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SCHOOL OF ENGINEERING

Feed Forward Neural Networks

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Pattern Recognition Lab, Friedrich-Alexander-Universität Erlangen-Nürnberg
April 21, 2020

Outline

Model

Perceptrons as Universal Function Approximators

From Activations to Classifications: Softmax Function

Optimization

Layer Abstraction

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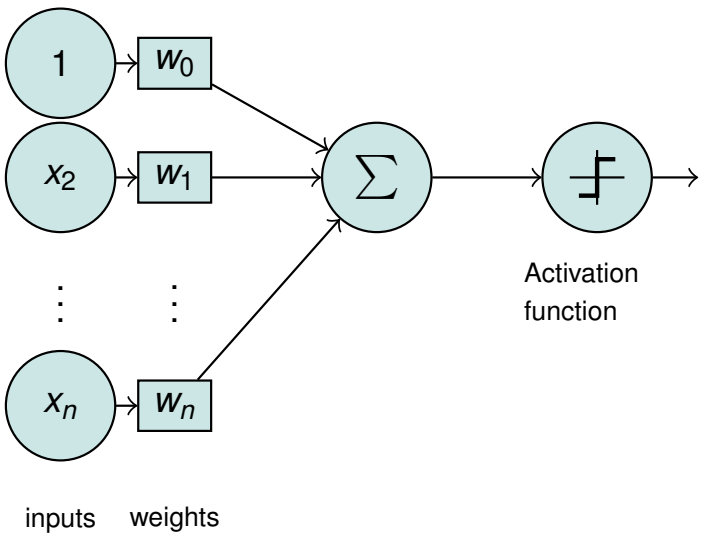
Model

Recap: Perceptrons

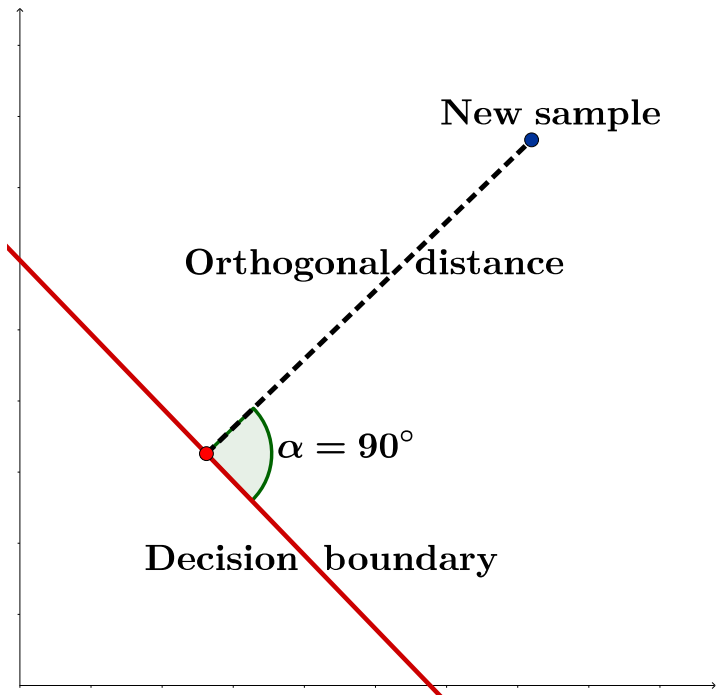
- Perceptron's decision rule:

$$\hat{y} = \text{sign}(\mathbf{w}^T \mathbf{x})$$

- Classification only depends on sign of distance

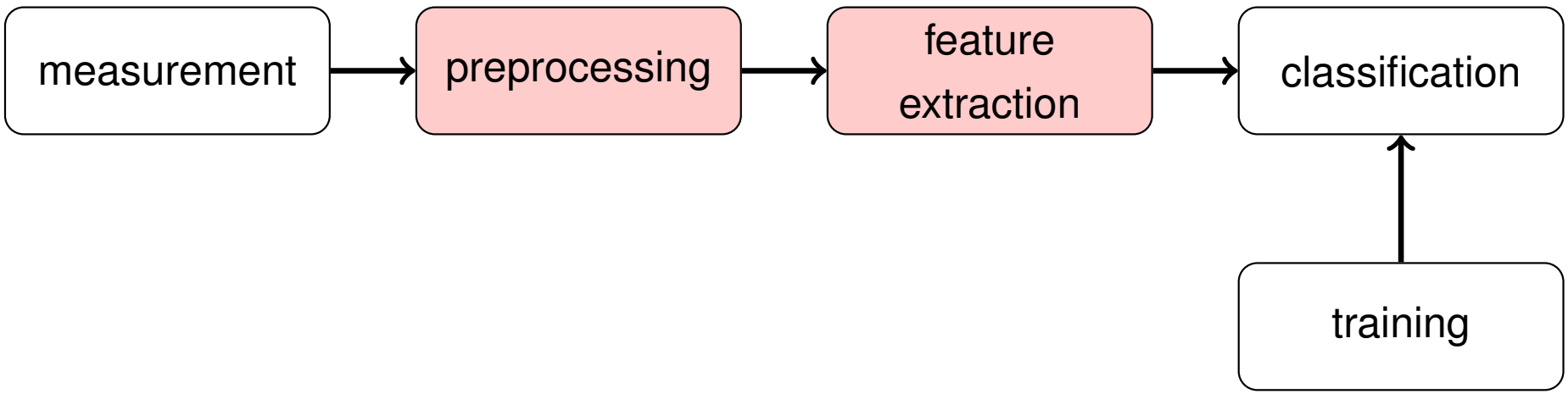


Perceptron



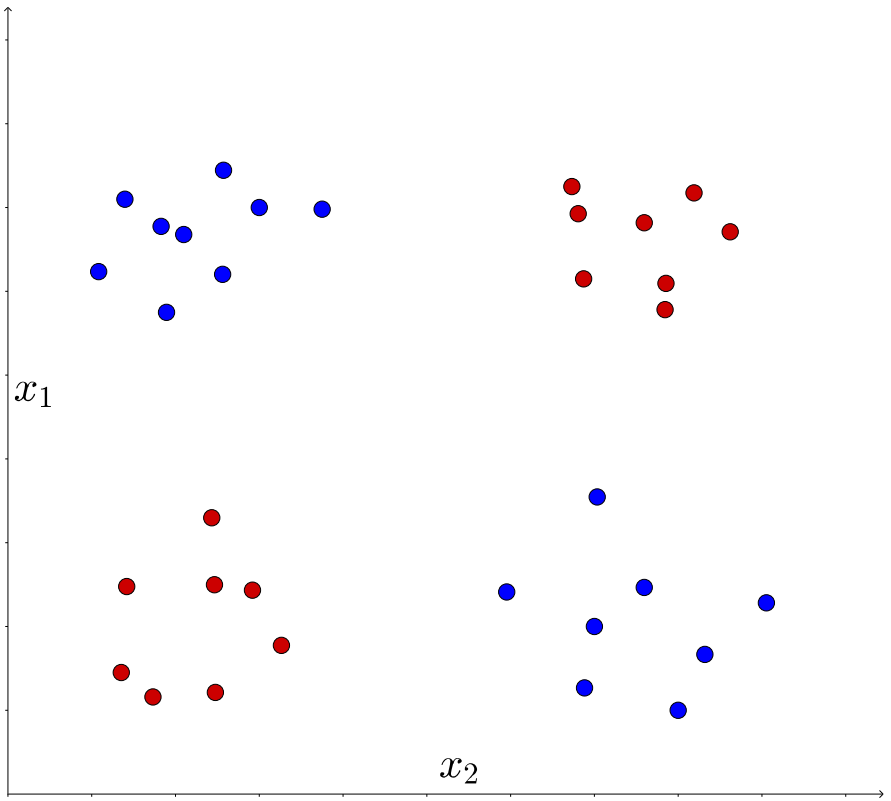
Linear decision boundary

Recap: Pattern Recognition Pipeline



- (Multi-layer) perceptron (today's lecture) still uses predefined features
- "Hand-crafted" feature design is replaced by **data driven feature learning** in state-of-the-art architectures (upcoming lectures)
- Most concepts are important across architectures!

XOR Problem

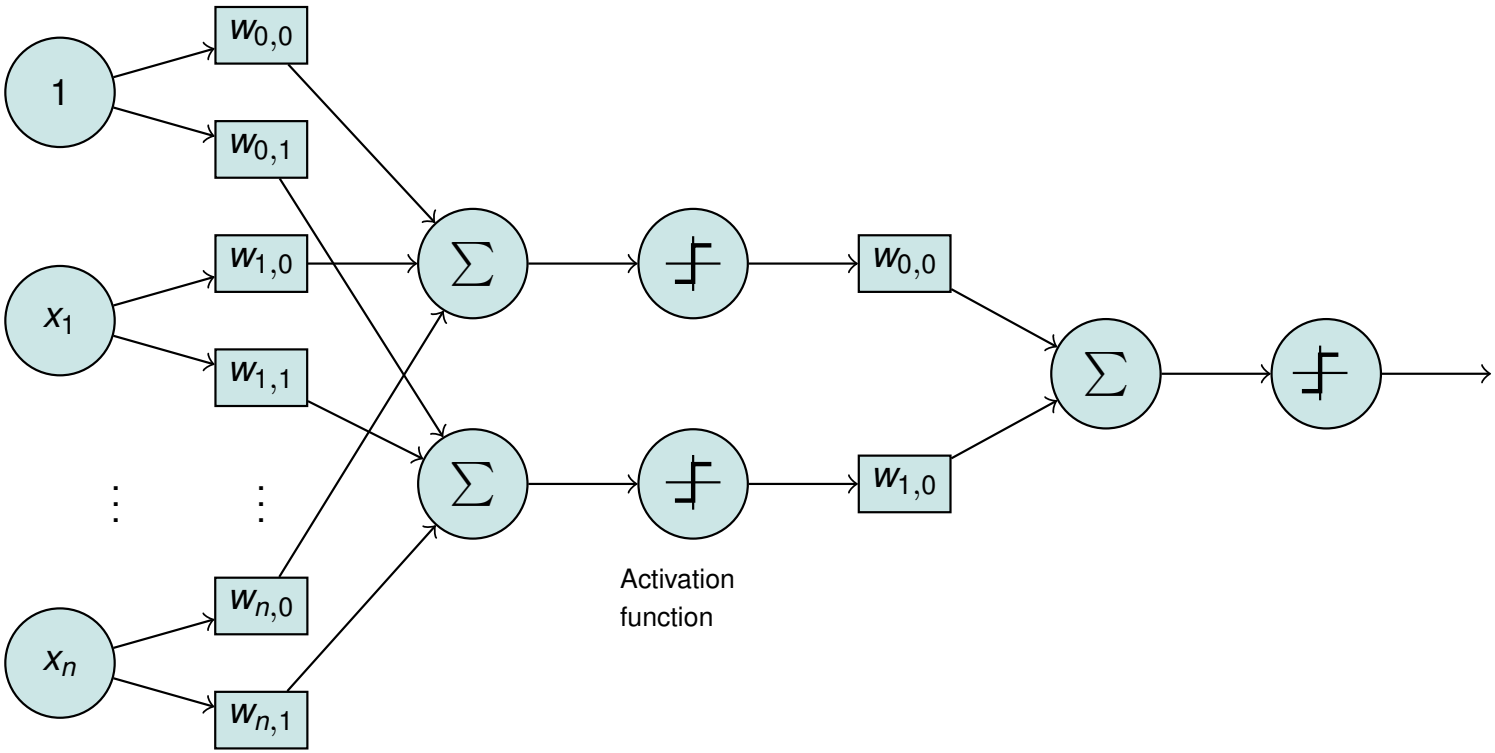


Samples from a XOR problem

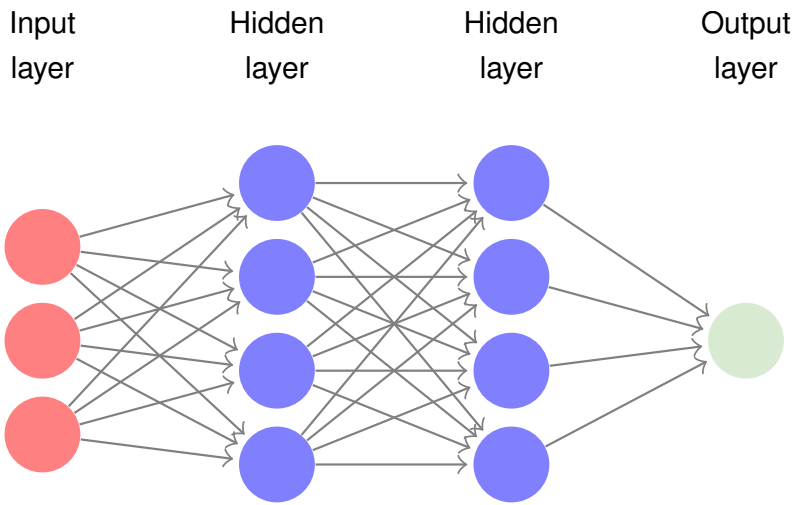
- XOR can’t be solved with a line
- 1969: "Perceptrons" described limitations of neural networks
- AI funding was cut heavily
- This became known as "AI winter"

Multi-Layer Perceptron

- A perceptron resembles a single neuron
- Idea: Use multiple neurons!
- This enables non-linear decision boundaries



Terminology



- Terms: Input layer, hidden layers, output layer
- A single hidden layer (of arbitrary width) can already be shown to be a **universal function approximator**
- Non-linear functions
  - are called activation functions in hidden layers
  - predict in the output layer and are used for the loss function

Perceptrons as Universal Function Approximators

Universal Approximation Theorem

- Let $\varphi(\cdot)$ be a non-constant, bounded and monotonically increasing function.
- For any $\varepsilon > 0$ and any continuous function f defined on a compact subset of $\mathbb{R}^m$, there exist an integer N, real constants $v_i, b_i \in \mathbb{R}$ and real vectors $w_i \in \mathbb{R}^m$ where $i = 1, \ldots, N$, such that

$$F(\mathbf{x}) = \sum_{i=1}^{N} v_i \varphi(\mathbf{w}_i^T \mathbf{x} + b_i) \quad \text{with}$$

$$|F(\mathbf{x}) - f(\mathbf{x})| < \varepsilon$$

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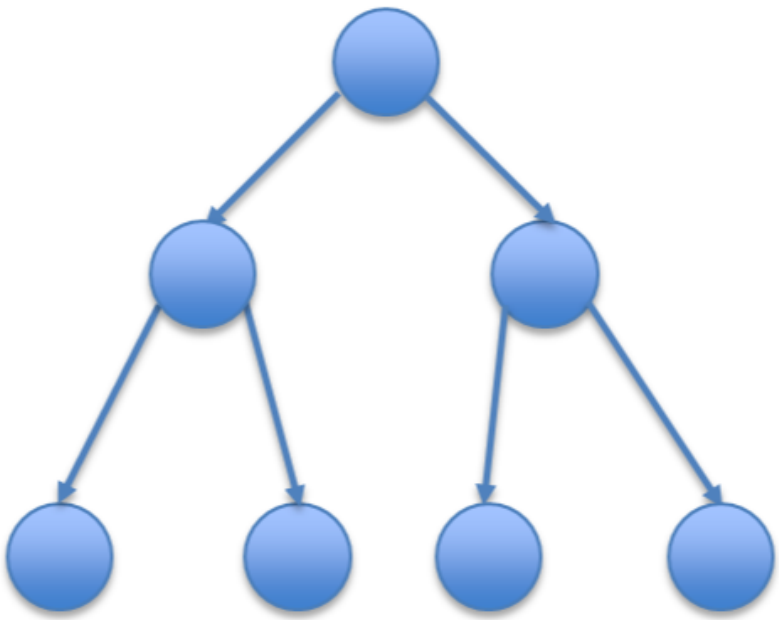
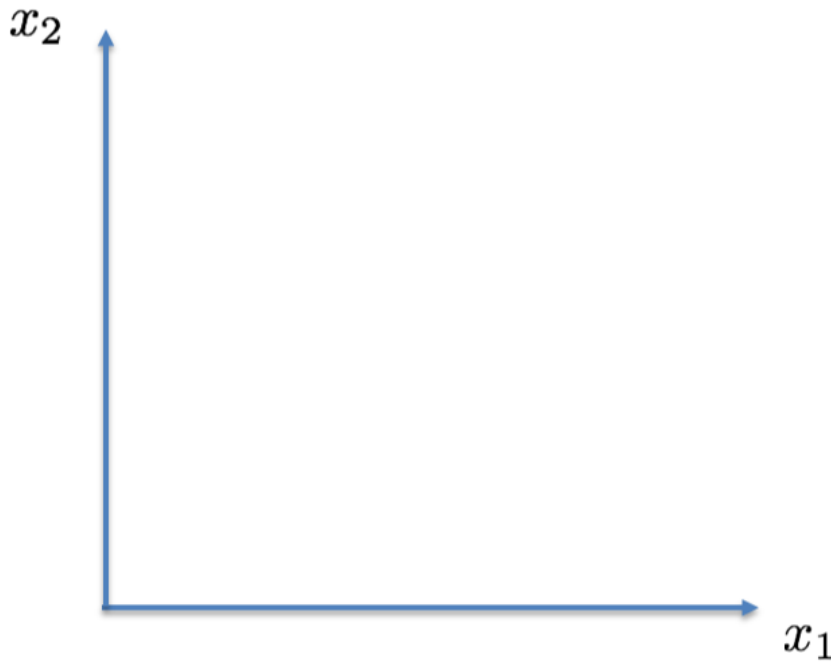
$\rightarrow$ We can approximate *any function with just one hidden layer* with a sensible activation function.

Classification Trees: Why do we need a universal approximator?





