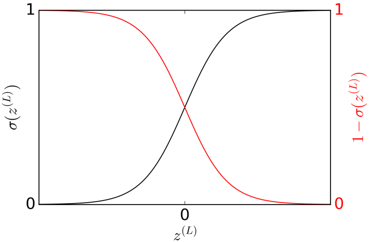

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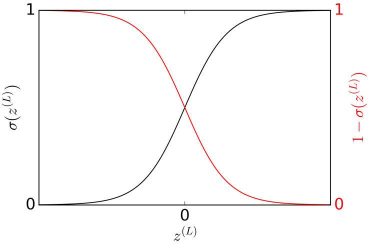

  - $\zeta(\cdot)$ is the softplus function

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

1 The Basics
- Example: Learning the XOR

2 Training
- Back Propagation

3 Neuron Design
- Cost Function & Output Neurons
- Hidden Neurons

4 Architecture Design
- Architecture Tuning

Back Propagation

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

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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 $\frac{\partial c^{(n)}}{\partial W_{i,j}^{(k)}} = \frac{\partial c^{(n)}}{\partial z_j^{(k)}} \cdot \frac{\partial z_j^{(k)}}{\partial W_{i,j}^{(k)}}$ starting from the ***deepest*** layer

Backward Pass I

- Conversely, we can get the first terms of $\frac{\partial c^{(n)}}{\partial W_{i,j}^{(k)}} = \frac{\partial c^{(n)}}{\partial z_j^{(k)}} \cdot \frac{\partial z_j^{(k)}}{\partial W_{i,j}^{(k)}}$ starting from the ***deepest*** layer
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  - Depending on the definition of functions $\mathrm{act}^{(L)}$ and $C^{(n)}$

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- When $k = L$, the evaluation varies from task to task
  - Depending on the definition of functions $\text{act}^{(L)}$ and $C^{(n)}$
- 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

$$\delta_j^{(k)} = \frac{\partial c^{(n)}}{\partial z_j^{(k)}} = \frac{\partial c^{(n)}}{\partial a_j^{(k)}} \cdot \frac{\partial a_j^{(k)}}{\partial z_j^{(k)}} = \frac{\partial c^{(n)}}{\partial a_j^{(k)}} \cdot \mathrm{act}'(z_j^{(k)})$$

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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*

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

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

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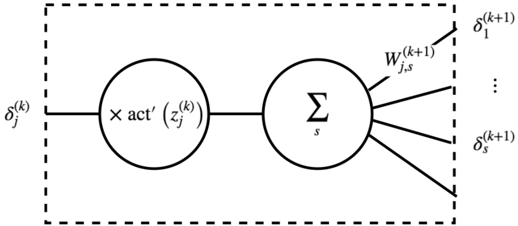

Backprop Algorithm (Minibatch Size $M = 1$)

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**

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

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

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**

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

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**

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

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

end

Backward pass:

Compute error signals

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

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

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

end

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

Backprop Algorithm (Minibatch Size $M > 1$)

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- Large width ($D^{(k)}$) at each layer

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- Large batch size

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  - Universal cost function
  - Different output units for different $\mathrm{P}(\mathbf{y} \mid \mathbf{x})$

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- The design of modern neurons is largely influenced by how an NN is trained
- Maximum likelihood principle:

$$\arg\max_{\Theta} \log \mathrm{P}(\mathbb{X}\,|\,\Theta) = \arg\min_{\Theta} \sum_i -\log \mathrm{P}(\boldsymbol{y}^{(i)}\,|\,\boldsymbol{x}^{(i)}, \Theta)$$

  - Universal cost function
  - Different output units for different $\mathrm{P}(\mathbf{y}\,|\,\mathbf{x})$
- Gradient-based optimization:
  - During SGD, the gradient

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

  should be sufficiently large before we get a satisfactory NN

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Negative Log Likelihood and Cross Entropy

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- Provides a consistent way to define output units

Sigmoid Units for Bernoulli Output Distributions

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  - $y \in \{0,1\}$ and $\rho \in (0,1)$

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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?

Vanishing Gradient Problem

- In backward pass of Backprop:

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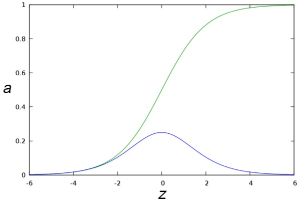

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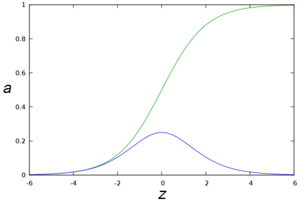

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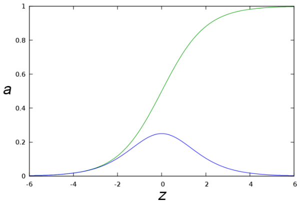

