THE UNIVERSITY OF BRITISH COLUMBIA

Topics in AI (CPSC 532L):
Multimodal Learning with Vision, Language and Sound

Lecture 2: Introduction to Deep Learning

Course **Logistics**

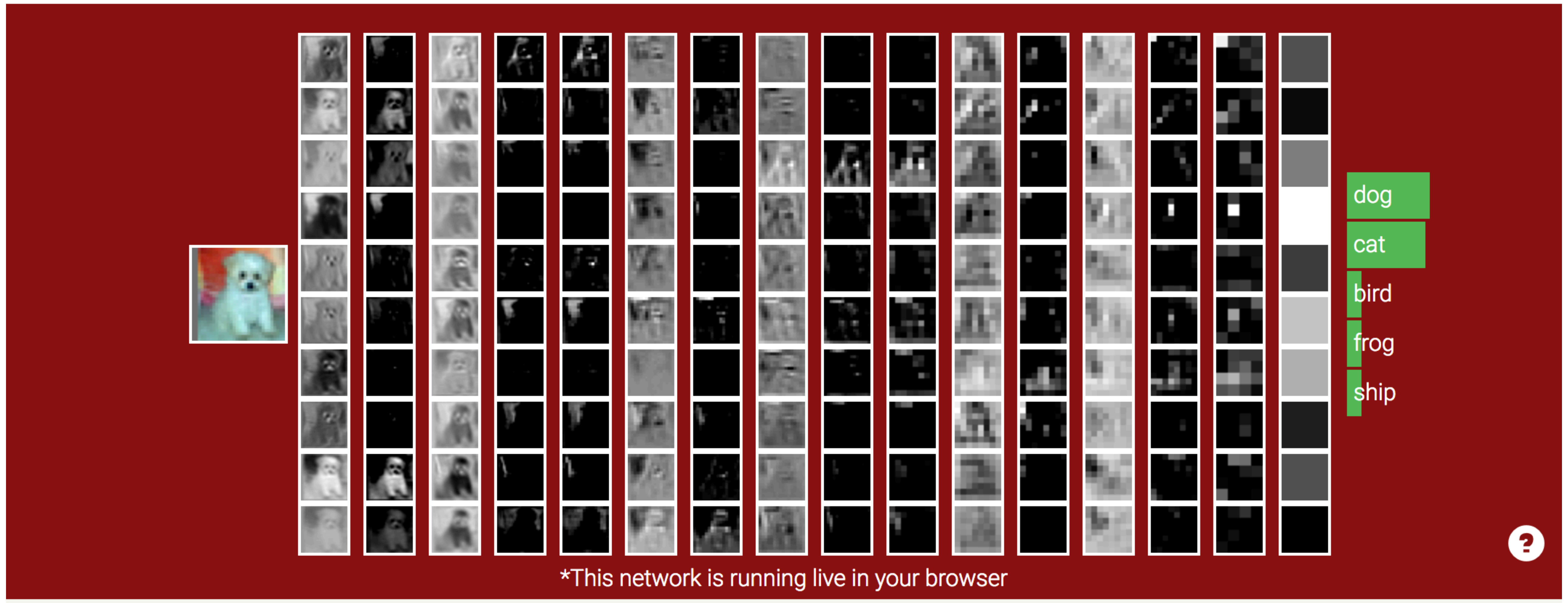
- Update on **course registrations** — 43 students registered (out of 40)
- Those who want to **audit** …
- **Piazza** registrations (all announcements and HW solutions will be there)
- **Assignment 1** is out (due date Monday, Jan 14 @ 11:59pm)
- Microsoft **Azure** credits and tutorial
- TA office hours will be posted by tonight (there will be one this week and next)

Introduction to **Deep Learning**

There is a **lot packed** into today's lecture (excerpts from a few lectures of CS231n)

CS231n: Convolutional Neural Networks for Visual Recognition

Spring 2017



if you want more details, check out CS231n lectures on-line

Covering: foundations and most important aspects of supervised DNNs

Not-covering: neuroscience background of deep learning, optimization (CPSC 340 & CPSC 540), and not a lot of theoretical underpinning


Disney · PIXAR
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Disney · PIXAR
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Linear **regression** (review)

	Inputs (features)					Outputs	
	production costs	promotional costs	genre of the movie	box office first week	total book sales	total revenue USA	total revenue international
Training Set	$x_1^{(1)}$	$x_2^{(1)}$	$x_3^{(1)}$	$x_4^{(1)}$	$x_5^{(1)}$	$y_1^{(1)}$	$y_2^{(1)}$
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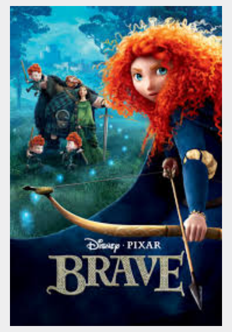

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Linear **regression** (review)

$$\hat{y}_j = \sum_i w_{ji} x_i + b_j$$

each output is a linear combination of inputs plus bias, easier to write in **matrix form**:

$$\hat{\mathbf{y}} = \mathbf{W}^T \mathbf{x} + \mathbf{b}$$

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Key to accurate prediction is **learning parameters** to minimize discrepancy with historical data

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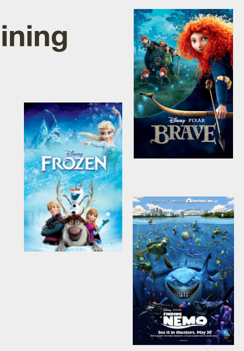