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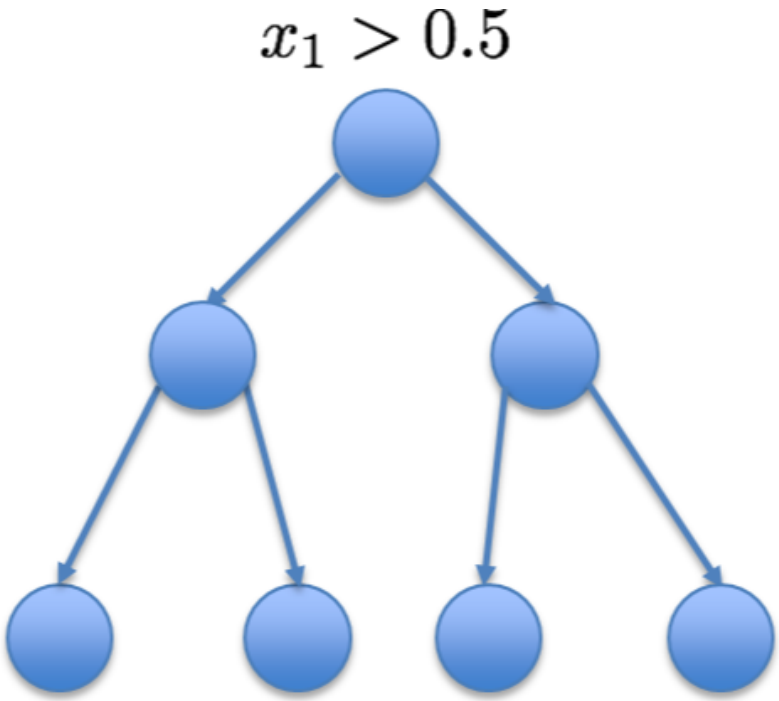

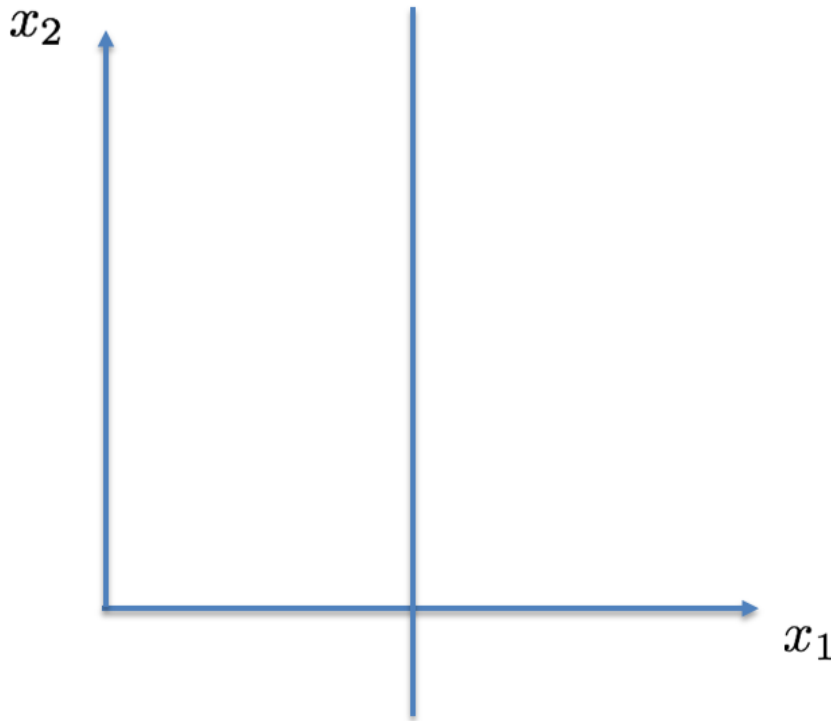

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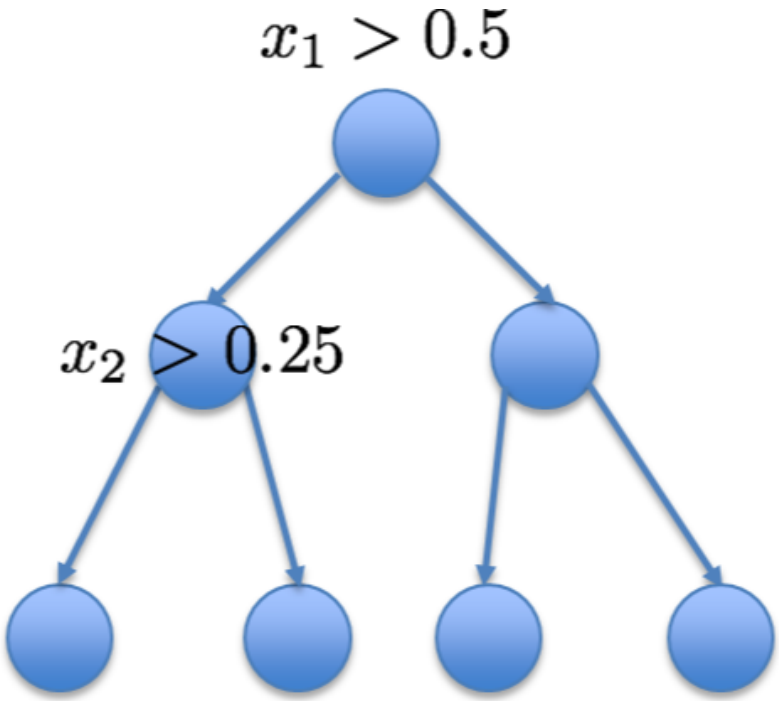

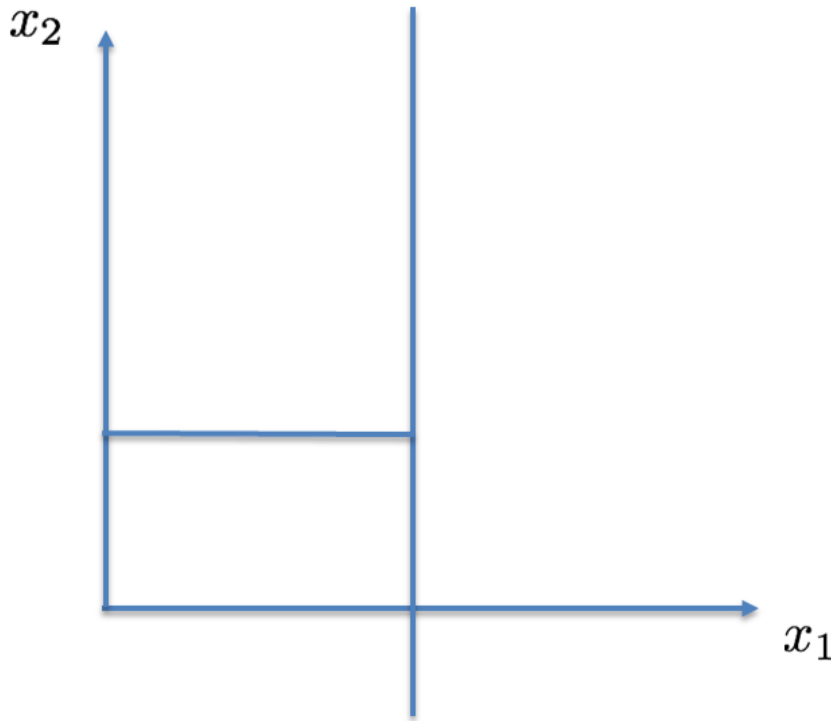

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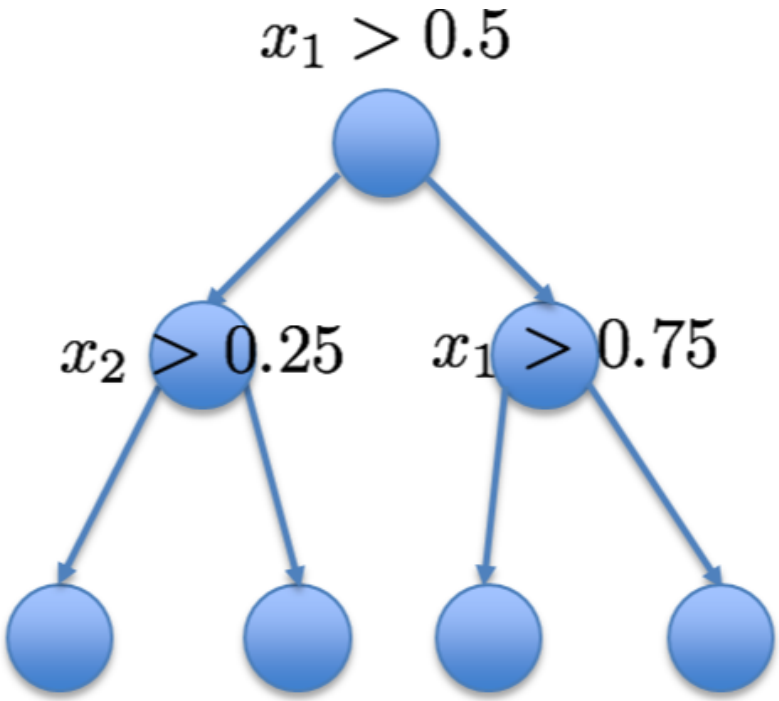

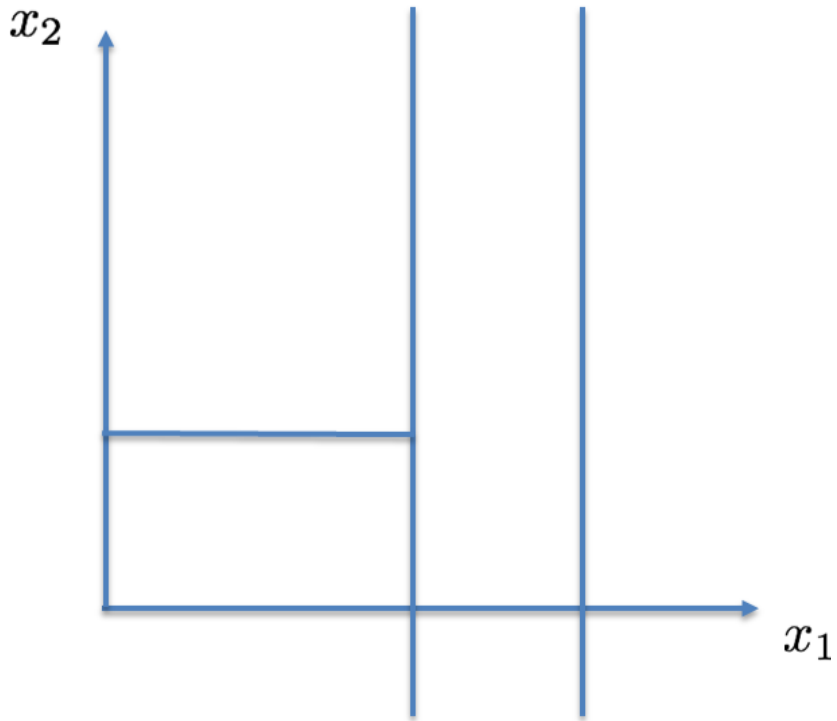

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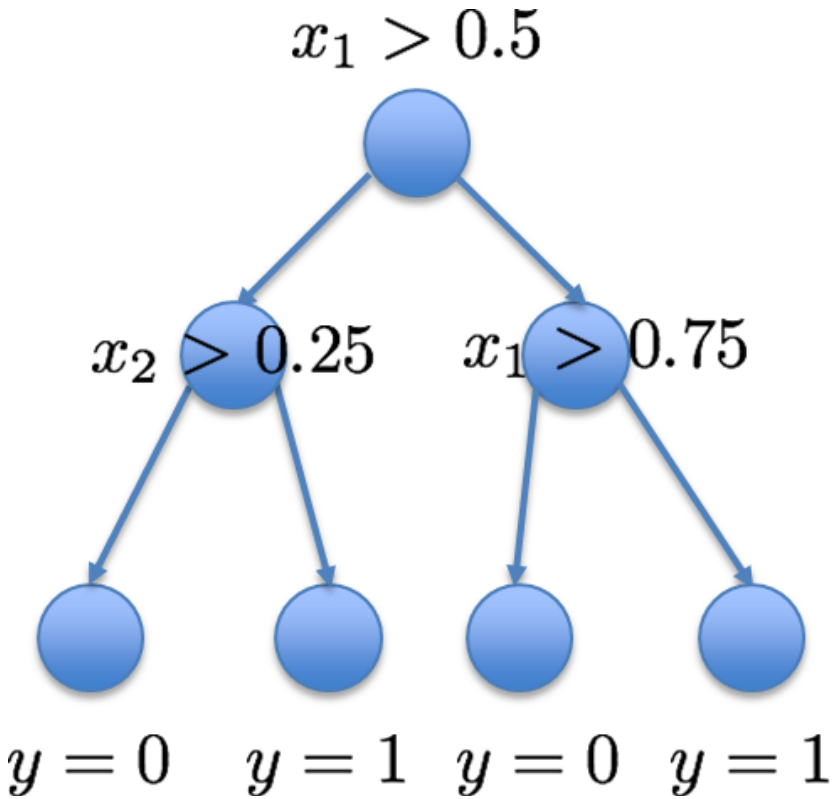
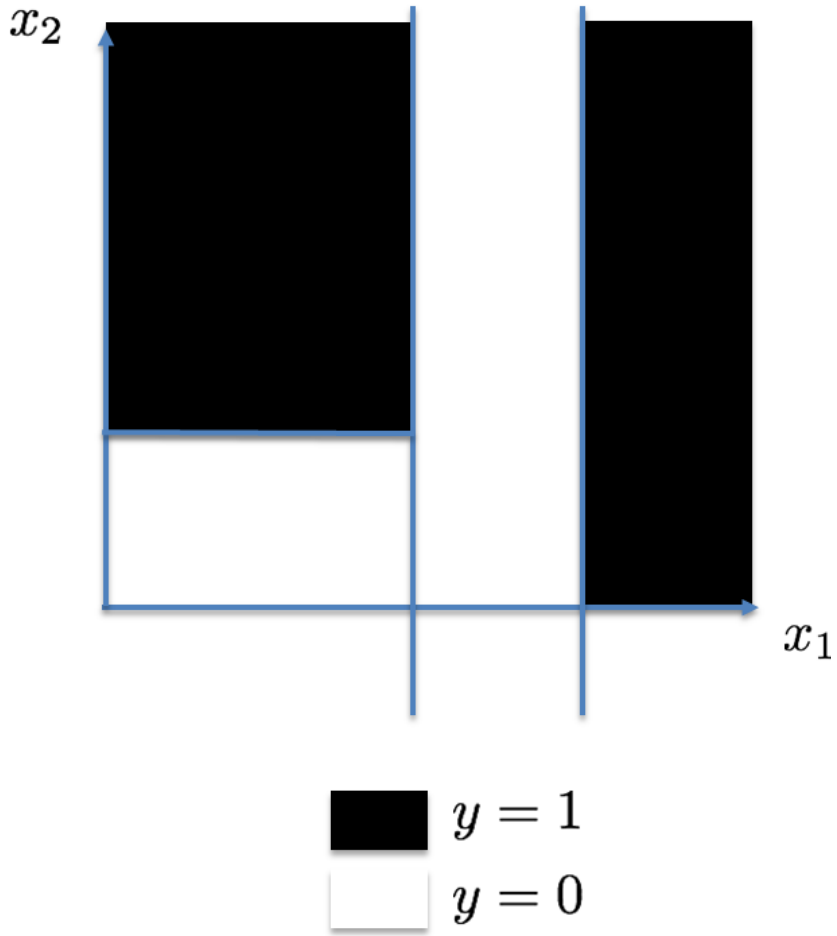
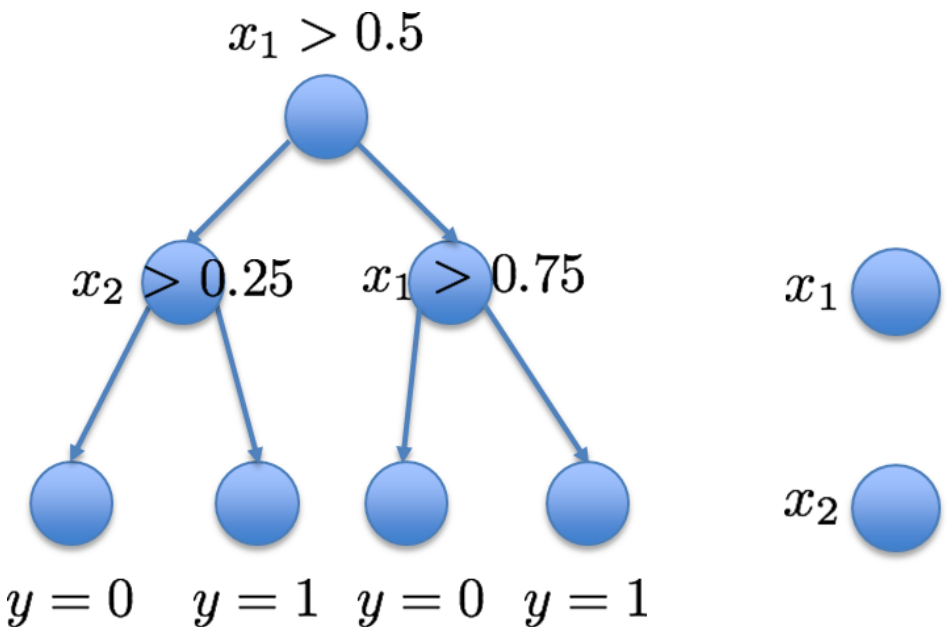




Classification Trees: Why do we need a universal approximator?

We can transform this into a network!

Classification Trees: Why do we need a universal approximator?



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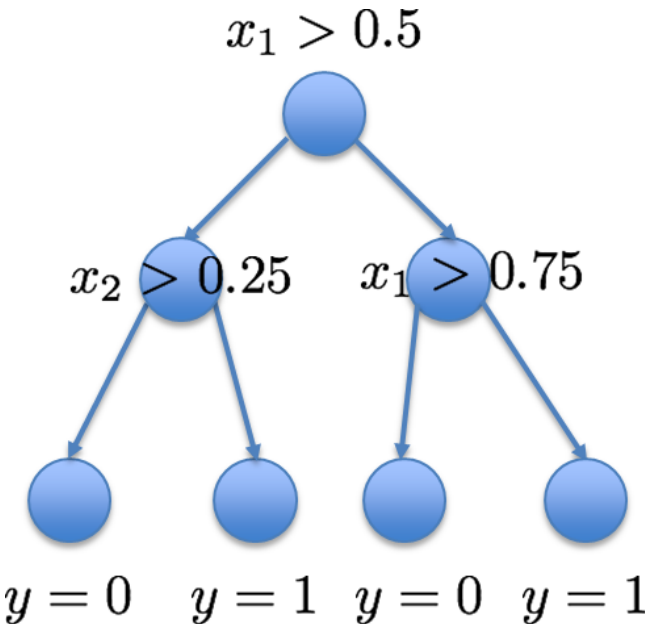

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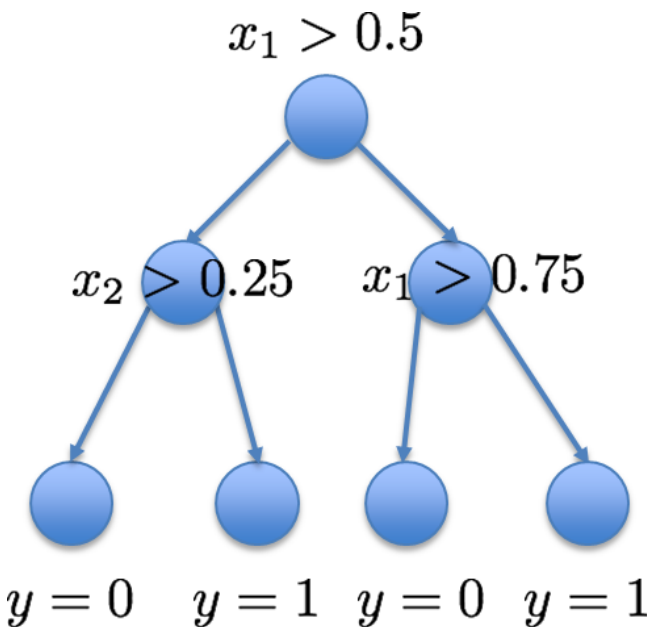

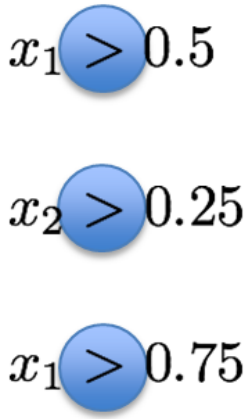

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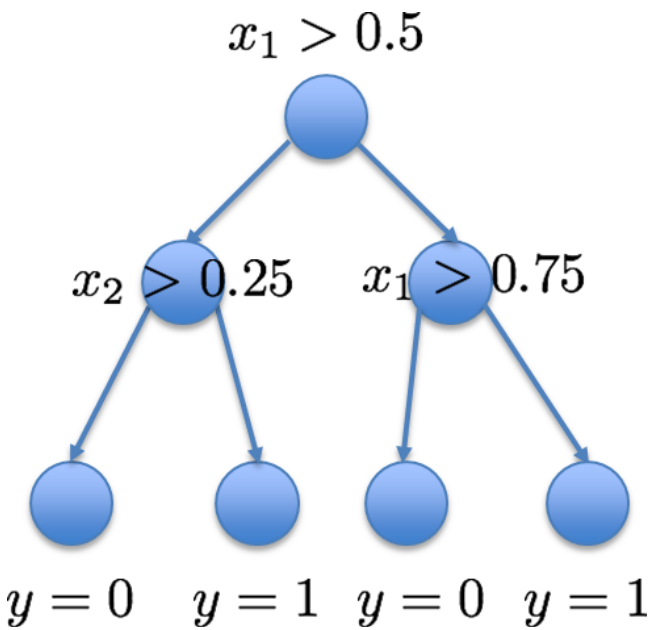