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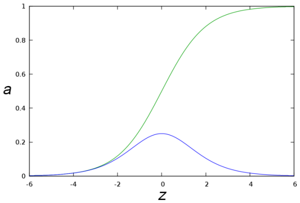
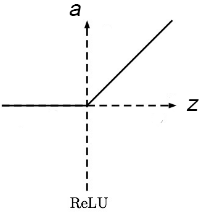


ReLU I



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

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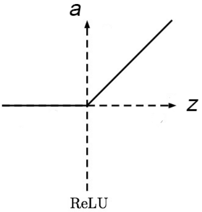

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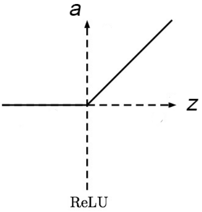

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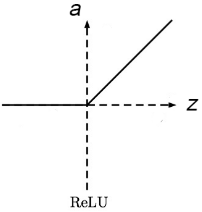

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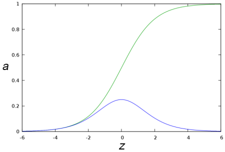
- What if $z^{(k)} = 0$?
- In practice, we usually assign 1 or 0 randomly
  - Floating points are not precise anyway

ReLU II

- Why piecewise linear?
  - To avoid vanishing gradient, we can modify $\sigma(\cdot)$ to make it steeper at middle such that $\sigma'(\cdot) > 1$



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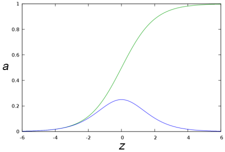

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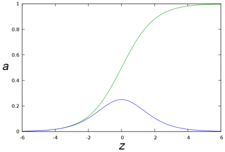

- The second derivative $\mathrm{ReLU}''(\cdot)$ is 0 everywhere
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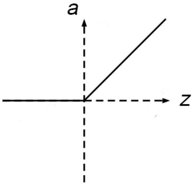
- Problem: for neurons with $\delta_j^{(k)} = 0$, theirs weights $\boldsymbol{W}_{:,j}^{(k)}$ will ***not*** be updated

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

- Improvement?

Leaky/Parametric ReLU



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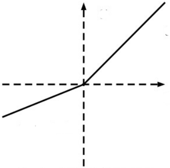
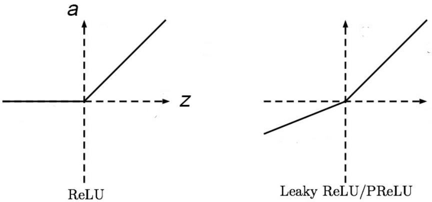

Leaky ReLU/PReLU

$$\mathrm{act}(z^{(k)}) = \max(\alpha \cdot z^{(k)}, z^{(k)}),$$

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

Leaky/Parametric ReLU



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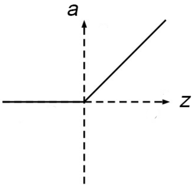

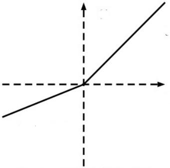

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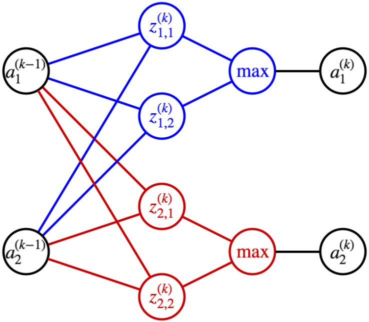
  - Usually a small value
  - Or domain-specific
- Example: ***absolute value rectification*** $\alpha = -1$
  - Used for object recognition from images
  - Seek features that are invariant under a polarity reversal of the input illumination
- ***Parametric ReLU*** (PReLU): α learned automatically by gradient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

Maxout Units I

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

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

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



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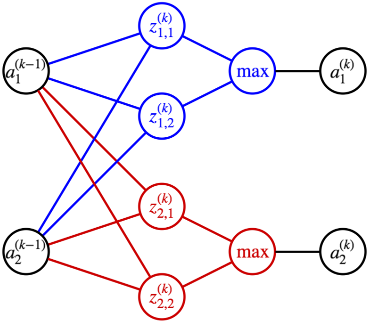
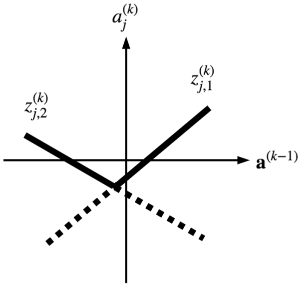
$$\mathrm{act}(\boldsymbol{z}^{(k)})_j = \max_s z_{j,s}$$