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$$\mathcal{L}(\mathbf{W}, \mathbf{b}) = \sum_{d=1}^{|D_{train}|} \underline{l(\hat{\mathbf{y}}^{(d)}, \mathbf{y}^{(d)})}$$

$$\mathbf{W}^*, \mathbf{b}^* = \arg\min \mathcal{L}(\mathbf{W}, \mathbf{b})$$

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$$\mathcal{L}(\mathbf{W}, \mathbf{b}) = \sum_{d=1}^{|D_{train}|} ||\underline{\hat{\mathbf{y}}^{(d)} - \mathbf{y}^{(d)}}||^2$$

$$\mathbf{W}^*, \mathbf{b}^* = \arg\min \mathcal{L}(\mathbf{W}, \mathbf{b})$$

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Linear **regression** (review) — Learning /w Least Squares

$$\mathcal{L}(\mathbf{W}, \mathbf{b}) = \sum_{d=1}^{|D_{train}|} \left|\left|\mathbf{W}^T \mathbf{x}^{(d)} + \mathbf{b} - \mathbf{y}^{(d)}\right|\right|^2$$

$$\mathbf{W}^*, \mathbf{b}^* = \arg\min \mathcal{L}(\mathbf{W}, \mathbf{b})$$

Solution:

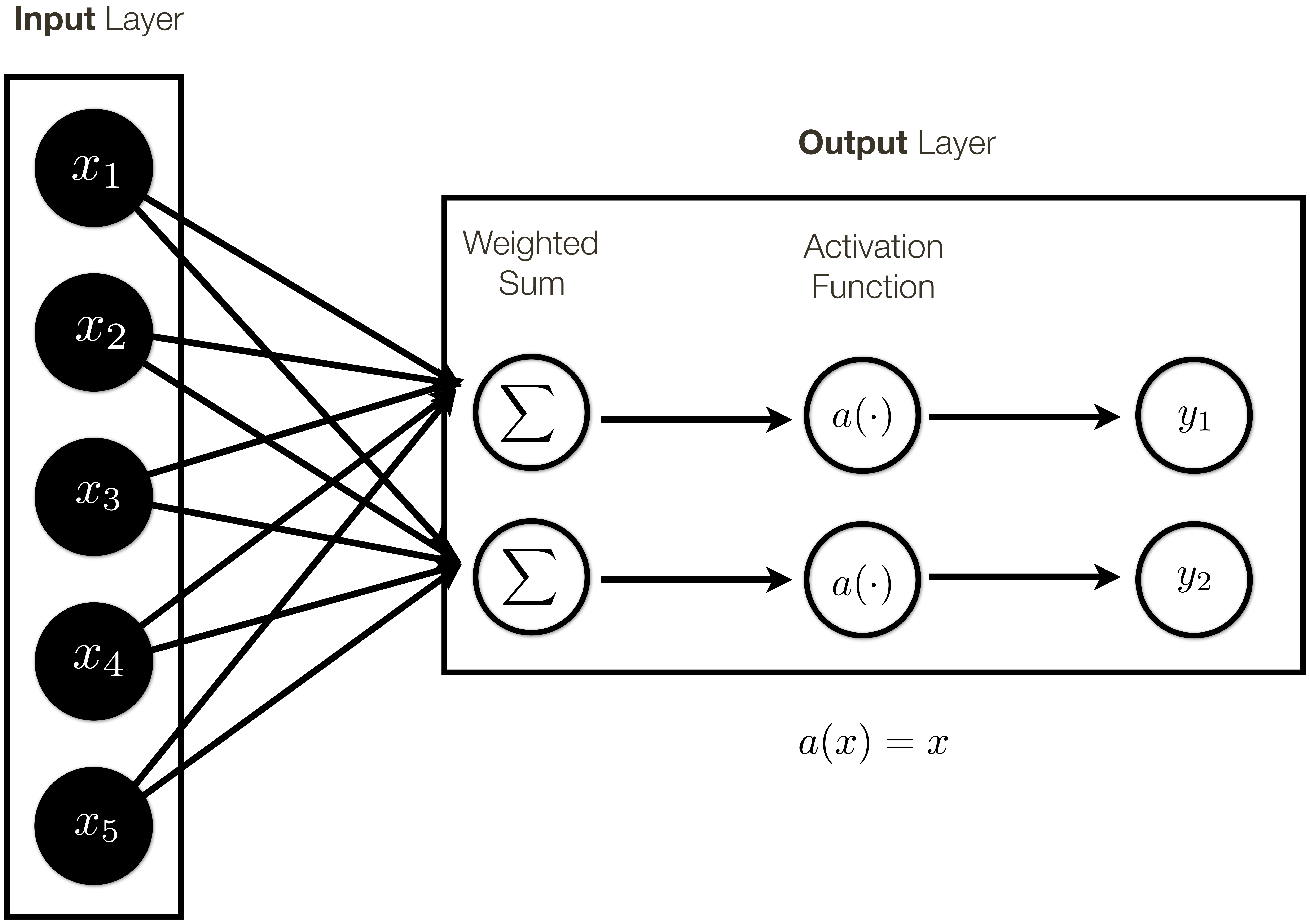
$$\frac{\partial \mathcal{L}(\mathbf{W}, \mathbf{b})}{\partial w_{ji}} = \frac{\partial}{\partial w_{ji}} \sum_{d=1}^{|D_{train}|} \left|\left|\mathbf{W}^T \mathbf{x}^{(d)} + \mathbf{b} - \mathbf{y}^{(d)}\right|\right|^2$$