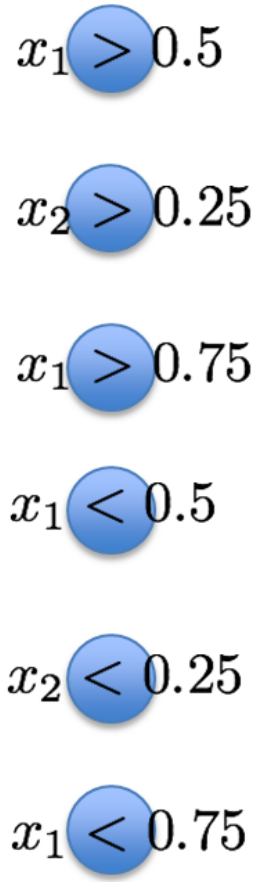

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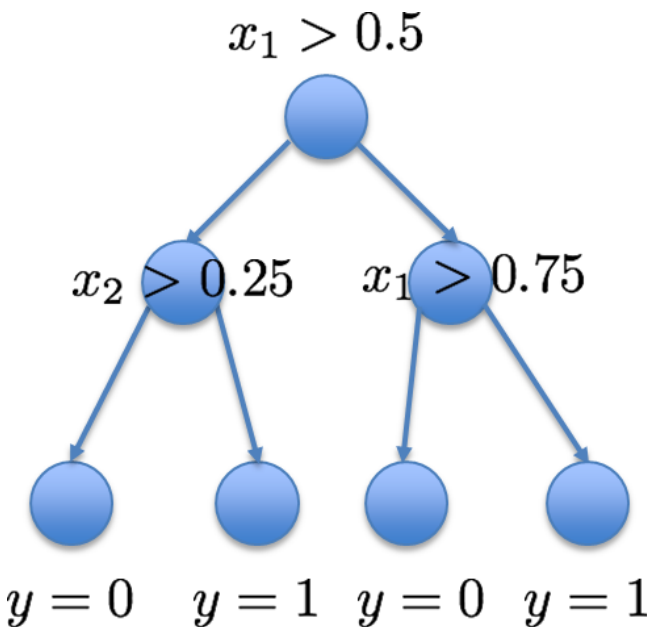

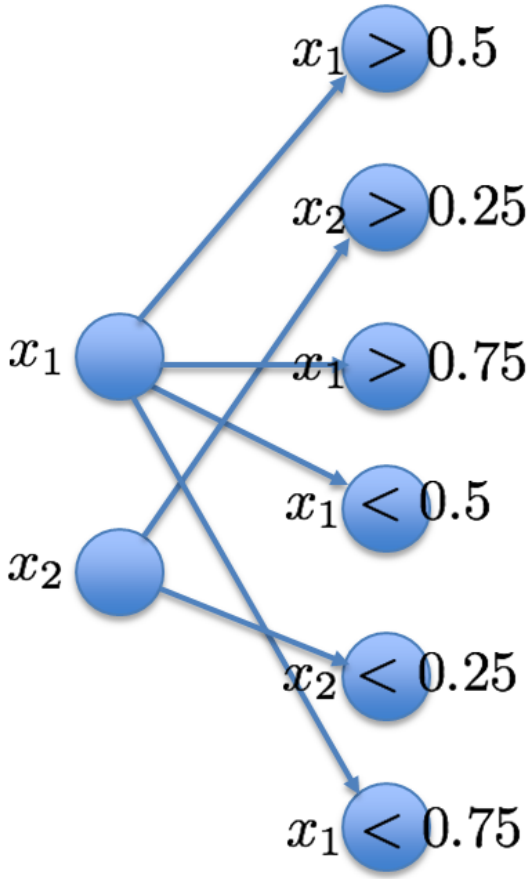

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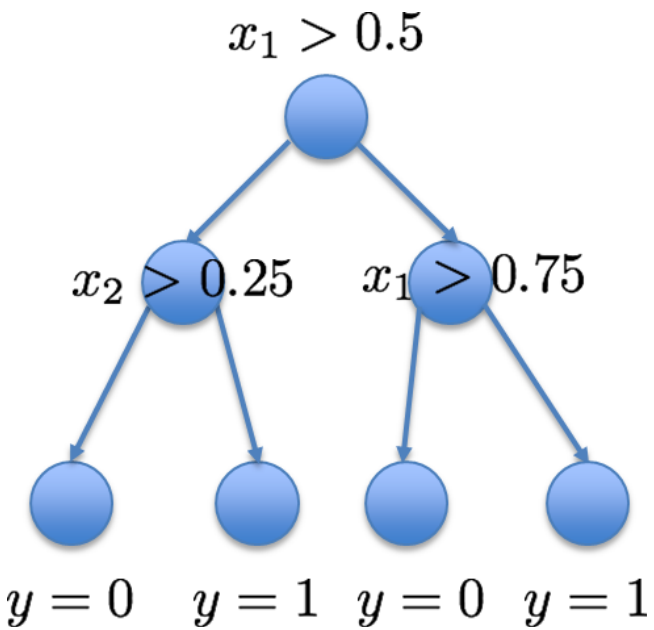

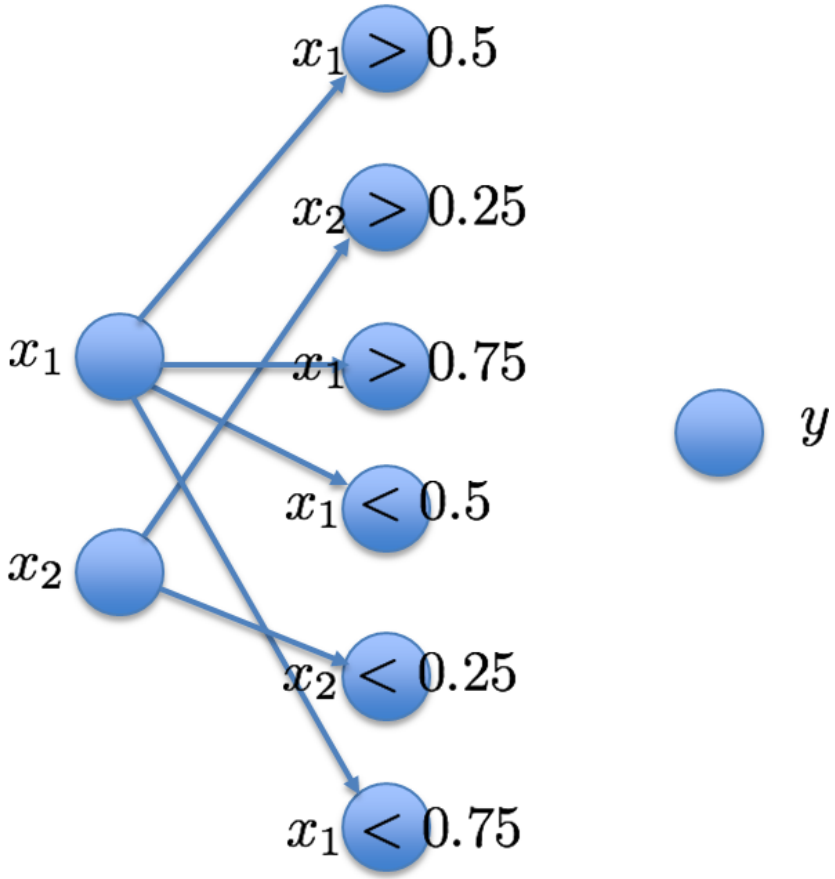

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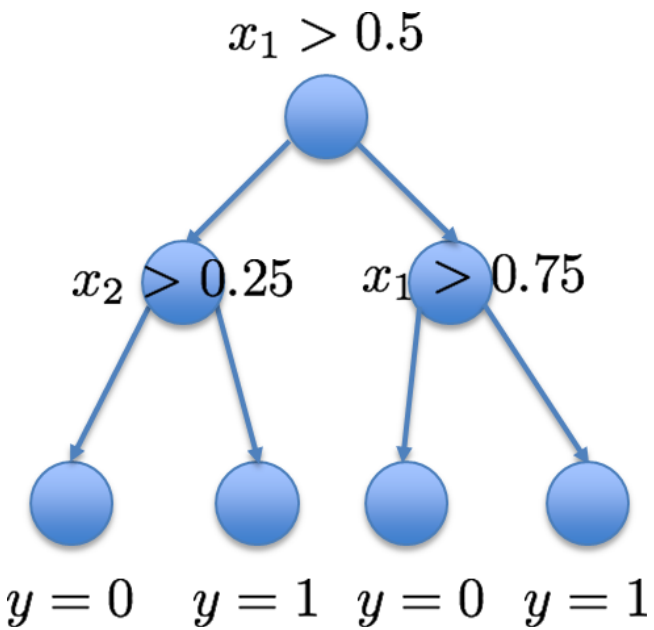

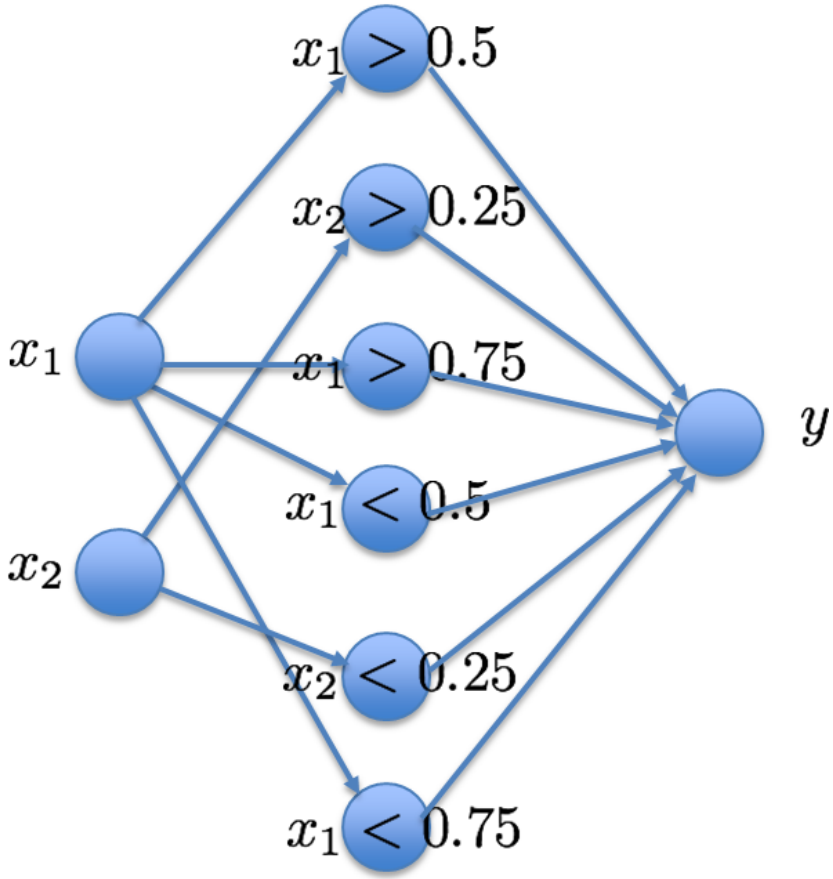

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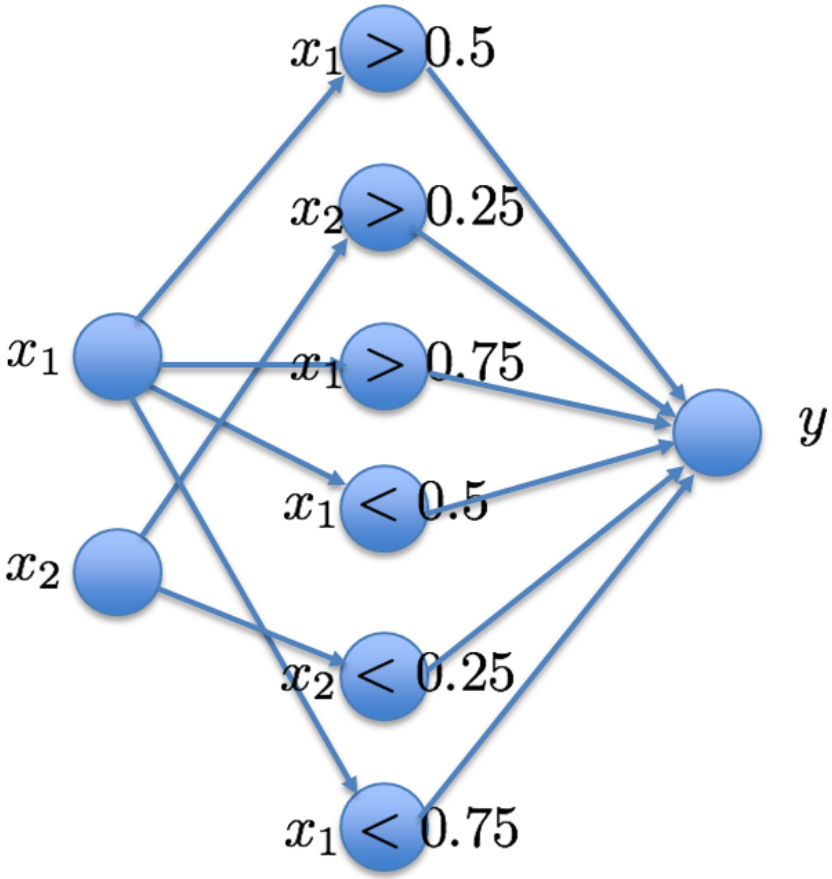

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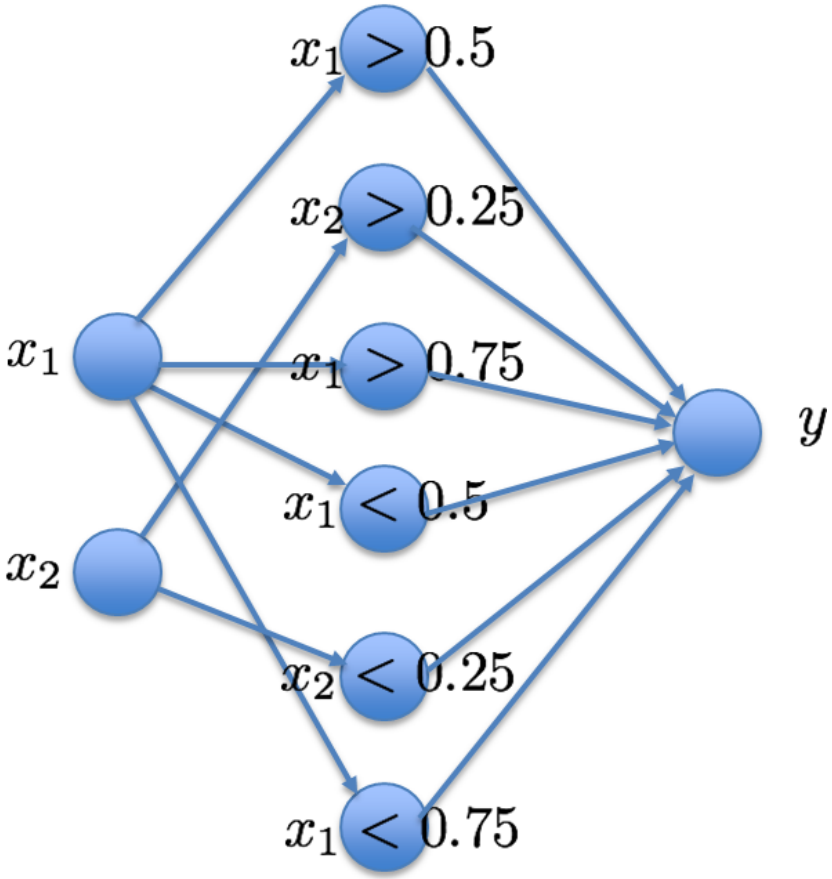

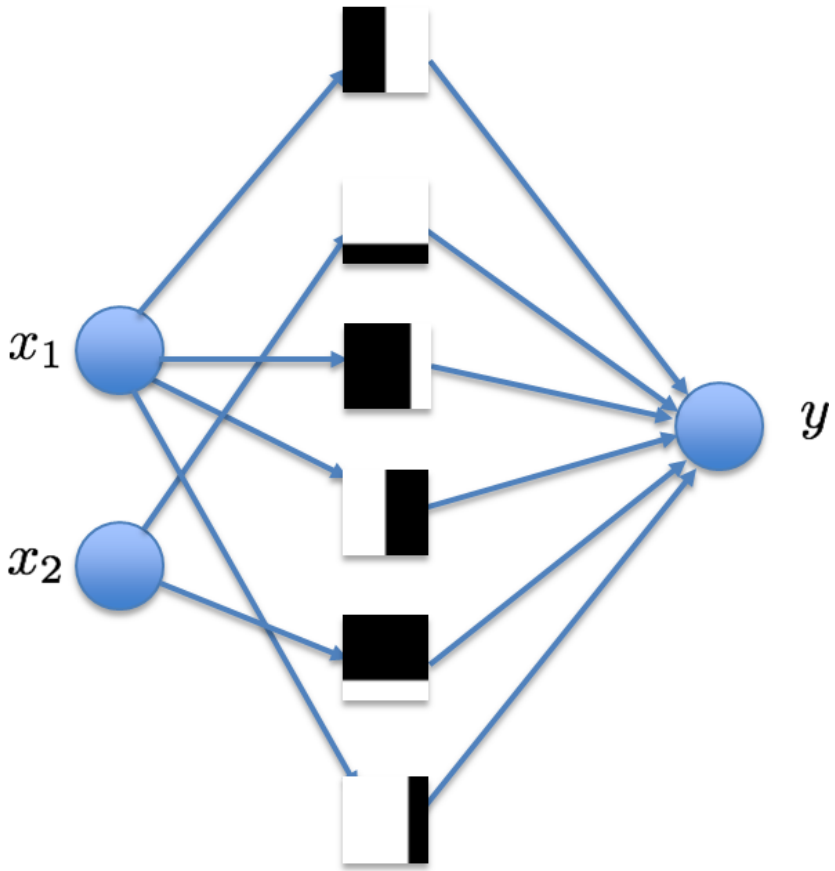

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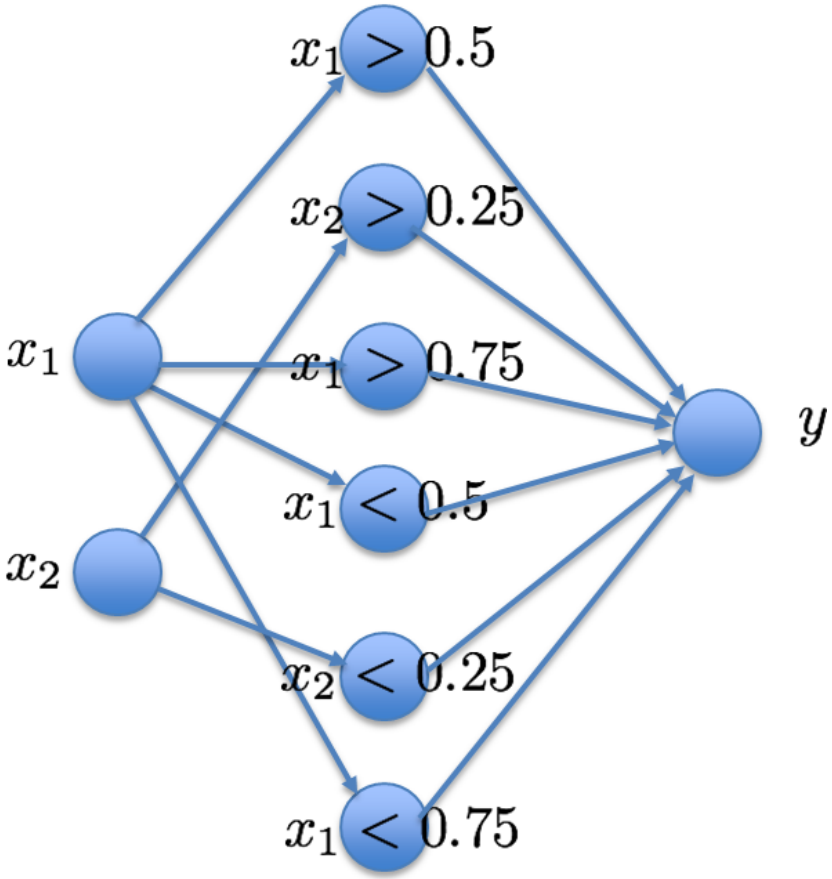