  - $\boldsymbol{a}^{(k-1)}$ is linearly mapped to multiple groups of $z_{j,:}^{(k)}$'s
- Learns a piecewise linear, convex activation function automatically
  - Covers both leaky ReLU and PReLU





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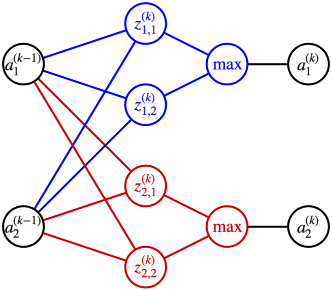

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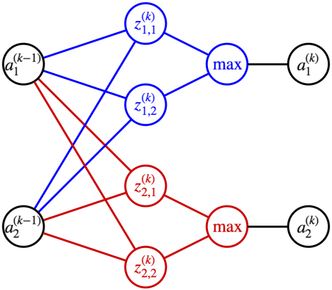

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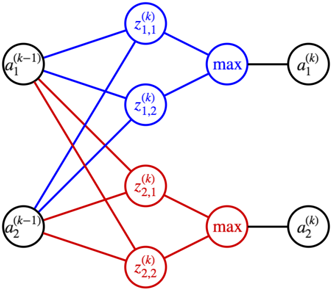

- Offers some "redundancy" that helps to resist the ***catastrophic forgetting*** phenomenon [2]
  - An NN may forget how to perform tasks that they were trained on in the past

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

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   - Example: Learning the XOR
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   - Back Propagation
3. Neuron Design
   - Cost Function & Output Neurons
   - Hidden Neurons
4. **Architecture Design**
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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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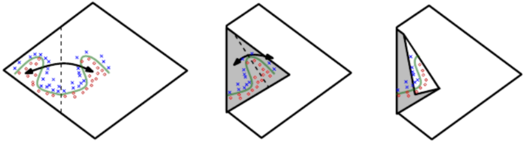
Exponential Gain in Number of Hidden Units

- Functions representable with a deep rectifier NN require an exponential number of hidden units in a shallow NN [6]
- 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

Deep ReLU Networks

- Activation-constant regions vs. output values [3]

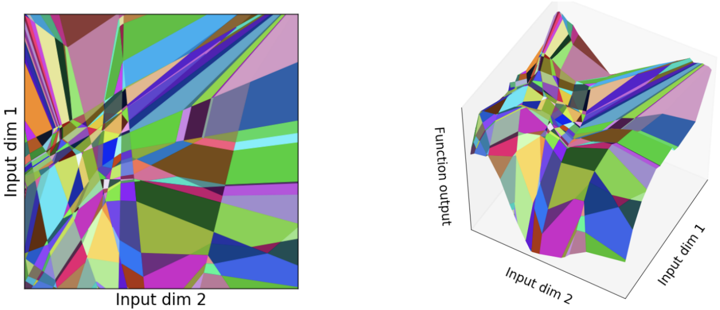


Figure 2: Function defined by a ReLU network of depth 5 and width 8 at initialization. Left: Partition of the input space into regions, on each of which the activation pattern of neurons is constant. Right: the function computed by the network, which is linear on each activation region.

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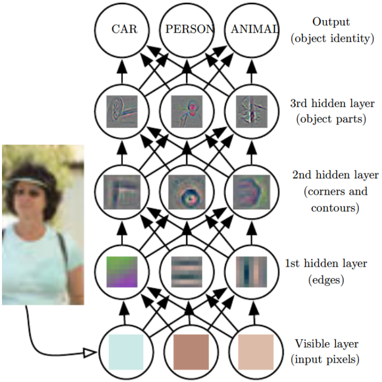
- When is the assumption valid? E.g., image recognition, natural language processing, etc.



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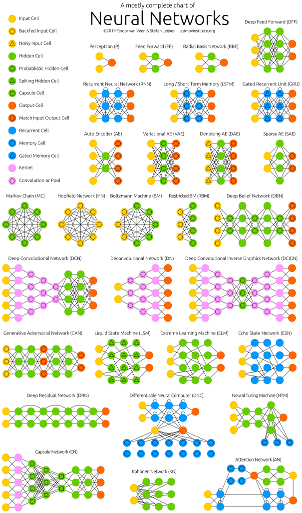

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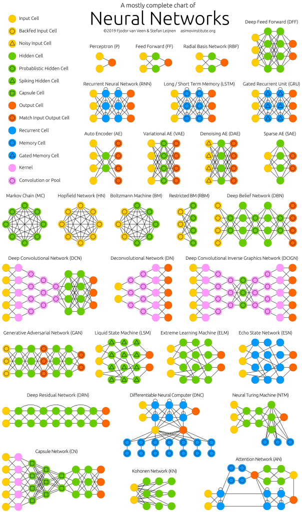
- Auto ML
  - The process of automating the above



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