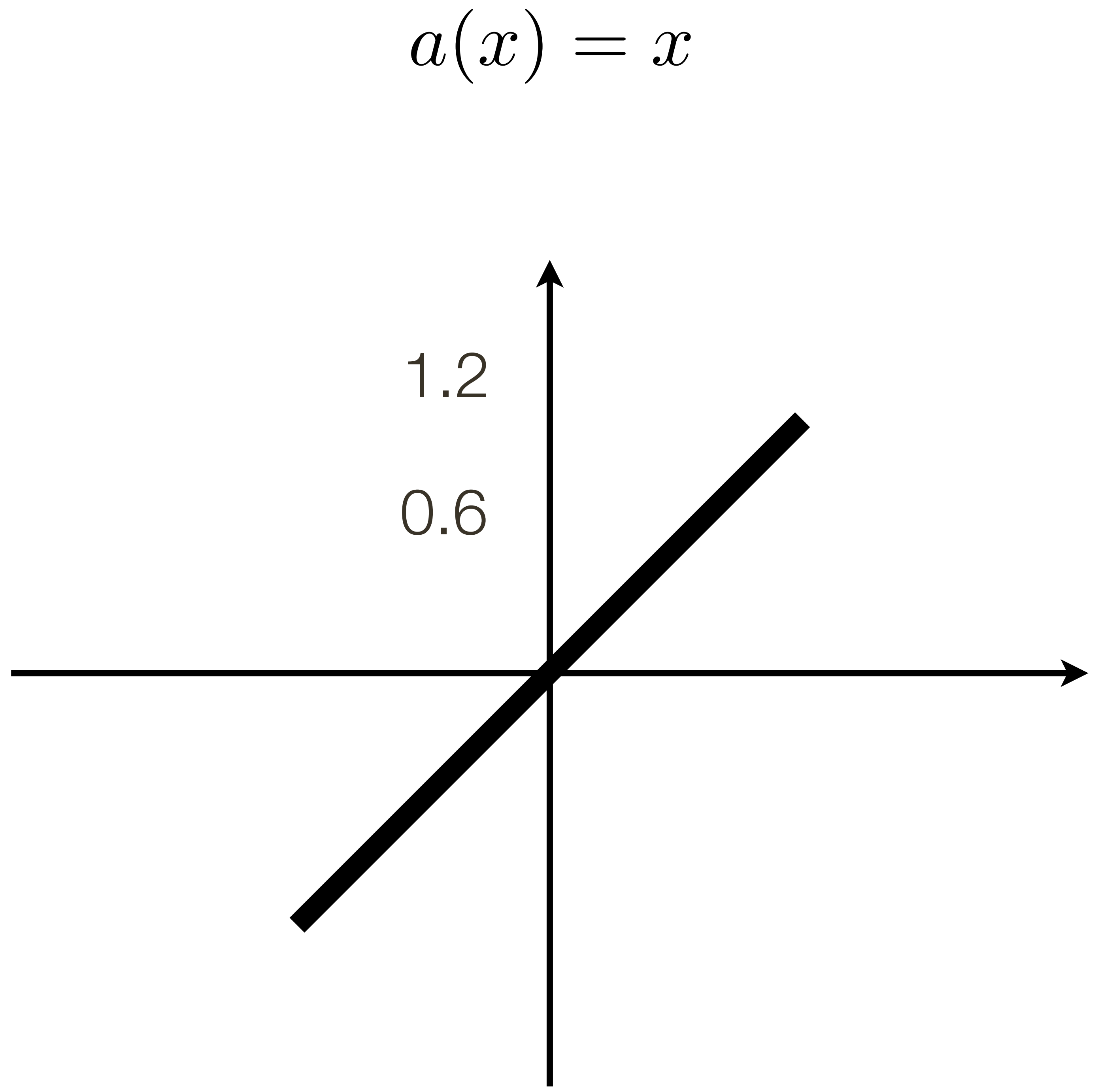
$$\frac{\partial \mathcal{L}(\mathbf{W}, \mathbf{b})}{\partial w_{ji}} = \frac{\partial}{\partial w_{ji}} \sum_{d=1}^{|D_{train}|} \left|\left|\mathbf{W}^T \mathbf{x}^{(d)} + \mathbf{b} - \mathbf{y}^{(d)}\right|\right|^2 = 0$$

after some operations $\longrightarrow$ $\mathbf{W}^* = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{Y}$