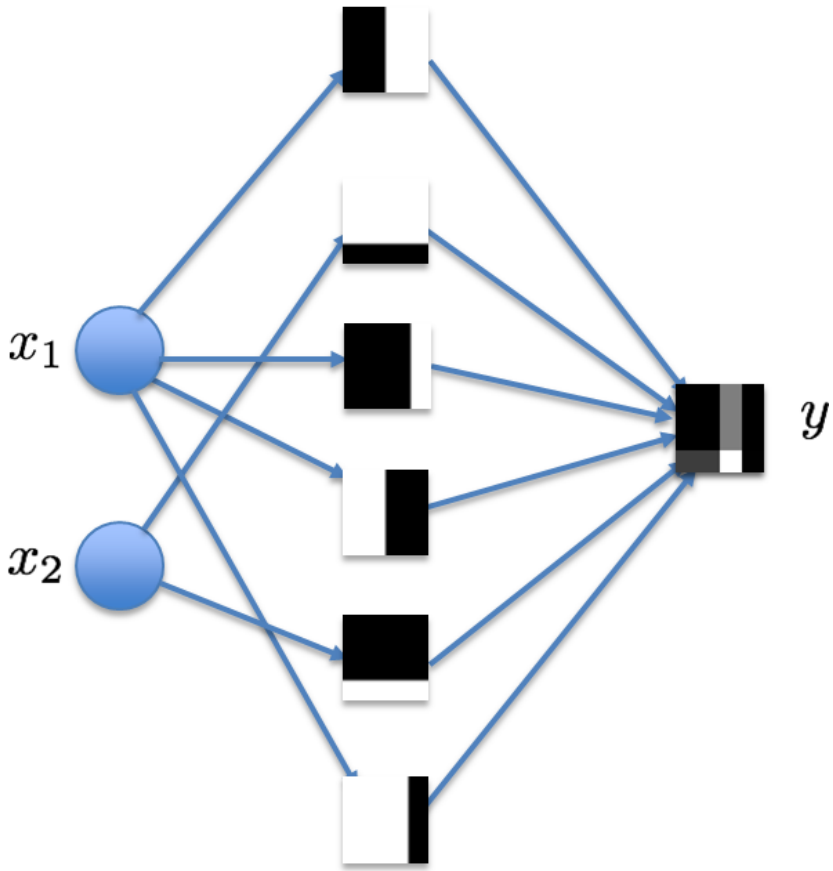

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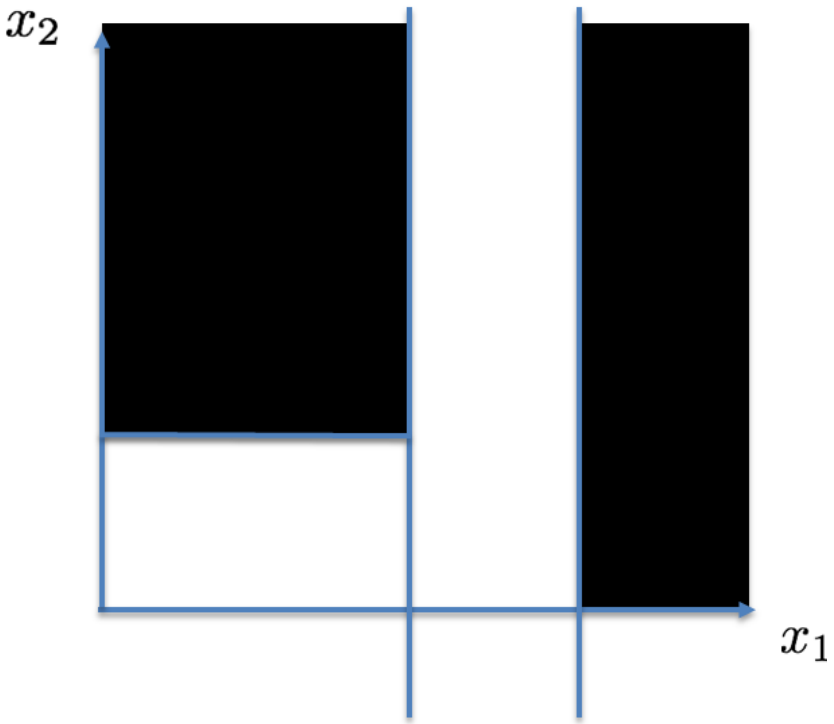

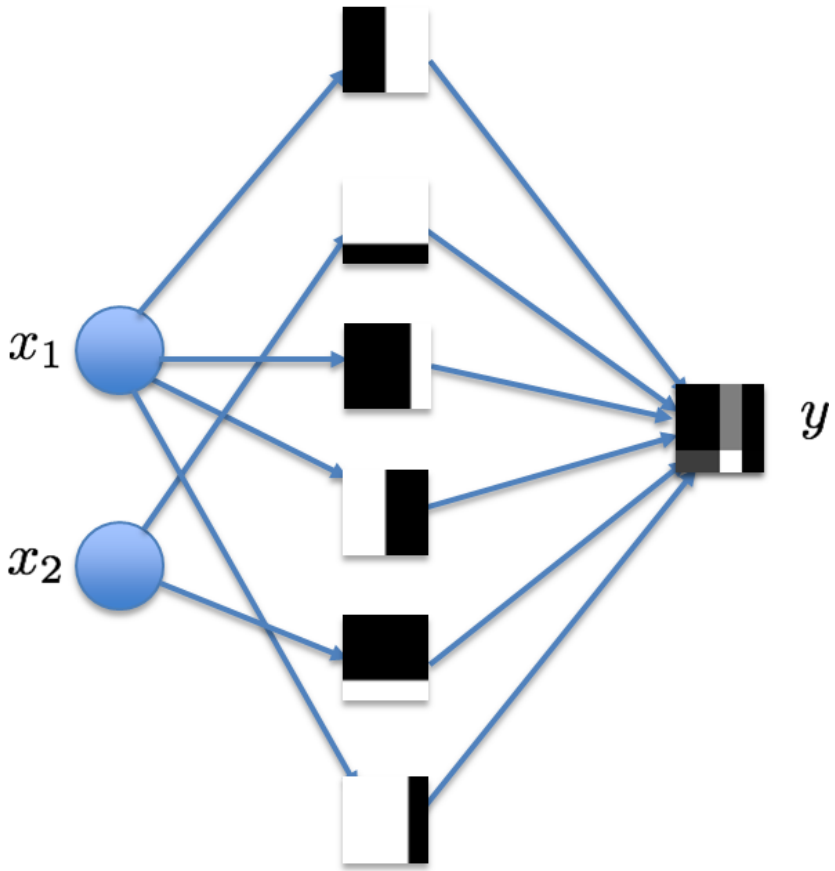

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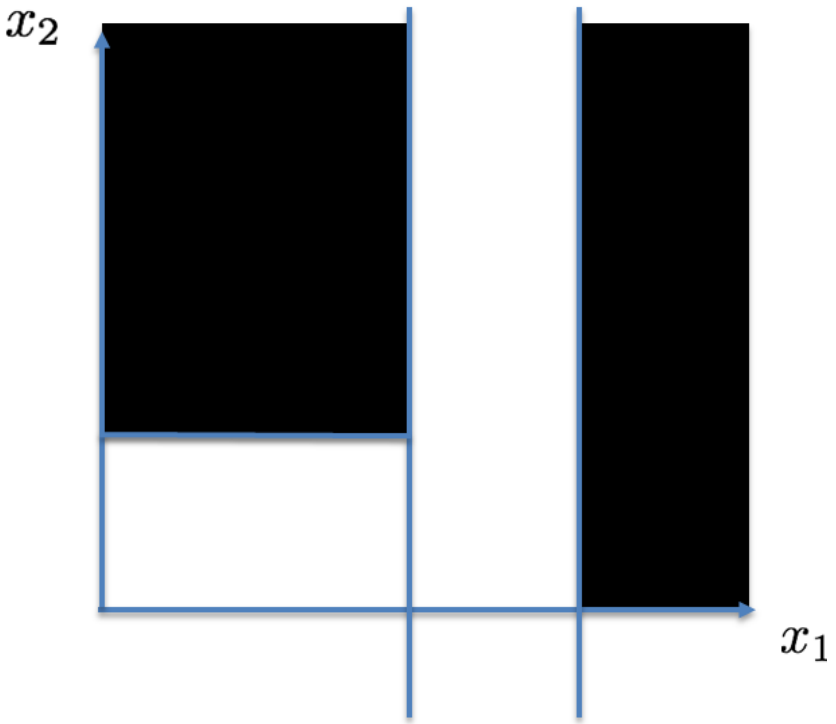

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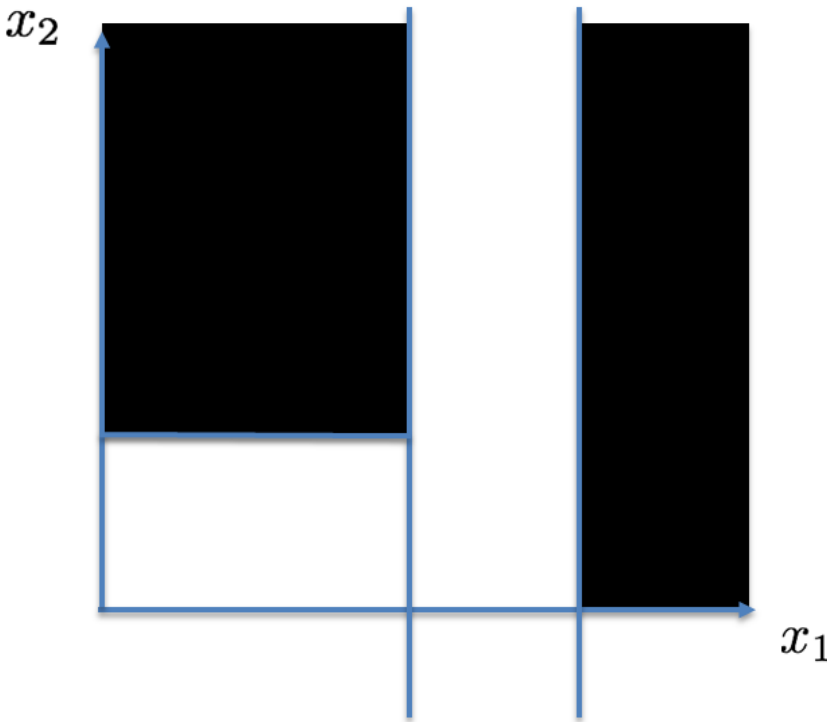

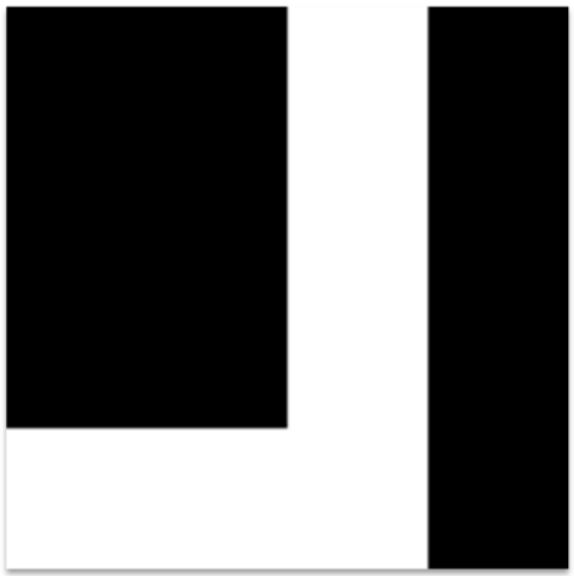

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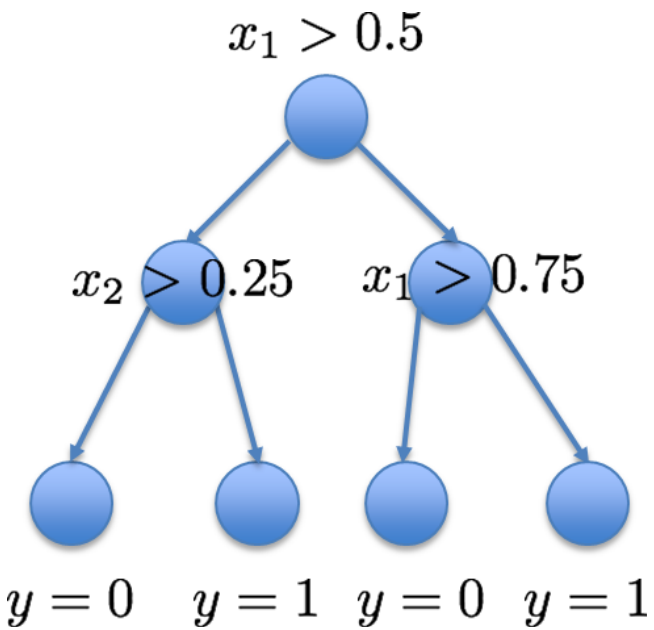

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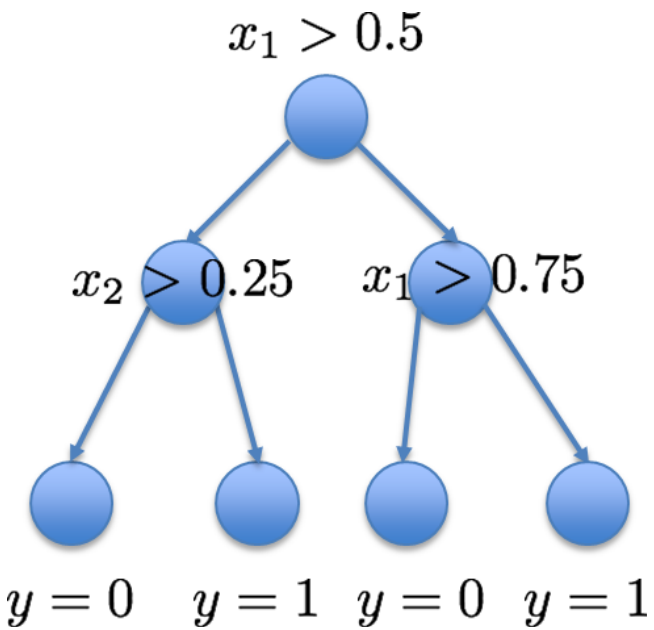

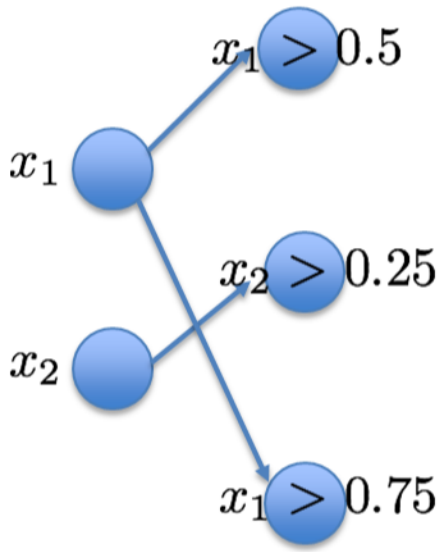

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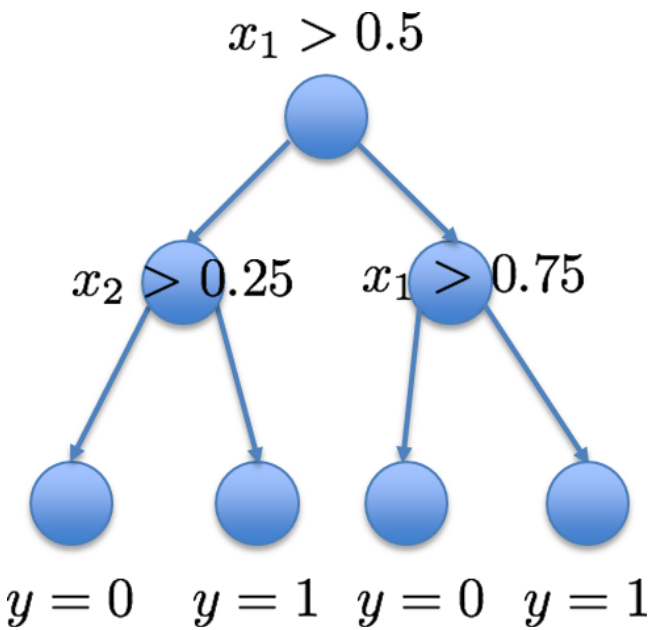

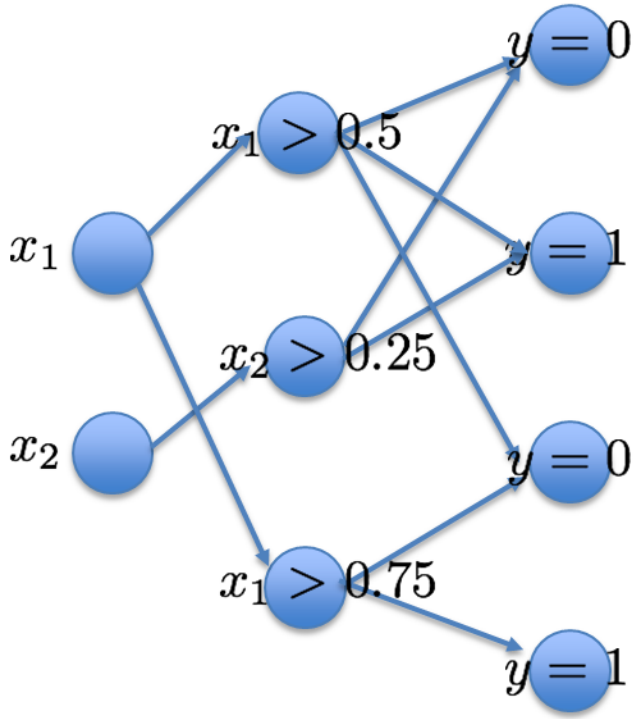

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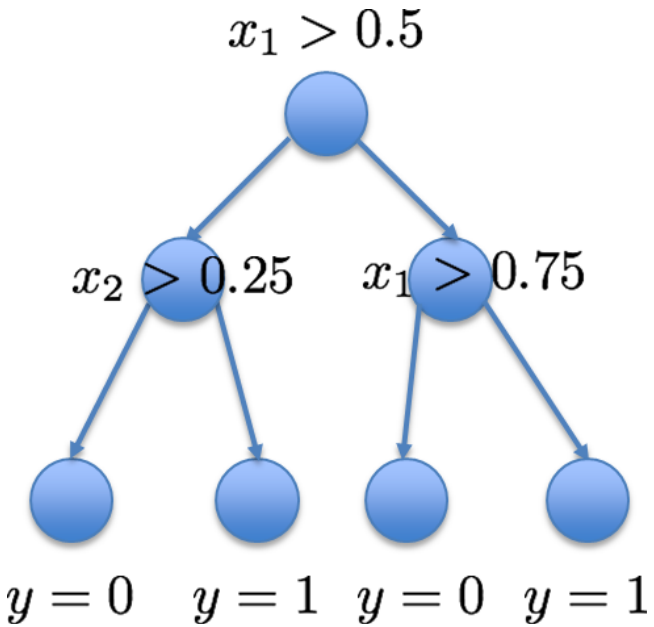

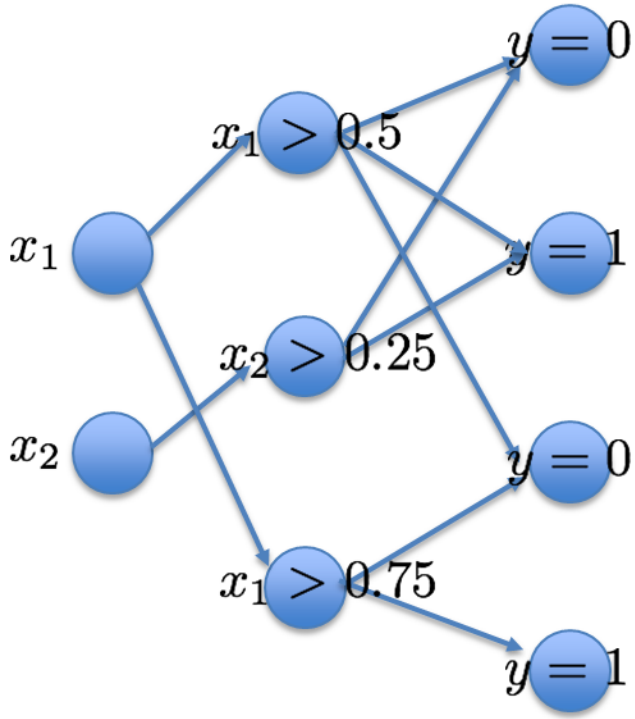

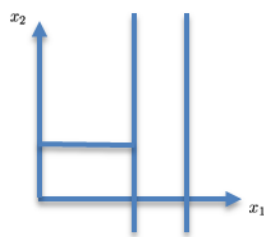

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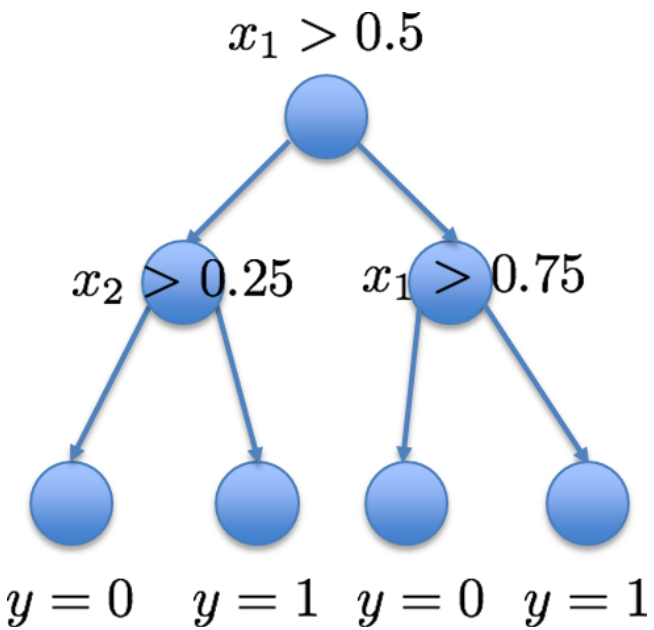