*slide adopted from V. Ordonex

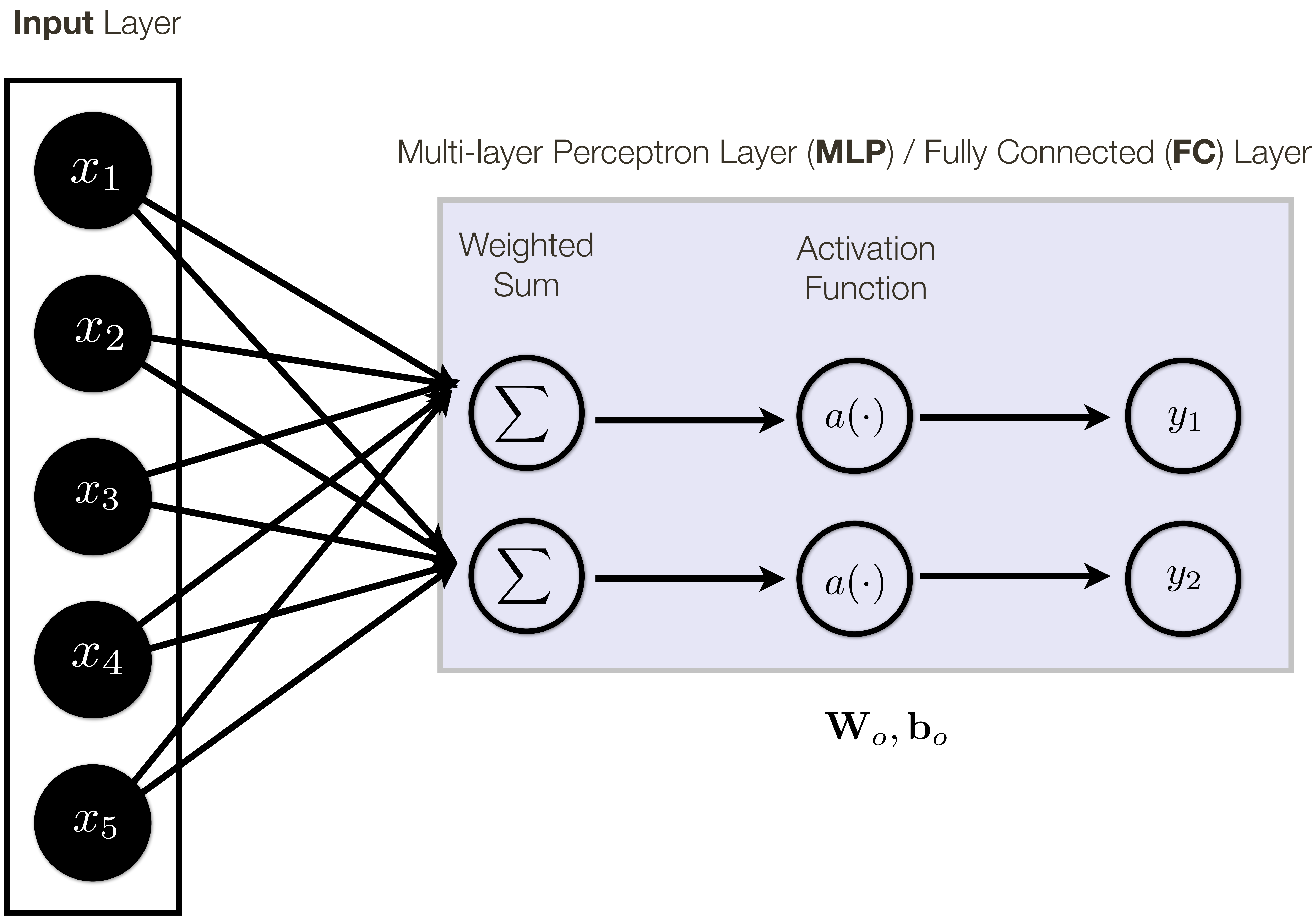
One-layer **Neural Network**





Linear Activation

One-layer **Neural Network**



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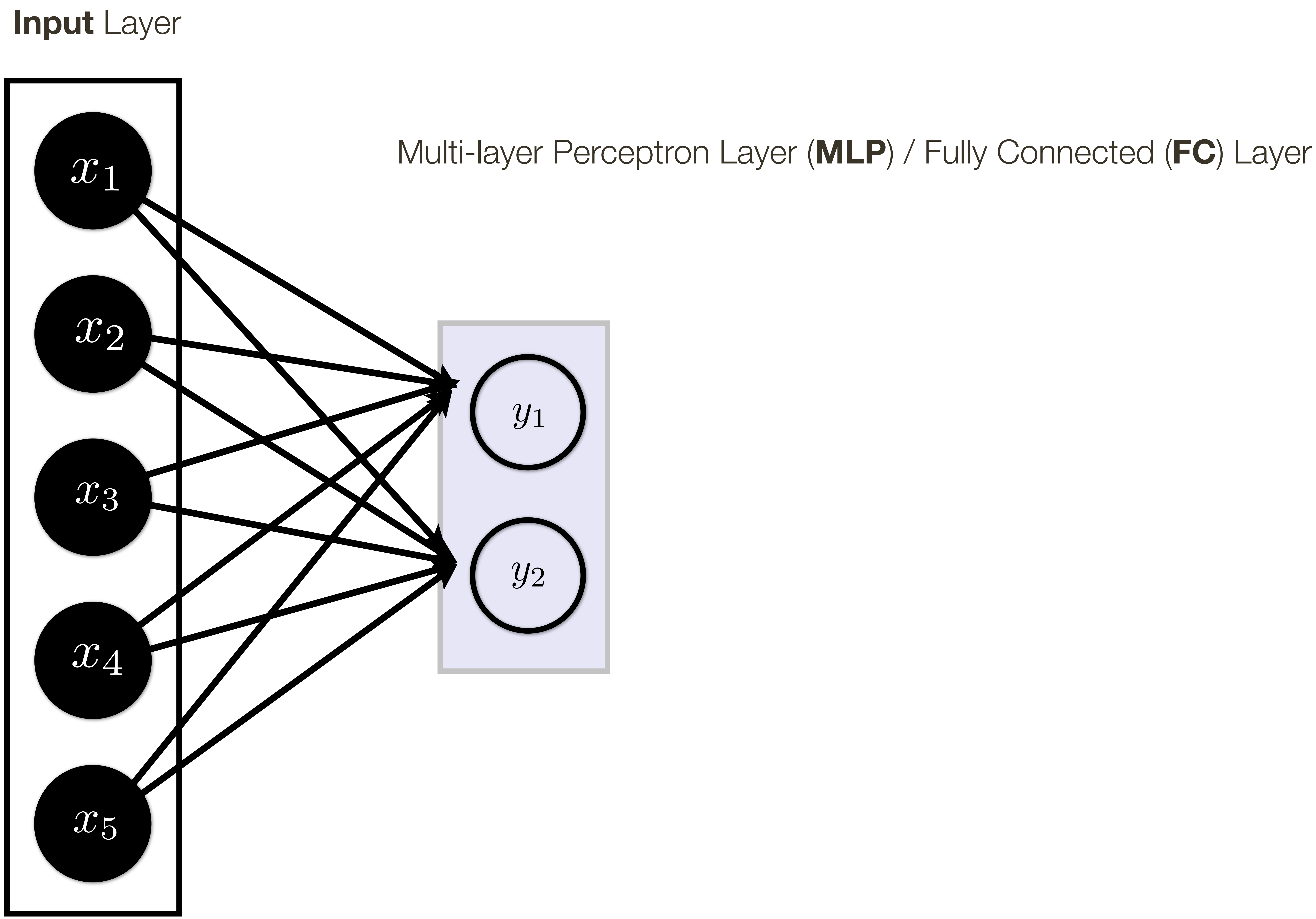
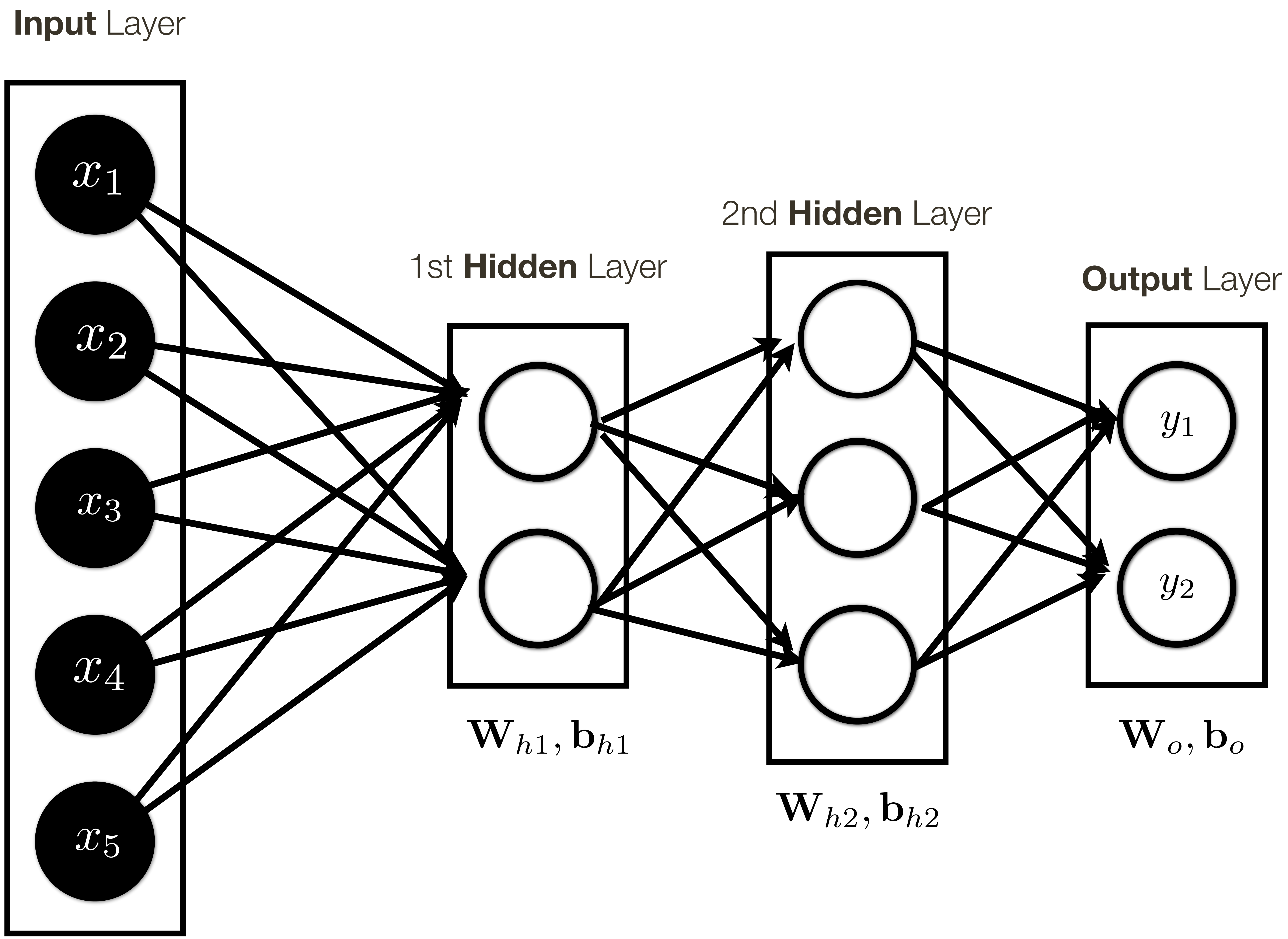


Multi-layer **Neural Network**



Neural Network **Intuition**

Question: What is a Neural Network?

Answer: Complex mapping from an input (vector) to an output (vector)

* slide from Marc'Aurelio Renzato

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Question: What does a hidden unit do?