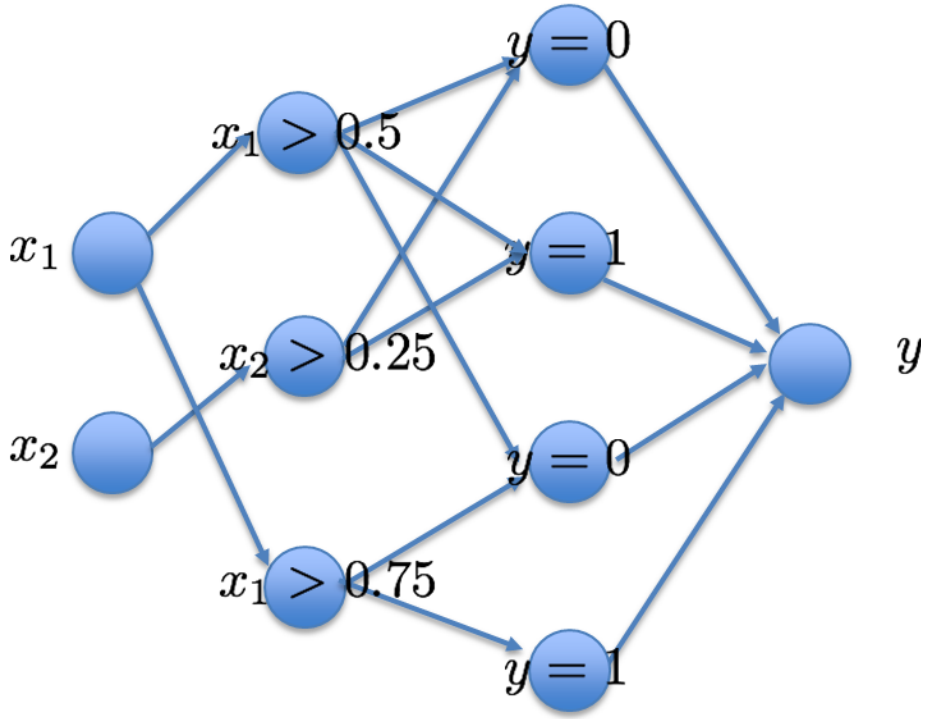

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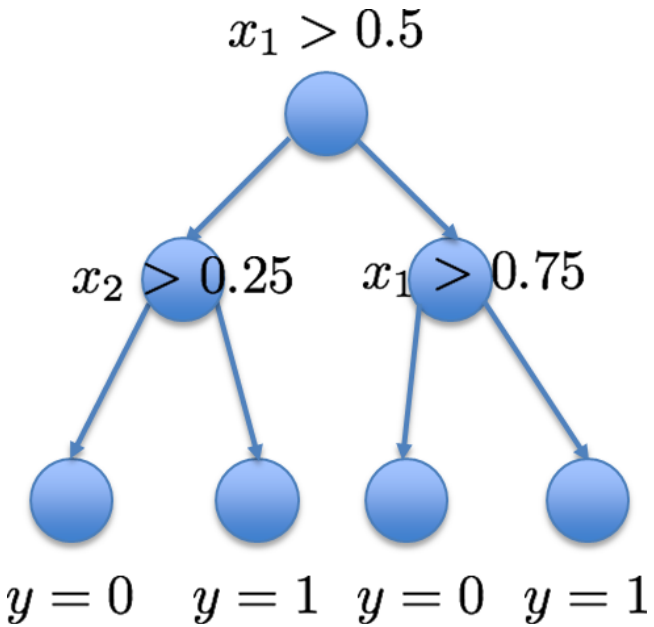

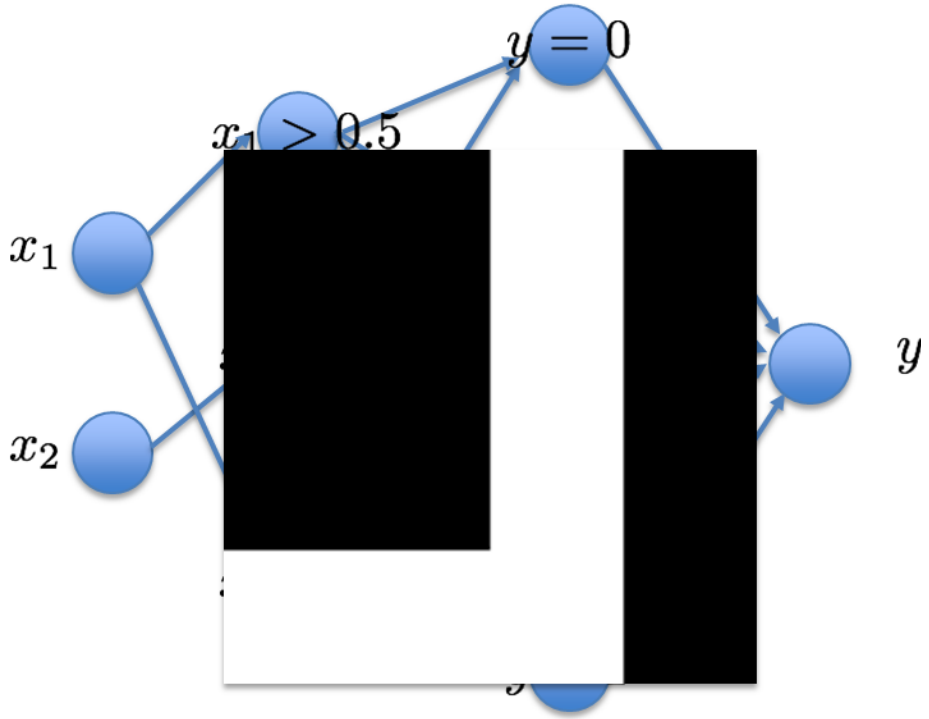

Universal Approximation Theorem

- Let $\varphi(\cdot)$ be a non-constant, bounded and monotonically increasing function.
- For any $\varepsilon > 0$ and any continuous function f defined on a compact subset of $\mathbb{R}^m$, there exist an integer N, real constants $v_i, b_i \in \mathbb{R}$ and real vectors $w_i \in \mathbb{R}^m$ where $i = 1, \ldots, N$, such that we can define:

$$F(\mathbf{x}) = \sum_{i=1}^{N} v_i \varphi(\mathbf{w}_i^T \mathbf{x} + b_i) \quad \text{with}$$

$$|F(\mathbf{x}) - f(\mathbf{x})| < \varepsilon$$

$\rightarrow$ We can approximate *any function with just one hidden layer* with a sensible activation function.

$\rightarrow$ **We have no idea *how*: how many nodes, how to train, ...**

NEXT TIME

ON DEEP LEARNING

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Feed Forward Neural Networks - Part 2

A. Maier, V. Christlein, K. Breininger, S. Vesal, F. Meister, C. Liu, S. Gündel, S. Jaganathan, N. Maul, M. Vornehm, L. Reeb, F. Thamm, M. Hoffmann, C. Bergler, F. Denzinger, W. Fu, B. Geissler, Z. Yang
Pattern Recognition Lab, Friedrich-Alexander-Universität Erlangen-Nürnberg
April 21, 2020

From Activations to Classifications: Softmax Function

Terminology

- So far: ground truth/estimated label is described by $y/\hat{y} \in \{-1, 1\}$.
- Instead, we can use a vector $\mathbf{y} = (y_1, \ldots, y_K)^T$ where $K = \#\text{classes}$.
- For exclusive classes, $\mathbf{y}$ looks as follows:

$$y_k = \begin{cases} 1 & \text{if } k \text{ is the index of the true class,} \\ 0 & \text{otherwise} \end{cases}$$

- Called **one-hot encoding**: Only one element is $\neq 0$.
- Classifier output $\hat{\mathbf{y}}$ can represent class probabilities.
- Better descriptor, especially for multi-class problems!

Softmax activation function

- The softmax function rescales a vector $\mathbf{x}$ using:

$$\hat{y}_k = \frac{\exp(x_k)}{\sum_{j=1}^{K} \exp(x_j)}$$

- $\hat{\mathbf{y}}$ has two properties:
  1. $\sum_{k=1}^{K} \hat{y}_k = 1$
  2. $\hat{y}_k \geq 0 \quad \forall \hat{y}_k \in \hat{\mathbf{y}}$
- These are two of Kolmogorov's axioms for a probability distribution.
- This allows to treat the output as normalized probabilities.
- The softmax function is also known as the normalized exponential function.

Softmax activation function

- The softmax function rescales a vector **x** using:

$$\hat{y}_k = \frac{\exp(x_k)}{\sum_{j=1}^{K} \exp(x_j)}$$

- Example: three-class problem

Label	x_k	$\exp(x_k)$	$\hat{y}_k$
Tiger			
Airplane			
Boat			

Softmax activation function

- The softmax function rescales a vector **x** using:

$$\hat{y}_k = \frac{\exp(x_k)}{\sum_{j=1}^{K} \exp(x_j)}$$

- Example: ~~three~~four-class problem

Label	x_k	$\exp(x_k)$	$\hat{y}_k$
Tiger			
Airplane			
Boat			
Heavy Metal			

Softmax activation function

- The softmax function rescales a vector **x** using:

$$\hat{y}_k = \frac{\exp(x_k)}{\sum_{j=1}^{K} \exp(x_j)}$$

- Example: ~~three~~four-class problem

Label	x_k	$\exp(x_k)$	$\hat{y}_k$
Tiger	-3.44		
Airplane	1.16		
Boat	-0.81		
Heavy Metal	3.91		

Softmax activation function

- The softmax function rescales a vector **x** using:

$$\hat{y}_k = \frac{\exp(x_k)}{\sum_{j=1}^{K} \exp(x_j)}$$

- Example: ~~three~~four-class problem

Label	x_k	$\exp(x_k)$	$\hat{y}_k$
Tiger	-3.44	0.03	
Airplane	1.16	3.19	
Boat	-0.81	0.44	
Heavy Metal	3.91	49.90	

Softmax activation function

- The softmax function rescales a vector **x** using:

$$\hat{y}_k = \frac{\exp(x_k)}{\sum_{j=1}^{K} \exp(x_j)}$$

- Example: ~~three~~four-class problem

Label	x_k	$\exp(x_k)$	$\hat{y}_k$
Tiger	-3.44	0.03	0.0006
Airplane	1.16	3.19	0.0596
Boat	-0.81	0.44	0.0083
Heavy Metal	3.91	49.90	0.9315

Loss functions

- The cross entropy H of probability distributions **p** and **q**

$$\mathrm{H}(\mathbf{p}, \mathbf{q}) = -\sum_{k=1}^{K} p_k \log(q_k)$$

- Based on H, we formulate a loss function L:

$$L(\mathbf{y}, \hat{\mathbf{y}}) = -\log(\hat{y}_k)|_{y_k=1}$$

- We will talk more about this during the next session!

"Softmax loss"

- Cross-entropy and the Softmax function typically appear together

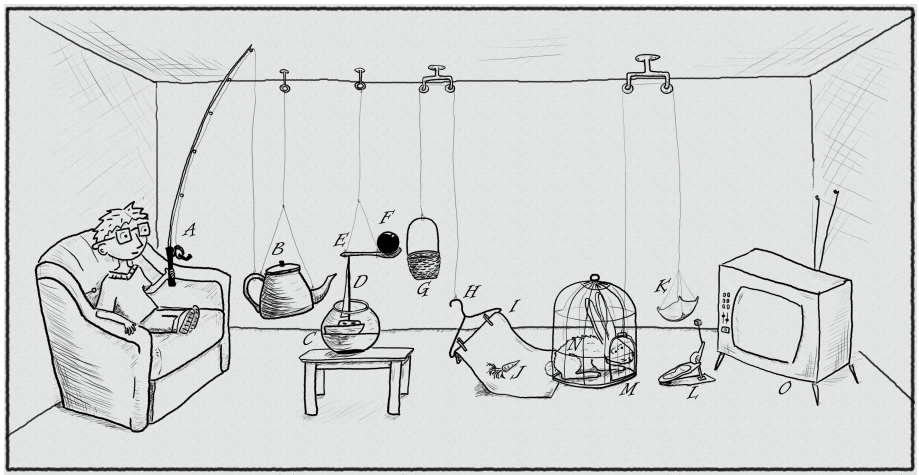
$$L(\mathbf{y}, \mathbf{x}) = -\log\left(\frac{\exp(x_k)}{\sum_{j=1}^{K}\exp(x_j)}\right)\Big|_{y_k=1}$$

- One-hot encoding very convenient ➔represents a histogram
- Naturally handles multiple class problems

Optimization

Credit Assignment Problem

- What do those two images have in common?



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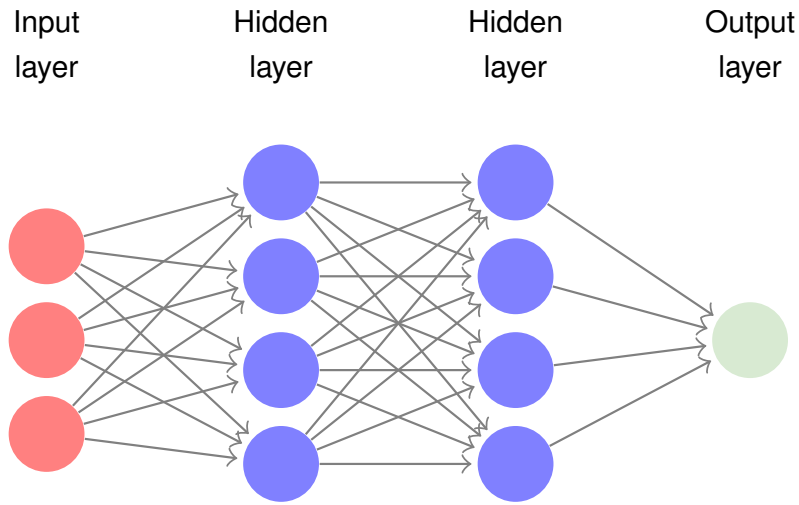
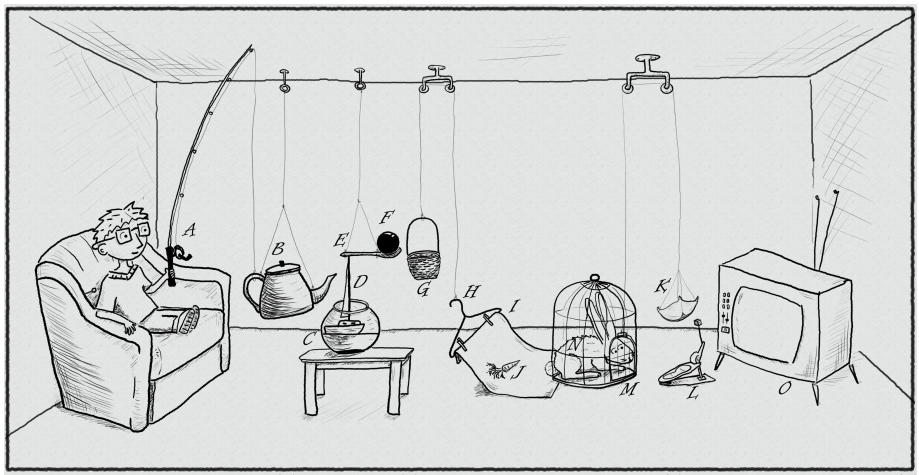


Credit Assignment Problem

- What do those two images have in common?



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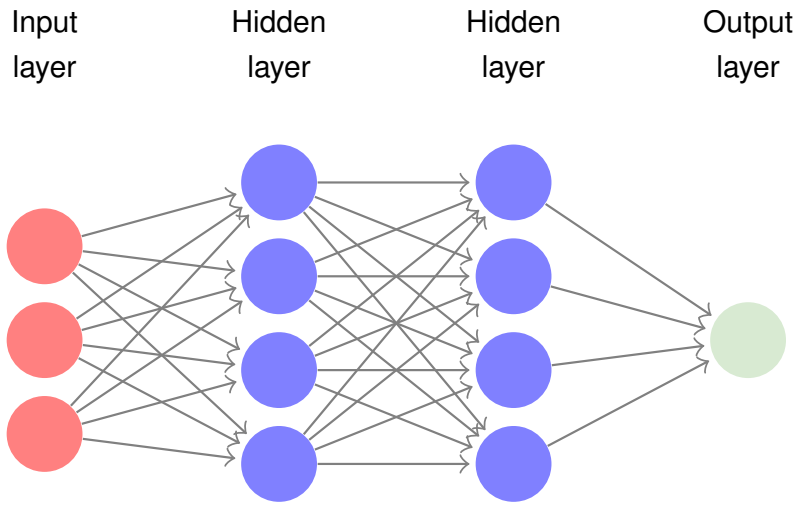


- If it doesn't work it's hard to know which parts to adjust.

Formalization as Optimization Problem

Goal: Find optimal weights $\mathbf{w}$ for all layers:

- Abstract the whole network as a function:

$$L(\mathbf{w}, \mathbf{x}, \mathbf{y})$$

- Consider all M training samples:

$$\mathbb{E}_{\mathbf{x},\mathbf{y}\sim\hat{p}_{\text{data}}(\mathbf{x},\mathbf{y})}\left[L(\mathbf{w}, \mathbf{x}, \mathbf{y})\right] = \frac{1}{M}\sum_{m=1}^{M} L(\mathbf{w}, \mathbf{x}, \mathbf{y})$$

- We now know what to do:

$$\underset{\mathbf{w}}{\text{minimize}} \quad \left\{L(\mathbf{w}, \mathbf{x}, \mathbf{y})\right\}$$

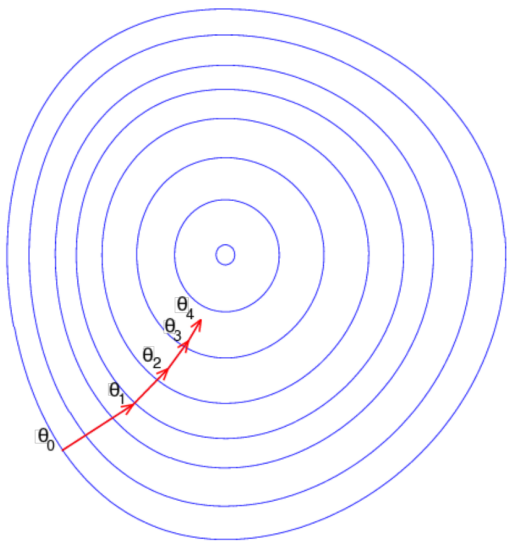
Gradient Descent

$$\underset{\mathbf{w}}{\text{argmin}} \left\{ \frac{1}{M} \sum_{m=1}^{M} L(\mathbf{w}, \mathbf{x}, \mathbf{y}) \right\}$$

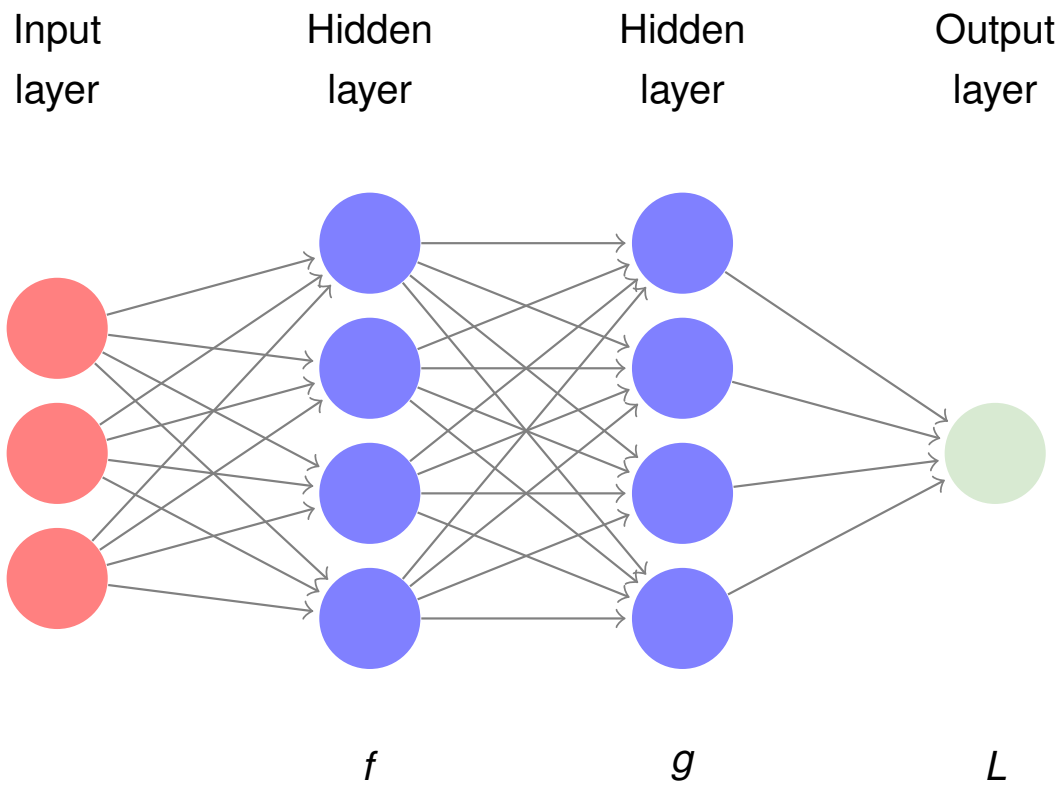
- Method of choice: Gradient Descent
  1. Initialize $\mathbf{w}$
  2. Iterate until convergence:

$$\mathbf{w}^{k+1} = \mathbf{w}^{k} - \eta \nabla_{\mathbf{w}} \frac{1}{M} \sum_{m=1}^{M} L(\mathbf{w}, \mathbf{x}, \mathbf{y})$$

  3. η is commonly referred to as the **learning rate**



What is this L we are trying to optimize?



- Complex network can be seen as composed functions:

$$L(\mathbf{w}, \mathbf{x}, \mathbf{y}) = L(g(f(\mathbf{x}, \mathbf{w}_f), \mathbf{w}_g), \mathbf{y})$$

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Feed Forward Neural Networks - Part 3

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April 21, 2020

How to Calculate Derivatives in Complex Neural Networks?

Example Problem

- Function: $\hat{y} = f(\mathbf{x}) = (2x_1 + 3x_2)^2 + 3$
- Evaluate $\frac{\partial}{\partial x_1} f \begin{pmatrix} 1 \\ 3 \end{pmatrix}$

Two algorithms:

- Finite differences
- Analytic derivative

Finite Differences

Definition of derivative:

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

Due to finite precision the symmetric definition is preferred:

$$f'(x) = \lim_{h \to 0} \frac{f\left(x+\frac{1}{2}h\right) - f\left(x-\frac{1}{2}h\right)}{h}$$

Example Problem

- Function: $\hat{y} = f(\mathbf{x}) = (2x_1 + 3x_2)^2 + 3$
- Evaluate $\frac{\partial}{\partial x_1} f \begin{pmatrix} 1 \\ 3 \end{pmatrix}$

$$f'(x) = \lim_{h \to 0} \frac{f\left(x + \frac{1}{2}h\right) - f\left(x - \frac{1}{2}h\right)}{h}$$

Let's calculate it:

- Set h to $2 \cdot 10^{-2}$

$$\frac{\partial}{\partial x_1} f \begin{pmatrix} 1 \\ 3 \end{pmatrix} = \frac{\left((2\left(1 + 10^{-2}\right) + 9\right)^2 + 3\right) - \left(\left(2\left(1 - 10^{-2}\right) + 9\right)^2 + 3\right)}{2 \cdot 10^{-2}}$$

Example Problem

- Function: $\hat{y} = f(\mathbf{x}) = (2x_1 + 3x_2)^2 + 3$
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$$\frac{\partial}{\partial x_1} f \begin{pmatrix} 1 \\ 3 \end{pmatrix} = \frac{\left(\left(2\left(1 + 10^{-2}\right) + 9\right)^2 + 3\right) - \left(\left(2\left(1 - 10^{-2}\right) + 9\right)^2 + 3\right)}{2 \cdot 10^{-2}}$$

$$= \frac{(124.4404 - 123.5604)}{2 \cdot 10^{-2}}$$

Example Problem

- Function: $\hat{y} = f(\mathbf{x}) = (2x_1 + 3x_2)^2 + 3$
- Evaluate $\frac{\partial}{\partial x_1} f \begin{pmatrix} 1 \\ 3 \end{pmatrix}$

$$f'(x) = \lim_{h \to 0} \frac{f\left(x + \frac{1}{2}h\right) - f\left(x - \frac{1}{2}h\right)}{h}$$

Let's calculate it:

- Set h to $2 \cdot 10^{-2}$

$$\begin{aligned}
\frac{\partial}{\partial x_1} f \begin{pmatrix} 1 \\ 3 \end{pmatrix} &= \frac{\left(\left(2\left(1 + 10^{-2}\right) + 9\right)^2 + 3\right) - \left(\left(2\left(1 - 10^{-2}\right) + 9\right)^2 + 3\right)}{2 \cdot 10^{-2}} \\
&= \frac{\left(124.4404 - 123.5604\right)}{2 \cdot 10^{-2}} \\
&= 43.9999
\end{aligned}$$

Finite Differences Summed up

- For practical use it often suffices to use $h = 1 \cdot 10^{-5}$
- For a more accurate derivative [7] use: $h = \epsilon_f^{\frac{1}{3}} \cdot x_c$
  - Where $\epsilon_f \approx 10^{-7}$
  - The characteristic scale is approximated as $x_c = x$
  - Prevent division by zero at $x = 0$

Conclusion

- **Easy** to use
- We only need to be able to **evaluate** functions
- Computationally **inefficient**
- **Frequently used** to check implementations

Analytic gradient

Example Problem

- Function: $\hat{y} = f(\mathbf{x}) = (2x_1 + 3x_2)^2 + 3$
- Evaluate $\frac{\partial}{\partial x_1} f \begin{pmatrix} 1 \\ 3 \end{pmatrix}$

Four analytic rules:

1. $\frac{d}{dx}\text{const} = 0$
2. Linearity: $\frac{d}{dx}$ is a linear operator
3. Monomials: $\frac{d}{dx} x^n = n \cdot x^{n-1}$
4. Chain rule: $\frac{d}{dx} f(g(x)) = \frac{d}{dg} f(g) \frac{d}{dx} g(x)$

Example Problem

- Function: $\hat{y} = f(\mathbf{x}) = (2x_1 + 3x_2)^2 + 3$
- Evaluate $\frac{\partial}{\partial x_1} f \begin{pmatrix} 1 \\ 3 \end{pmatrix}$

1. $\frac{d}{dx}\text{const} = 0$
2. $\frac{d}{dx}$ is linear
3. $\frac{d}{dx} x^n = n \cdot x^{n-1}$
4. $\frac{d}{dx} f(g(x)) = \frac{d}{dg} f(g) \cdot \frac{d}{dx} g(x)$

Let's calculate it:

Example Problem

- Function: $\hat{y} = f(\mathbf{x}) = (2x_1 + 3x_2)^2 + 3$
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4. $\frac{d}{dx} f(g(x)) = \frac{d}{dg} f(g) \cdot \frac{d}{dx} g(x)$

Let's calculate it:

$$\frac{\partial}{\partial x_1} f \begin{pmatrix} 1 \\ 3 \end{pmatrix} = \frac{\partial}{\partial x_1} (2x_1 + 9)^2$$

Rules 1 and 2

Example Problem

- Function: $\hat{y} = f(\mathbf{x}) = (2x_1 + 3x_2)^2 + 3$
- Evaluate $\frac{\partial}{\partial x_1} f \begin{pmatrix} 1 \\ 3 \end{pmatrix}$

1. $\frac{d}{dx}\text{const} = 0$
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4. $\frac{d}{dx} f(g(x)) = \frac{d}{dg} f(g) \cdot \frac{d}{dx} g(x)$

Let's calculate it:

$$\frac{\partial}{\partial x_1} f \begin{pmatrix} 1 \\ 3 \end{pmatrix} = \frac{\partial}{\partial x_1} (2x_1 + 9)^2 \qquad \text{Rules 1 and 2}$$

$$= \frac{\partial}{\partial z} (z)^2 \frac{\partial}{\partial x_1} (2x_1 + 9) \qquad \text{Rule 4 and } 2x_1 + 9 = z$$

Example Problem

- Function: $\hat{y} = f(\mathbf{x}) = (2x_1 + 3x_2)^2 + 3$
- Evaluate $\frac{\partial}{\partial x_1} f \begin{pmatrix} 1 \\ 3 \end{pmatrix}$

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Let's calculate it:

$$\frac{\partial}{\partial x_1} f \begin{pmatrix} 1 \\ 3 \end{pmatrix} = \frac{\partial}{\partial x_1} (2x_1 + 9)^2 \qquad \text{Rules 1 and 2}$$

$$= \frac{\partial}{\partial z} (z)^2 \frac{\partial}{\partial x_1} (2x_1 + 9) \qquad \text{Rule 4 and } 2x_1 + 9 = z$$

$$= 2(2x_1 + 9) \frac{\partial}{\partial x_1} (2x_1 + 9) \qquad \text{Rule 3}$$

Example Problem

- Function: $\hat{y} = f(\mathbf{x}) = (2x_1 + 3x_2)^2 + 3$
- Evaluate $\frac{\partial}{\partial x_1} f \begin{pmatrix} 1 \\ 3 \end{pmatrix}$

1. $\frac{d}{dx}\text{const} = 0$
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$$= \frac{\partial}{\partial z} (z)^2 \frac{\partial}{\partial x_1} (2x_1 + 9) \qquad \text{Rule 4 and } 2x_1 + 9 = z$$

$$= 2(2x_1 + 9) \frac{\partial}{\partial x_1} (2x_1 + 9) \qquad \text{Rule 3}$$

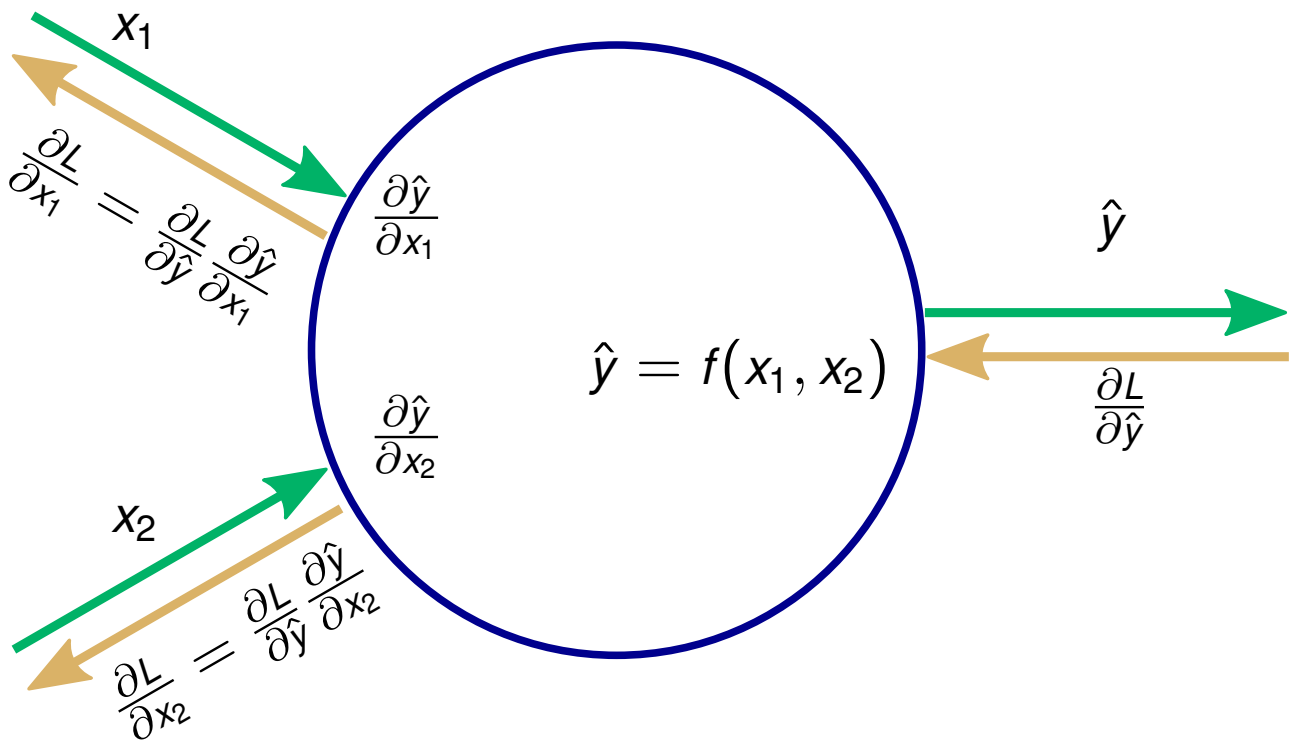
$$= 2(2x_1 + 9) \cdot 2 = 44 \qquad \text{Rules 1 and 2 and } x_1 = 1$$

Analytic Gradient Summed up

- **Chain rule** and **Linearity** enable to **decompose** complex functions
- Analytic formulas have to be calculated manually
- Computationally more **efficient** than finite differences

Can we compute analytic gradients automatically?

Backpropagation Algorithm



1. Forward pass: Compute activations
2. Backward pass: Recursively apply chain rule

Example Problem

- Function: $\hat{y} = f(\mathbf{x}) = (2x_1 + 3x_2)^2 + 3$
- Evaluate $\frac{\partial}{\partial x_1} f \begin{pmatrix} 1 \\ 3 \end{pmatrix}$

$$\frac{d}{dx} f(g(x)) = \frac{d}{dg} f(g) \frac{d}{dx} g(x)$$

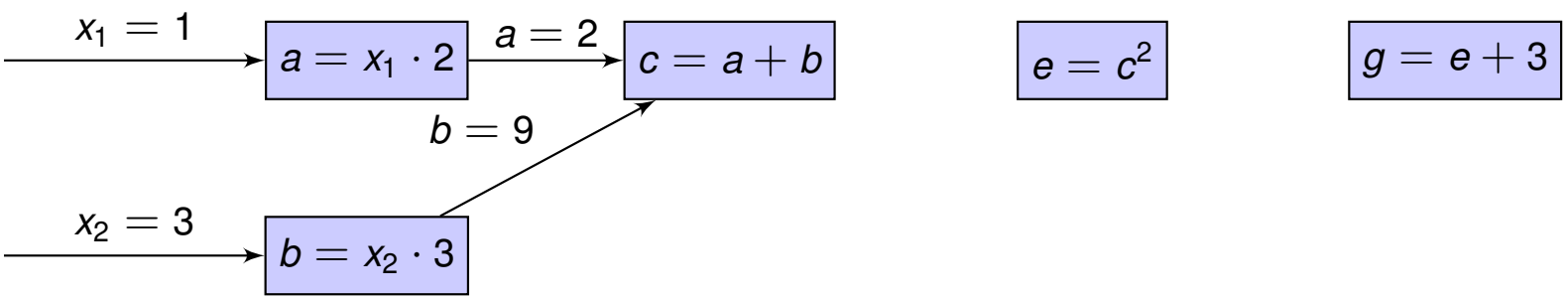
$x_1 = 1 \rightarrow a = x_1 \cdot 2$ $\quad c = a + b$ $\quad e = c^2$ $\quad g = e + 3$

$x_2 = 3 \rightarrow b = x_2 \cdot 3$

Example Problem

- Function: $\hat{y} = f(\mathbf{x}) = (2x_1 + 3x_2)^2 + 3$
- Evaluate $\frac{\partial}{\partial x_1} f \begin{pmatrix} 1 \\ 3 \end{pmatrix}$

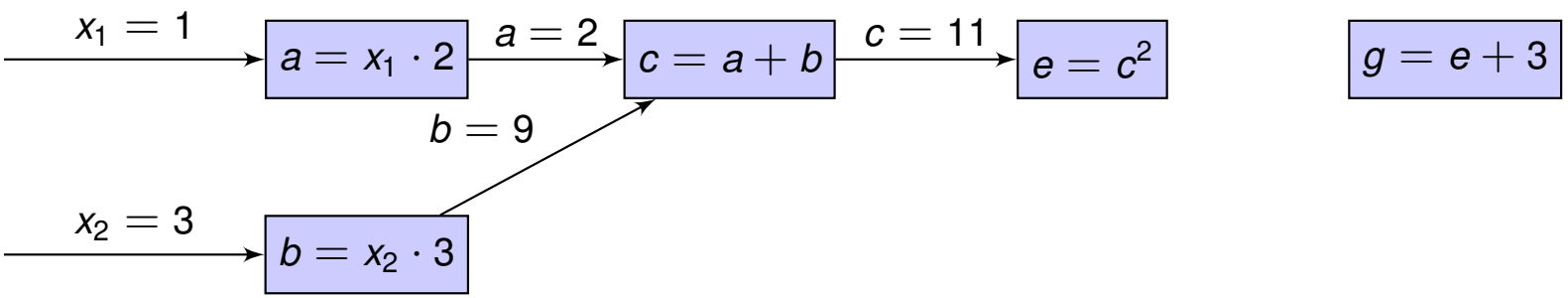
$$\frac{d}{dx} f(g(x)) = \frac{d}{dg} f(g) \frac{d}{dx} g(x)$$



Example Problem

- Function: $\hat{y} = f(\mathbf{x}) = (2x_1 + 3x_2)^2 + 3$
- Evaluate $\frac{\partial}{\partial x_1} f \begin{pmatrix} 1 \\ 3 \end{pmatrix}$

$$\frac{d}{dx} f(g(x)) = \frac{d}{dg} f(g) \frac{d}{dx} g(x)$$



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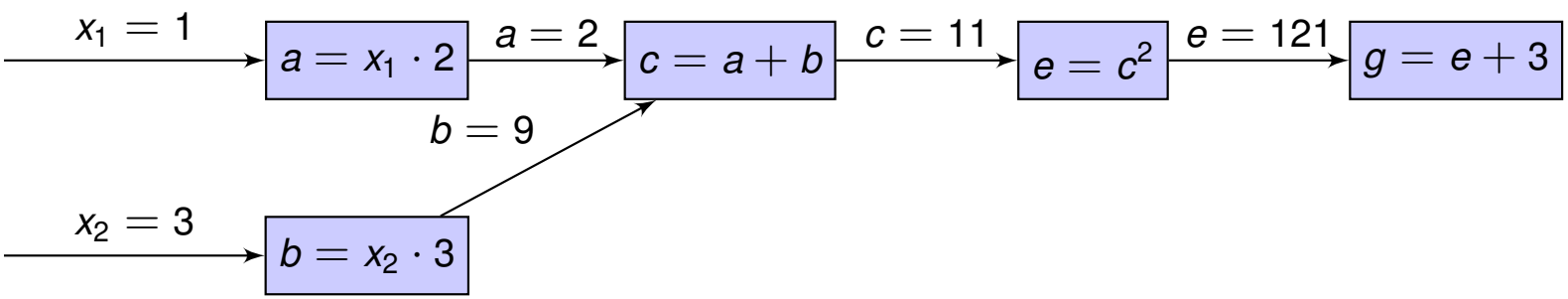