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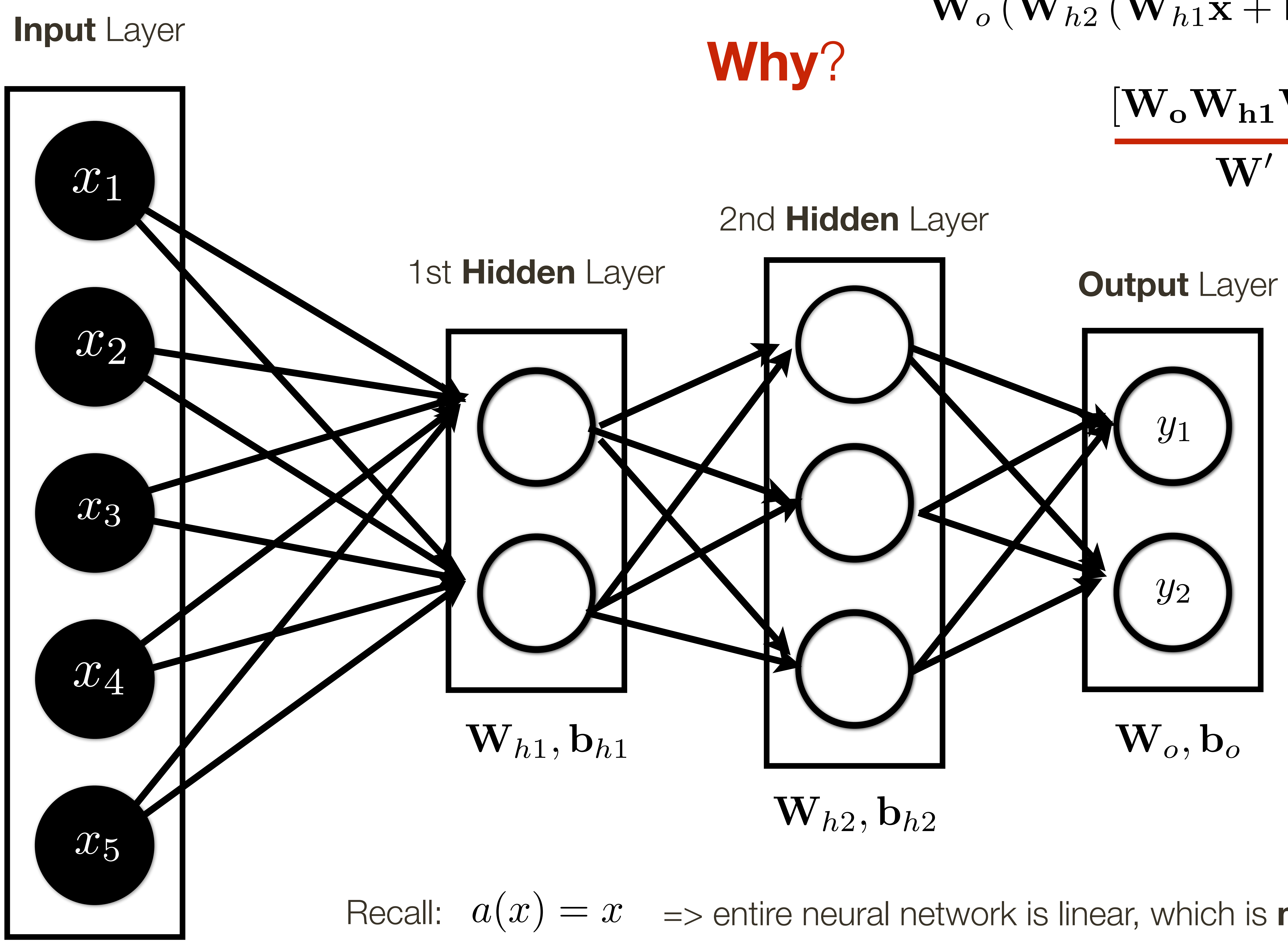
Question: Why have many layers?