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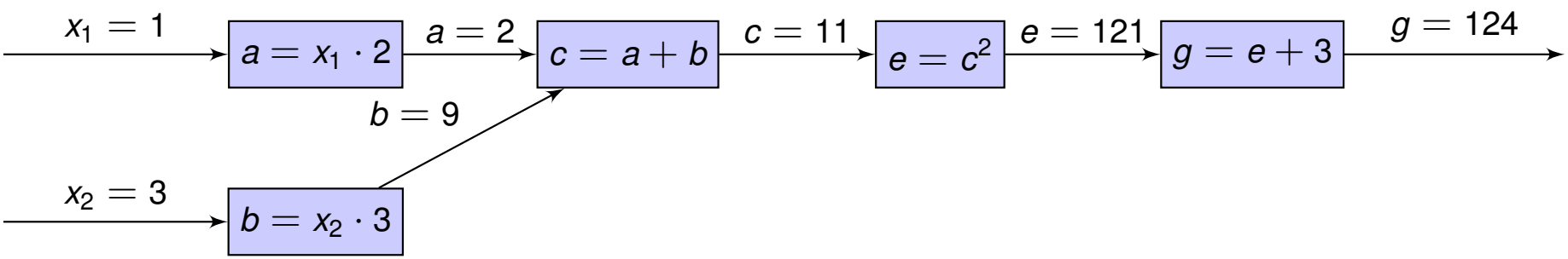

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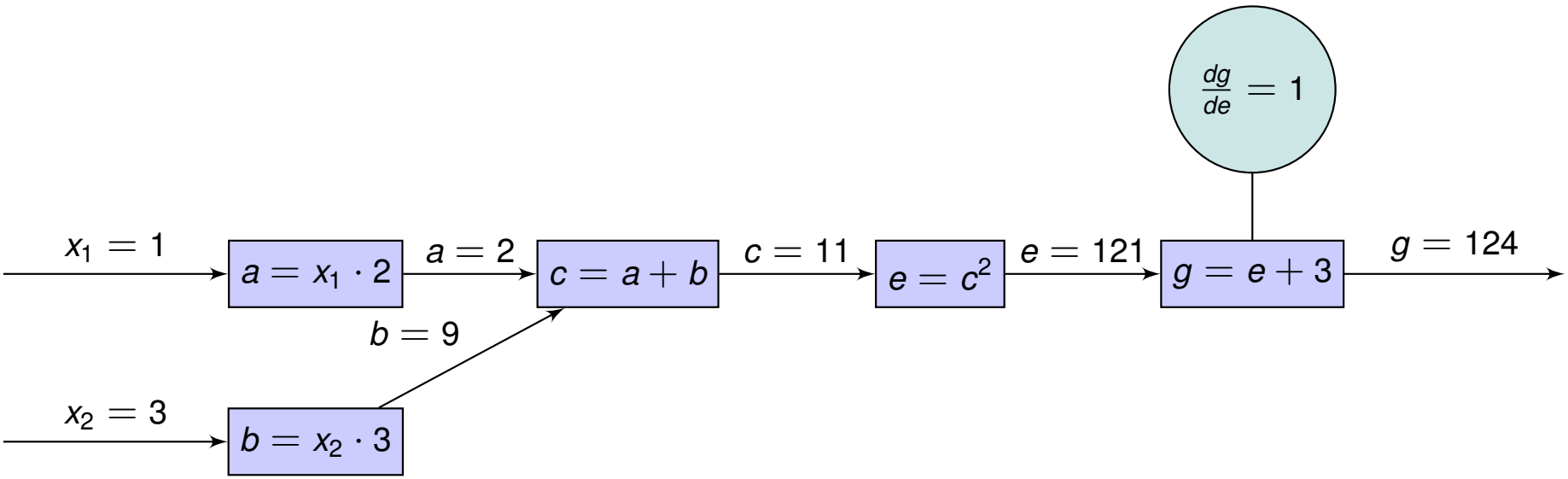

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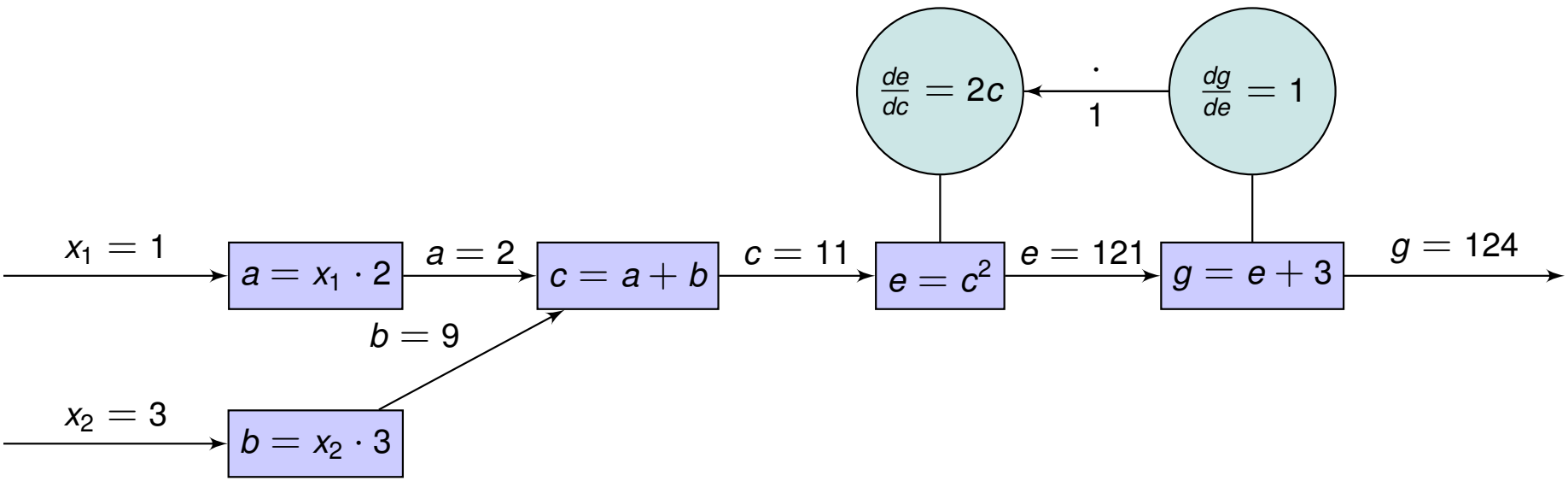

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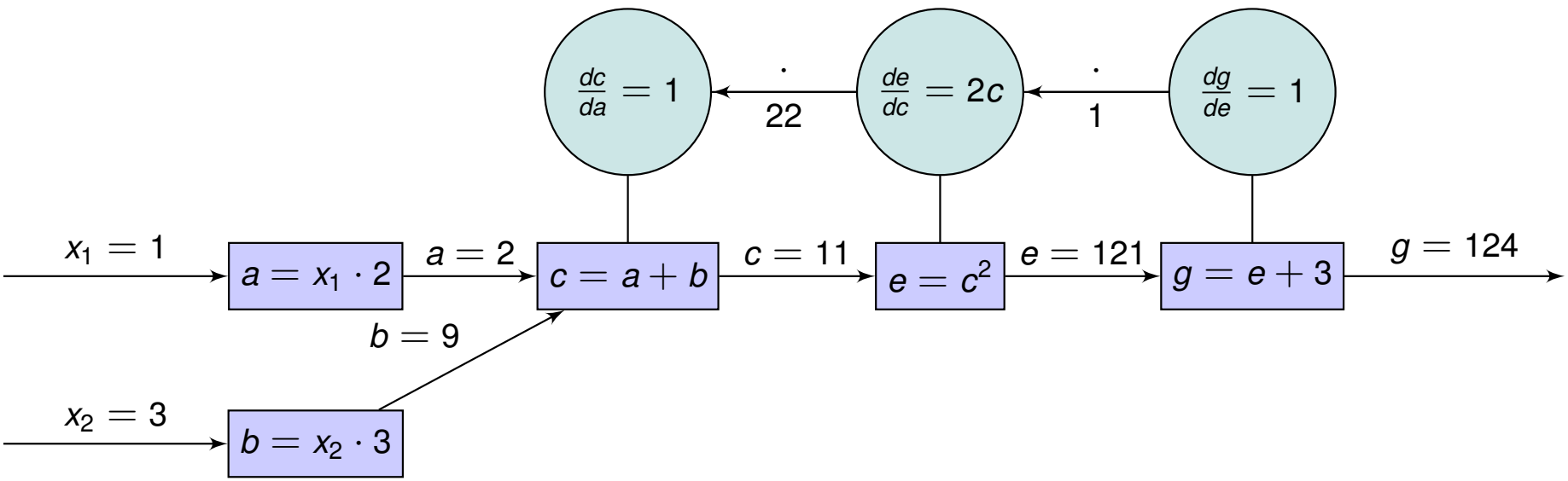

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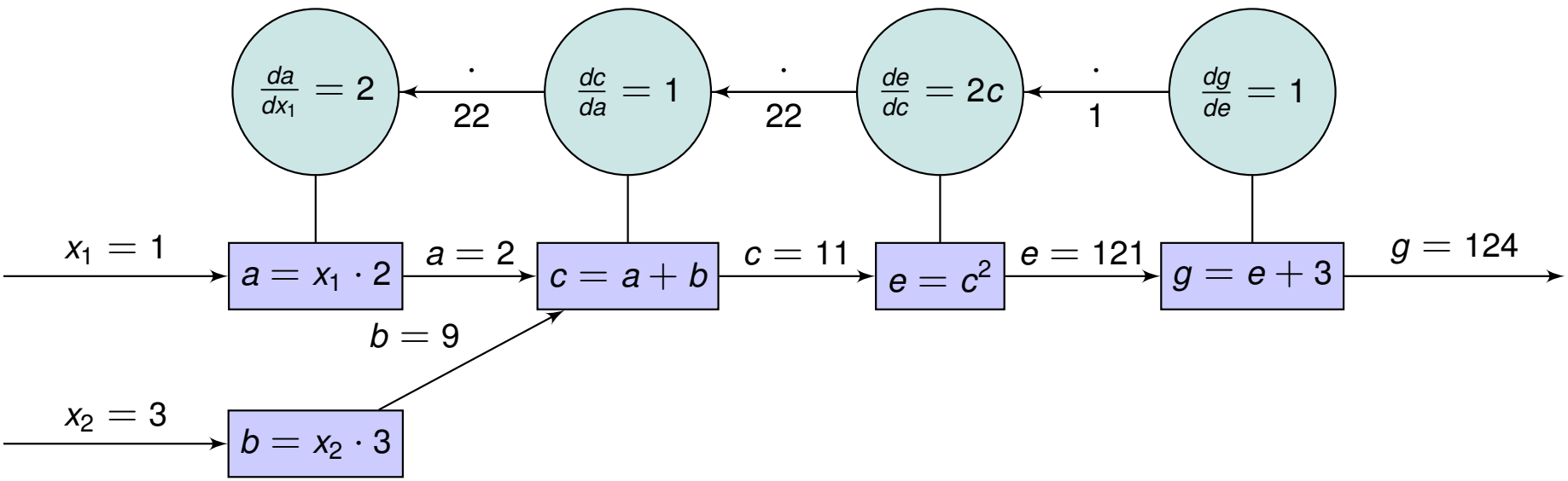

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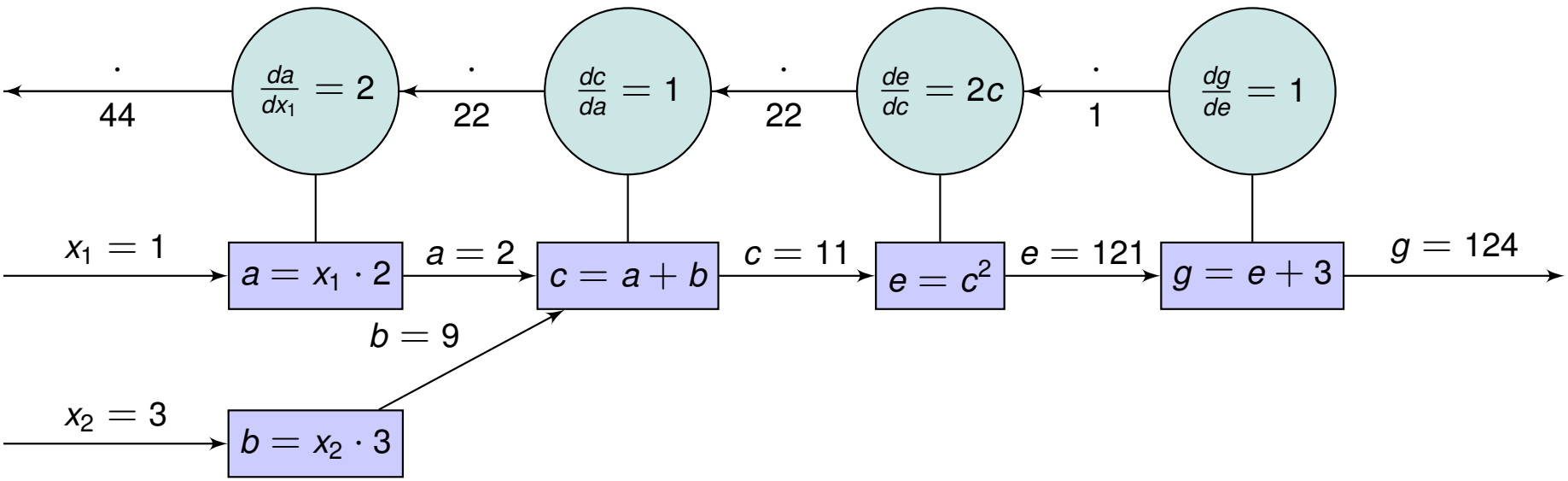
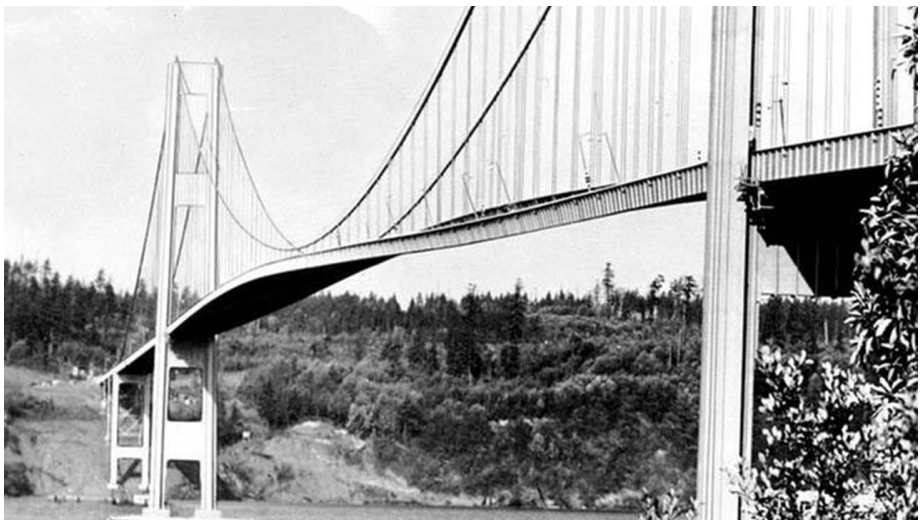
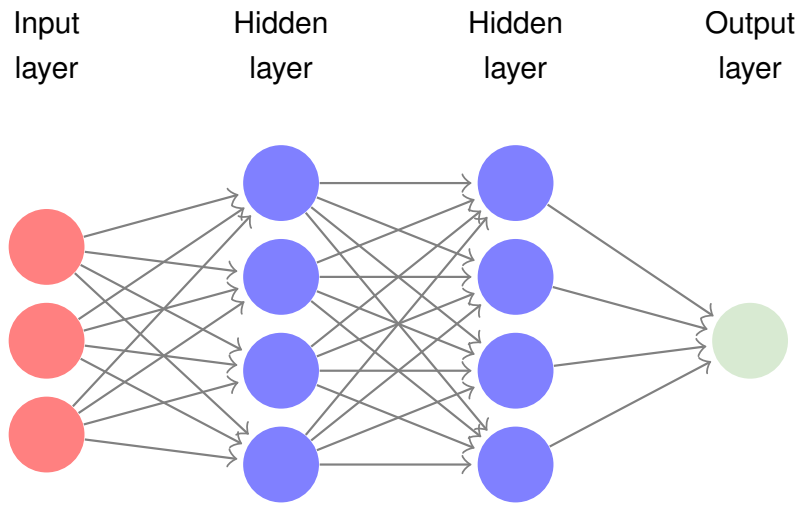


Stability Problem

- What do those two images have in common?

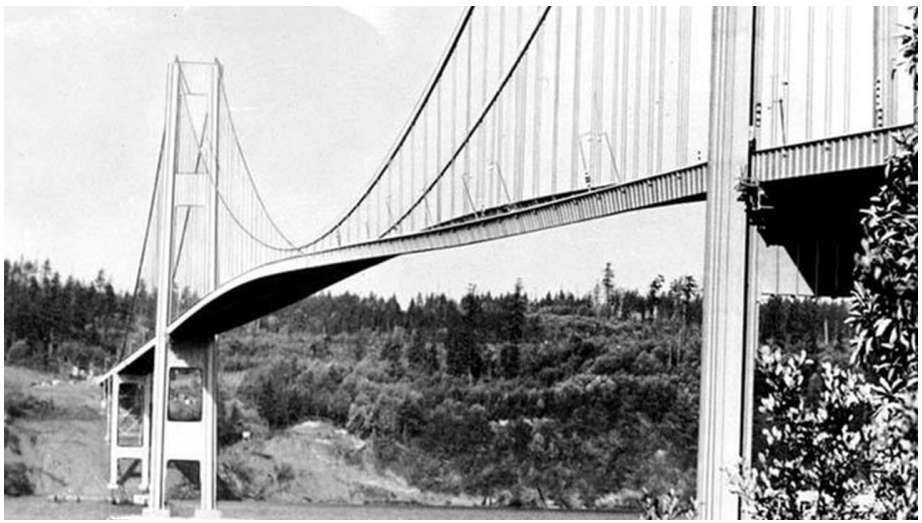


Click for video

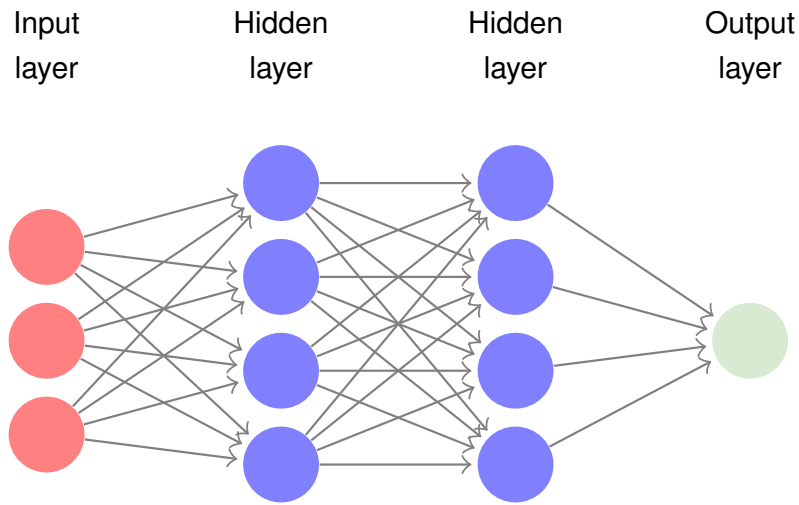


Stability Problem

- What do those two images have in common?

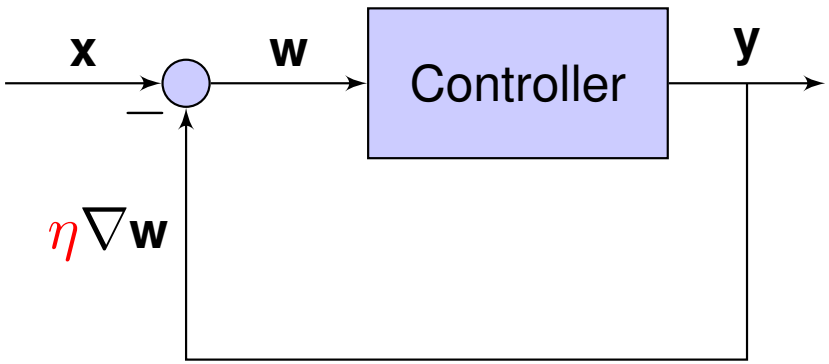


Click for video

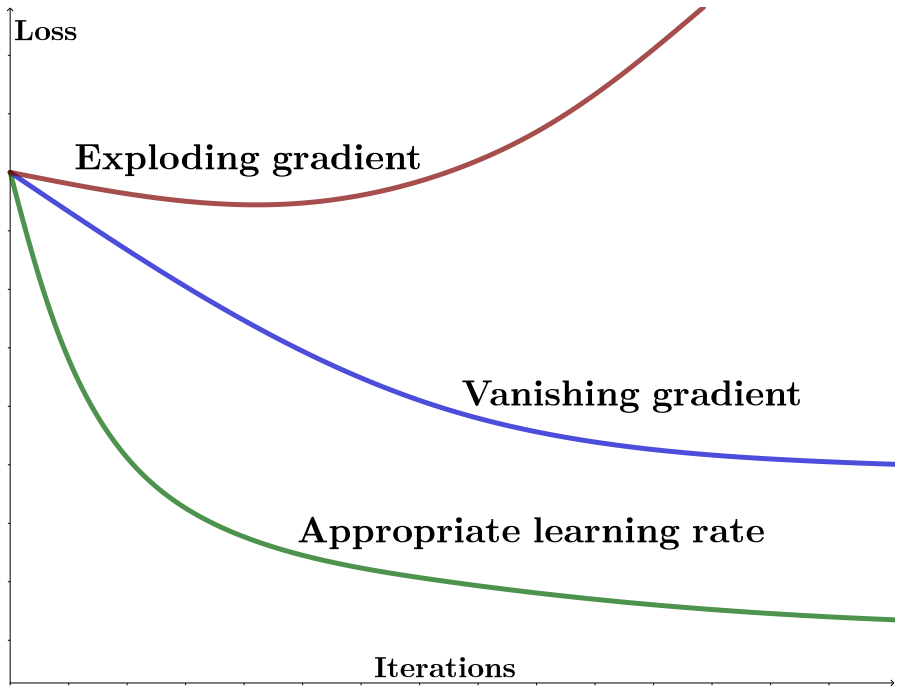


- Both suffer from positive feedback!
- This can cause disaster

Feedback loop



Analogy to control theory



- If η is too high $\rightarrow$ **positive feedback** $\rightarrow$ loss grows **without bounds**
- If η is too small $\rightarrow$ **negative feedback** $\rightarrow$ **gradient vanishes**
- Choice of η is **critical** for learning

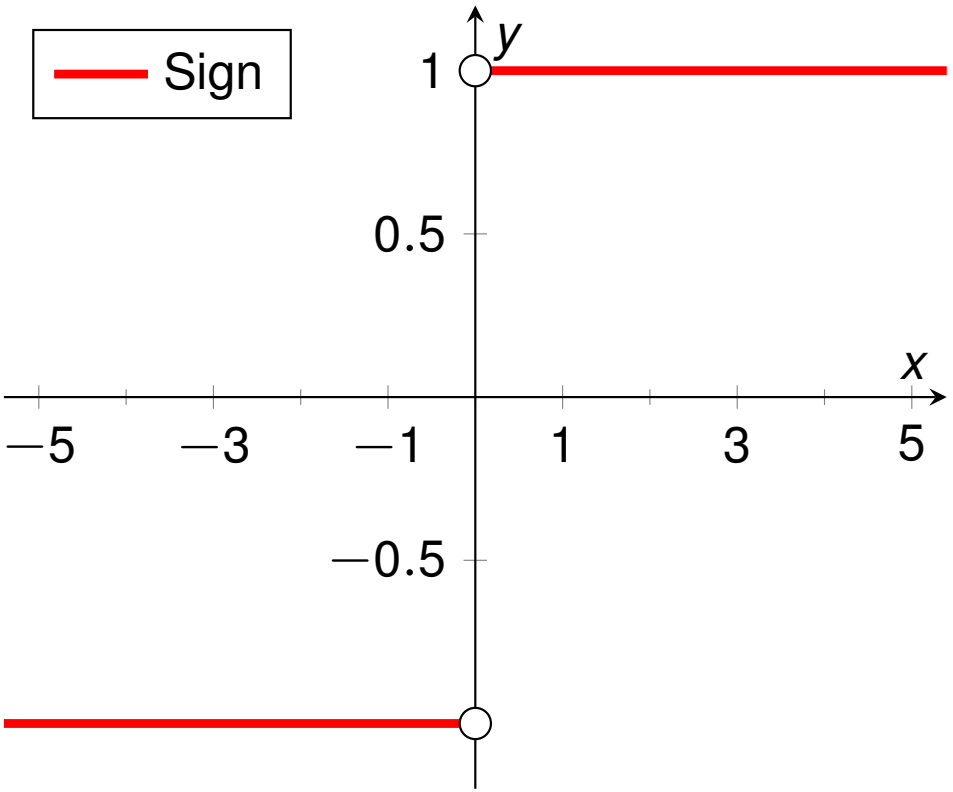
Backpropagation Summed up

- Built around the **chain rule**
- Uses a **forward-pass** through the function
- Computationally very **efficient** by using a **dynamic programming** approach
- Is **no training algorithm**, because it just computes a gradient

Consequences

- Product of partials $\rightarrow$ numerical **errors multiply**
- Product of partials $\rightarrow$ **vanishing** or **exploding** gradient

About the sign Activation Function



Sign

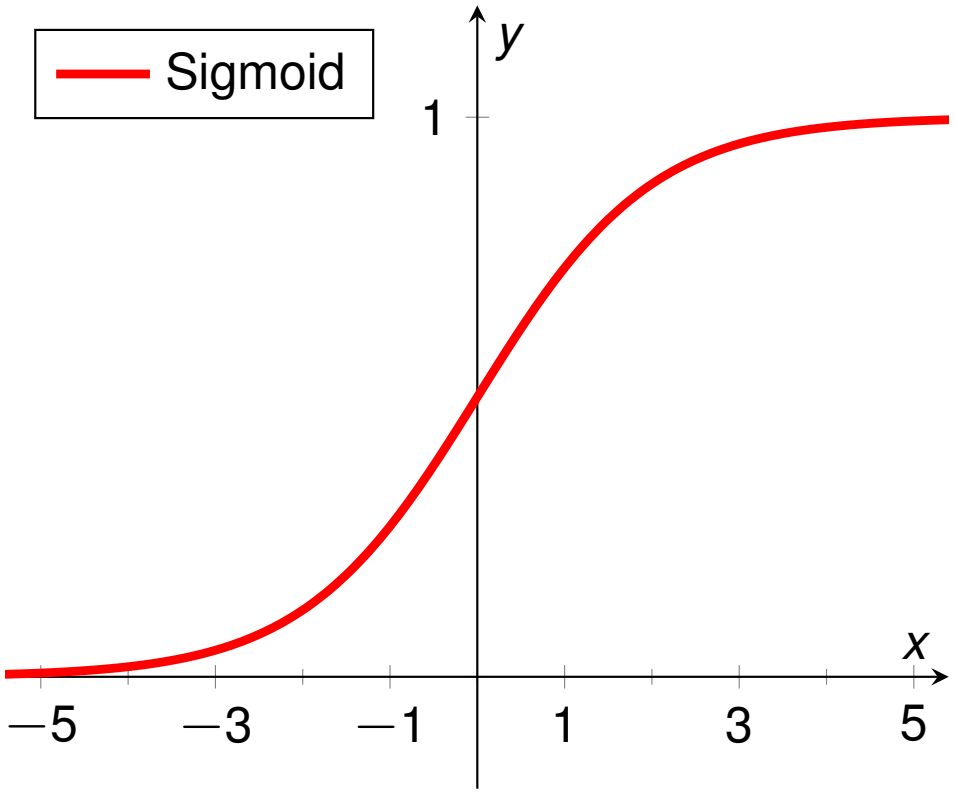
$$f(x) = \begin{cases} +1 & \text{for } x \geq 0 \\ -1 & \text{for } x < 0 \end{cases}$$

$$f'(x) = 2\delta(x)$$

\+ Normalized output

− Gradient vanishes almost everywhere!

Smooth Activation Function



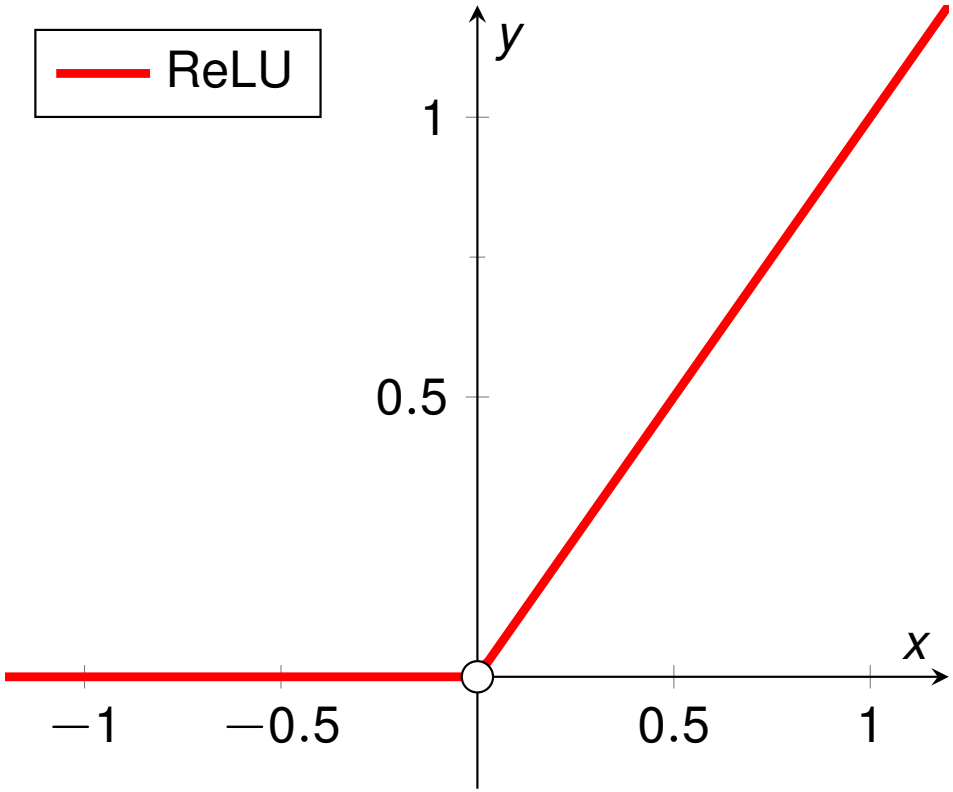
Sigmoid (logistic function)

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

$$f'(x) = f(x)(1 - f(x))$$

+ Normalized output
− Gradient still eventually vanishes

Piecewise-linear Activation Function



Rectified Linear Unit (ReLU)

$$f(x) = \max(0, x)$$

$$f'(x) = \begin{cases} 1 & \text{if } x > 0 \\ 0 & \text{else} \end{cases}$$

\+ Less vanishing gradient

NEXT TIME

ON DEEP LEARNING

FRIEDRICH-ALEXANDER-
UNIVERSITÄT
ERLANGEN-NÜRNBERG

SCHOOL OF ENGINEERING

Feed Forward Neural Networks - Part 4

A. Maier, V. Christlein, K. Breininger, S. Vesal, F. Meister, C. Liu, S. Gündel, S. Jaganathan, N. Maul, M. Vornehm, L. Reeb, F. Thamm, M. Hoffmann, C. Bergler, F. Denzinger, W. Fu, B. Geissler, Z. Yang
Pattern Recognition Lab, Friedrich-Alexander-Universität Erlangen-Nürnberg
April 21, 2020

Layer Abstraction

From Graphs of Nodes to Graphs of Layers

- We introduced **layers** but computed everything on individual nodes
- It is convenient to add further abstraction
- But how can we express this?

Recall: Single neuron

- Add a bias unit to $\mathbf{x} \in \mathbb{R}^{N-1}$ by adding a dimension with $x_n = 1$
- This is a connection from every input element to the single output element:

$$\hat{y} = \mathbf{w}^T \mathbf{x}$$

Representing the connections

- Assume we have M neurons $\rightarrow$ M sets of weights: $\mathbf{w}_m$ for $m \in \{1, \ldots, M\}$

$$\hat{y_m} = \mathbf{w}_m^T \mathbf{x}$$

- We rewrite this operation as matrix-vector multiplication:

$$\hat{\mathbf{y}} = \mathbf{W}\mathbf{x}$$

- This is known as **fully connected layer**.
- It represents any arbitrary connection topology between layers.
- We can describe back-propagation in this more abstract view as well!

Fully Connected Layer

$$\begin{pmatrix} \hat{y}_1 \\ \hat{y}_2 \end{pmatrix} = \begin{bmatrix} w_{11} & w_{12} & w_{13} \\ w_{21} & w_{22} & w_{23} \end{bmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

- The forward-pass is:

$$\hat{\mathbf{y}} = \mathbf{W}\mathbf{x}$$

- After the forward-pass through all layers, we can compute a loss that depends on our loss function L.
- We need two gradients for the backward-pass:
  - Gradient with respect to the weights: $\frac{\partial \mathbf{L}}{\partial \mathbf{W}}$ for gradient descend
  - Gradient with respect to the inputs: $\frac{\partial \mathbf{L}}{\partial \mathbf{x}}$ for backpropagation

Fully Connected Layer Summed up

- Can represent any connection topology
- Enables higher level view concentrating on layers instead of nodes
- Is a matrix multiplication:

$$\hat{\mathbf{y}} = \mathbf{W}\mathbf{x}$$

- Its gradient with respect to the weights:

$$\frac{\partial L}{\partial \mathbf{W}} = \frac{\partial L}{\partial \hat{\mathbf{y}}} \frac{\partial \hat{\mathbf{y}}}{\partial \mathbf{W}} = \frac{\partial L}{\partial \hat{\mathbf{y}}} \mathbf{x}^T$$

- Its gradient with respect to the input:

$$\frac{\partial L}{\partial \mathbf{x}} = \frac{\partial L}{\partial \hat{\mathbf{y}}} \frac{\partial \hat{\mathbf{y}}}{\partial \mathbf{x}} = \mathbf{W}^T \frac{\partial L}{\partial \hat{\mathbf{y}}}$$

Fully Connected Layer: Simple example

- Assume we are looking at a simple network (no activation function) with the forward pass:

$$\hat{\mathbf{y}} = \mathbf{W}\mathbf{x}$$

- We try to find parameters $\mathbf{W}$ that minimize the following loss function:

$$L(\mathbf{x}, \mathbf{W}, \mathbf{y}) = \frac{1}{2}\|\mathbf{W}\mathbf{x} - \mathbf{y}\|_2^2$$

- Then simply: $\frac{\partial L}{\partial \hat{\mathbf{y}}} = \hat{\mathbf{y}} - \mathbf{y} = \mathbf{W}\mathbf{x} - \mathbf{y}$
- The gradient with respect to the weights: $\frac{\partial L}{\partial \mathbf{W}} = (\mathbf{W}\mathbf{x} - \mathbf{y})\mathbf{x}^T$
- The gradient with respect to the inputs: $\frac{\partial L}{\partial \mathbf{x}} = \mathbf{W}^T(\mathbf{W}\mathbf{x} - \mathbf{y})$

Linear Network in Matrix notation

$$L(\mathbf{W}_1, \mathbf{W}_2, \mathbf{W}_3) = \frac{1}{2} \left\| \mathbf{W}_3 \mathbf{W}_2 \mathbf{W}_1 \mathbf{x} - \mathbf{y} \right\|_2^2$$

Linear Network in Matrix notation

$$L(\mathbf{W}_1, \mathbf{W}_2, \mathbf{W}_3) = \frac{1}{2} \left\| \mathbf{W}_3 \mathbf{W}_2 \mathbf{W}_1 \mathbf{x} - \mathbf{y} \right\|_2^2$$

$$\frac{\partial L(\mathbf{W}_1, \mathbf{W}_2, \mathbf{W}_3)}{\partial \mathbf{W}_1} =$$

Linear Network in Matrix notation

$$L(\mathbf{W}_1, \mathbf{W}_2, \mathbf{W}_3) = \frac{1}{2} \left\| \mathbf{W}_3 \mathbf{W}_2 \mathbf{W}_1 \mathbf{x} - \mathbf{y} \right\|_2^2$$

$$\frac{\partial L(\mathbf{W}_1, \mathbf{W}_2, \mathbf{W}_3)}{\partial \mathbf{W}_1} = (\mathbf{W}_3 \mathbf{W}_2)^T (\mathbf{W}_3 \mathbf{W}_2 \mathbf{W}_1 \mathbf{x} - \mathbf{y}) \mathbf{x}^T$$

Linear Network in Matrix notation

$$L(\mathbf{W}_1, \mathbf{W}_2, \mathbf{W}_3) = \frac{1}{2} \|\mathbf{W}_3 \mathbf{W}_2 \mathbf{W}_1 \mathbf{x} - \mathbf{y}\|_2^2$$

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Linear Network in Matrix notation

$$L(\mathbf{W}_1, \mathbf{W}_2, \mathbf{W}_3) = \frac{1}{2} \|\mathbf{W}_3 \mathbf{W}_2 \mathbf{W}_1 \mathbf{x} - \mathbf{y}\|_2^2$$

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$$\frac{\partial L(\mathbf{W}_1, \mathbf{W}_2, \mathbf{W}_3)}{\partial \mathbf{W}_2}$$

Linear Network in Matrix notation

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$$\frac{\partial L(\mathbf{W}_1, \mathbf{W}_2, \mathbf{W}_3)}{\partial \mathbf{W}_2} = \mathbf{W}_3^T (\mathbf{W}_3 \mathbf{W}_2 \mathbf{W}_1 \mathbf{x} - \mathbf{y}) (\mathbf{W}_1 \mathbf{x})^T$$

Linear Network in Matrix notation

$$L(\mathbf{W}_1, \mathbf{W}_2, \mathbf{W}_3) = \frac{1}{2}\|\mathbf{W}_3\mathbf{W}_2\mathbf{W}_1\mathbf{x} - \mathbf{y}\|_2^2$$

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$$\frac{\partial L(\mathbf{W}_1, \mathbf{W}_2, \mathbf{W}_3)}{\partial \mathbf{W}_3} = (\mathbf{W}_3\mathbf{W}_2\mathbf{W}_1\mathbf{x} - \mathbf{y})(\mathbf{W}_2\mathbf{W}_1\mathbf{x})^T$$

Summary

- **Softmax activation** function with **cross entropy loss** mostly go together as "Softmax Loss".
- **Gradient descent** is our default training algorithm in deep learning.
- We can compute gradients using **finite differences** to check our implementation.
- We use the **backpropagation** algorithm to compute gradients efficiently.
- The **fully connected** layer is the most general connectivity between layers in a feed-forward neural network.

NEXT TIME

ON DEEP LEARNING

- Problem adapted loss functions
- Sophisticated optimization routines
- Optimization adapted to the needs of every single parameter
- An argument why neural networks shouldn't perform well
- Some very recent insights why they do perform well

Comprehensive Questions

- Name a loss function for multi-class classification in deep learning.
- Explain how this loss function works.
- How can you check if the derivative implementation of a loss function is correct?
- What does backpropagation do?
- How does backpropagation work?
- Explain the exploding and vanishing gradient problems.
- Why is the signum function not used in deep learning?

Further Reading

- Link - The original paper popularizing ReLUs
- Link - The original paper popularizing backpropagation
- Link - Bishop - Mathematical compendium for machine learning
- Link - Blog article putting backpropagation in a very general context

References

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[1] R. O. Duda, P. E. Hart, and D. G. Stork. Pattern Classification. John Wiley and Sons, inc., 2000.

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