Answer: 1) More layers = more complex functional mapping

2) More efficient due to distributed representation

* slide from Marc'Aurelio Renzato

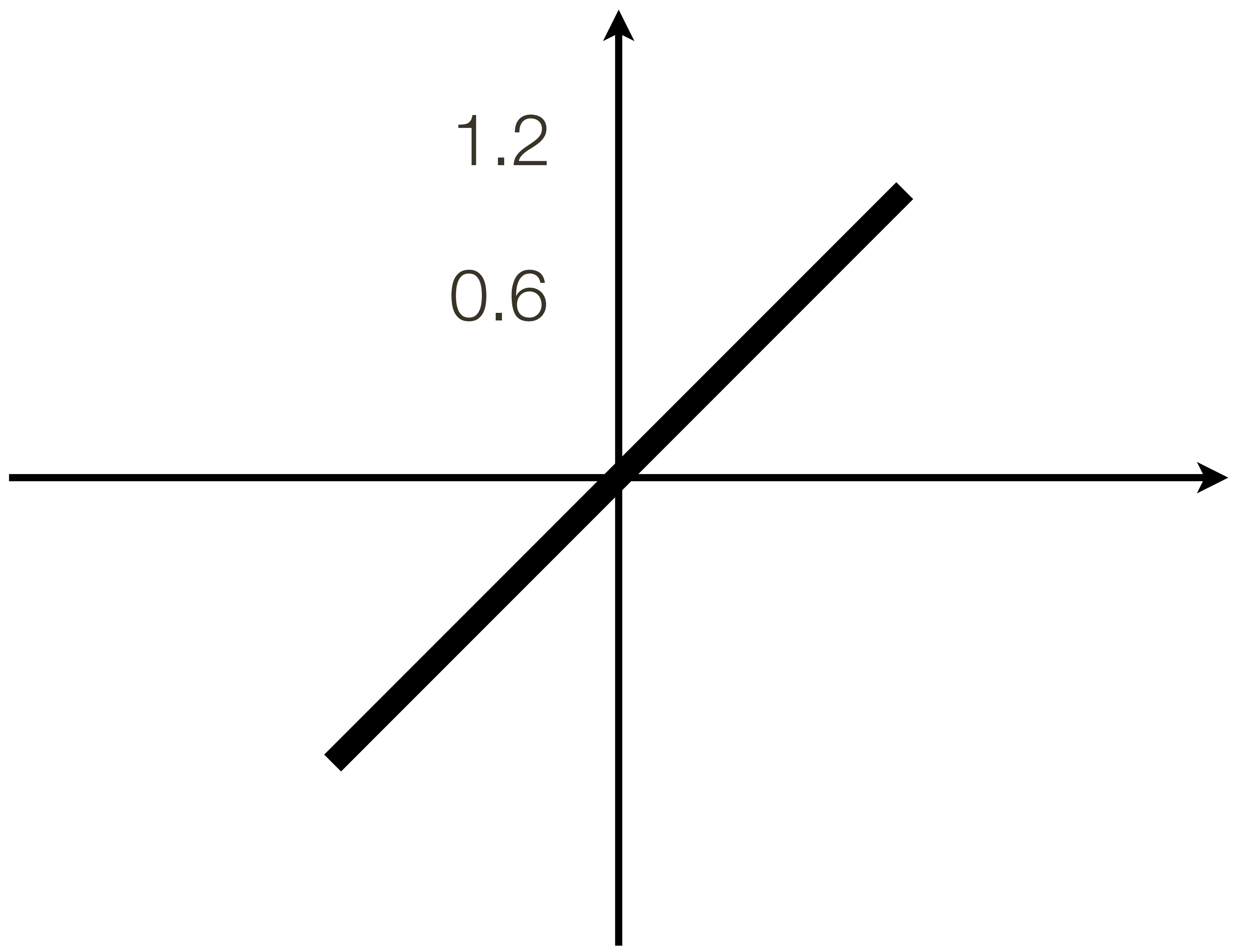
Multi-layer **Neural Network**



Why?

$$\mathbf{W}_o\left(\mathbf{W}_{h2}\left(\mathbf{W}_{h1}\mathbf{x} + \mathbf{b}_{h1}\right) + \mathbf{b}_{h2}\right) + \mathbf{b}_o =$$

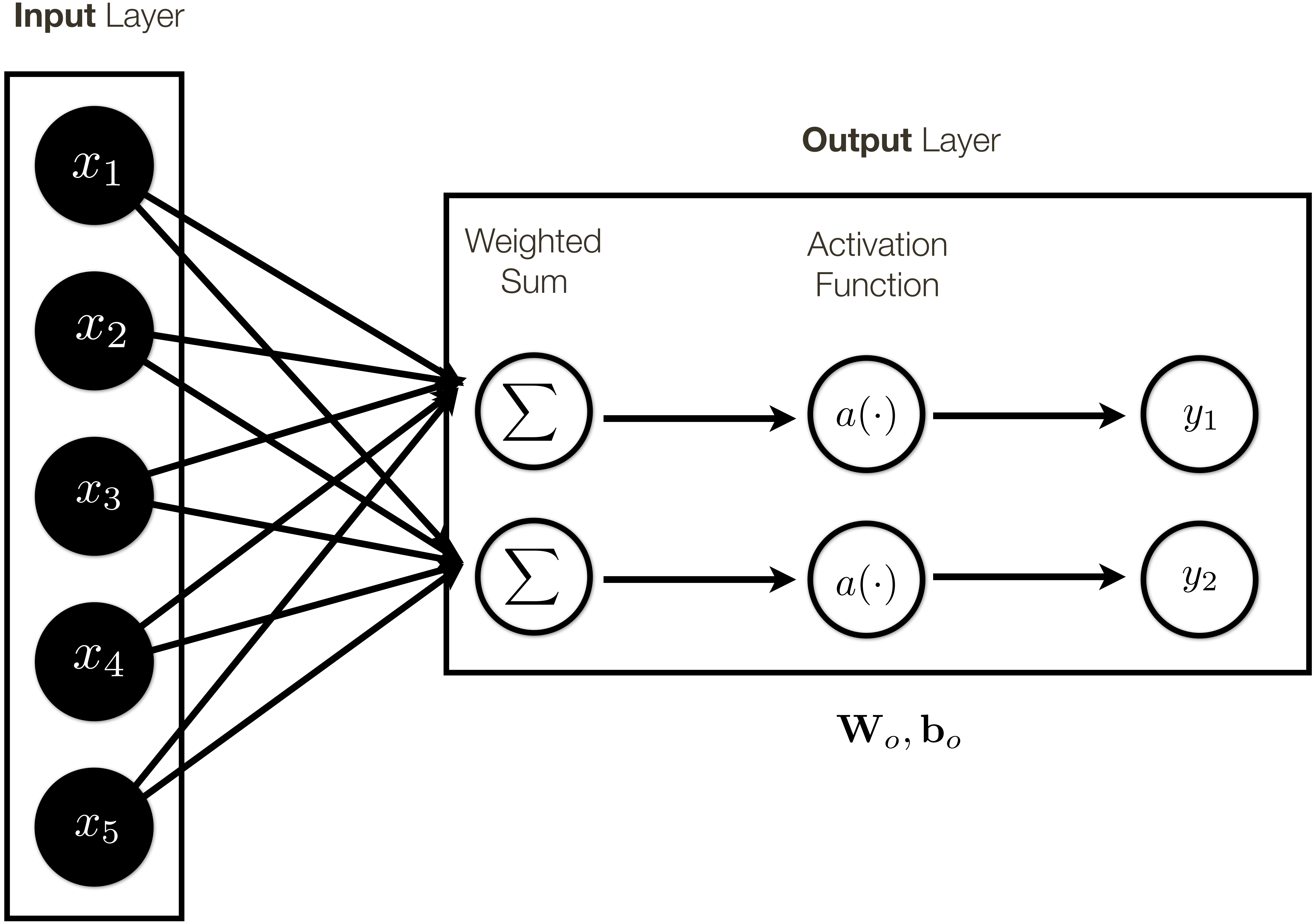
$$\underbrace{\left[\mathbf{W_o W_{h1} W_{h2}}\right]}_{\mathbf{W}'}\mathbf{x} + \underbrace{\left[\mathbf{W_o W_{h1} b}_{h1} + \mathbf{W_o b}_{h2} + \mathbf{b}_o\right]}_{\mathbf{b}'}$$



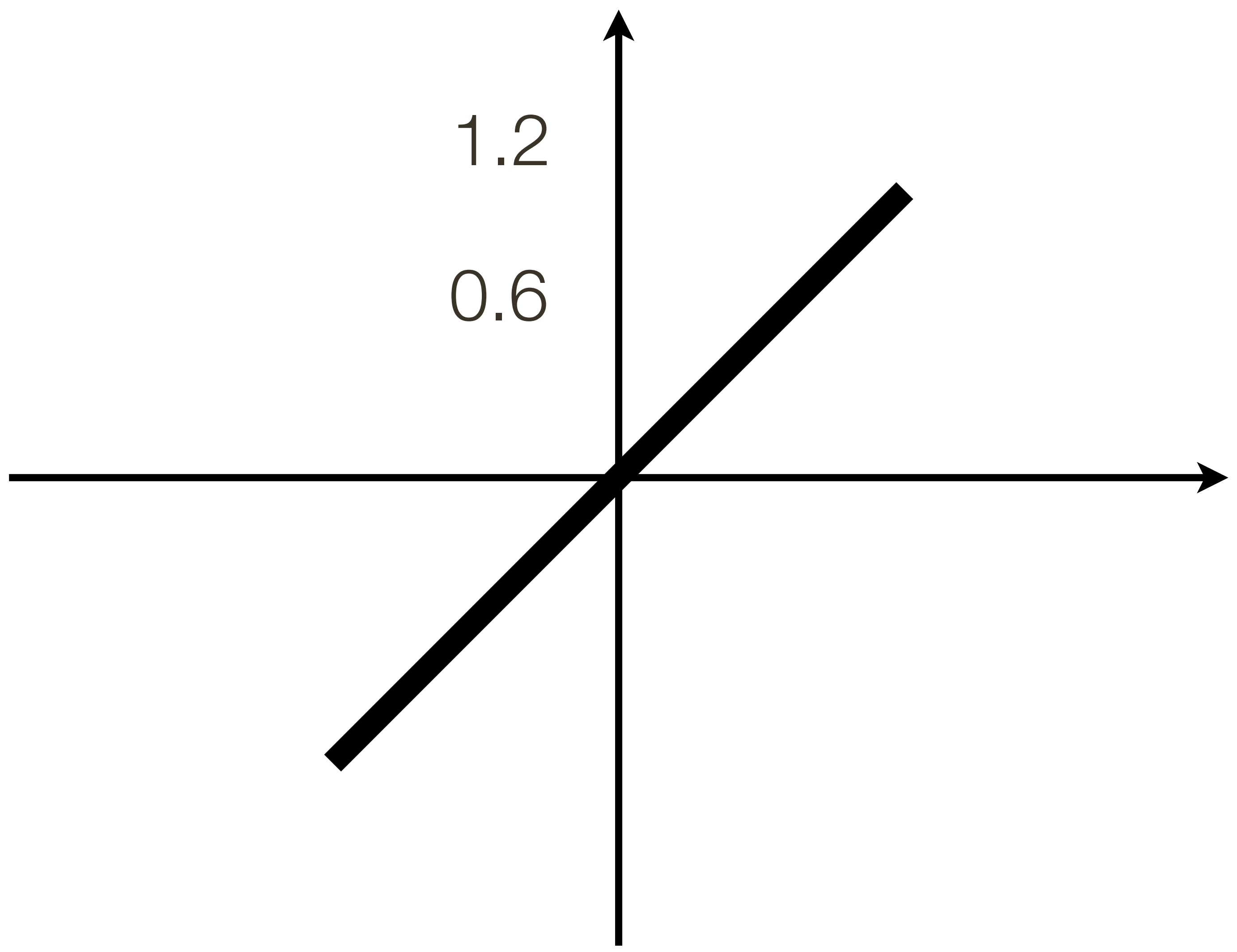
Linear Activation

Recall: $a(x) = x$ => entire neural network is linear, which is **not expressive**

One-layer **Neural Network**



$a(x) = x$



Linear Activation

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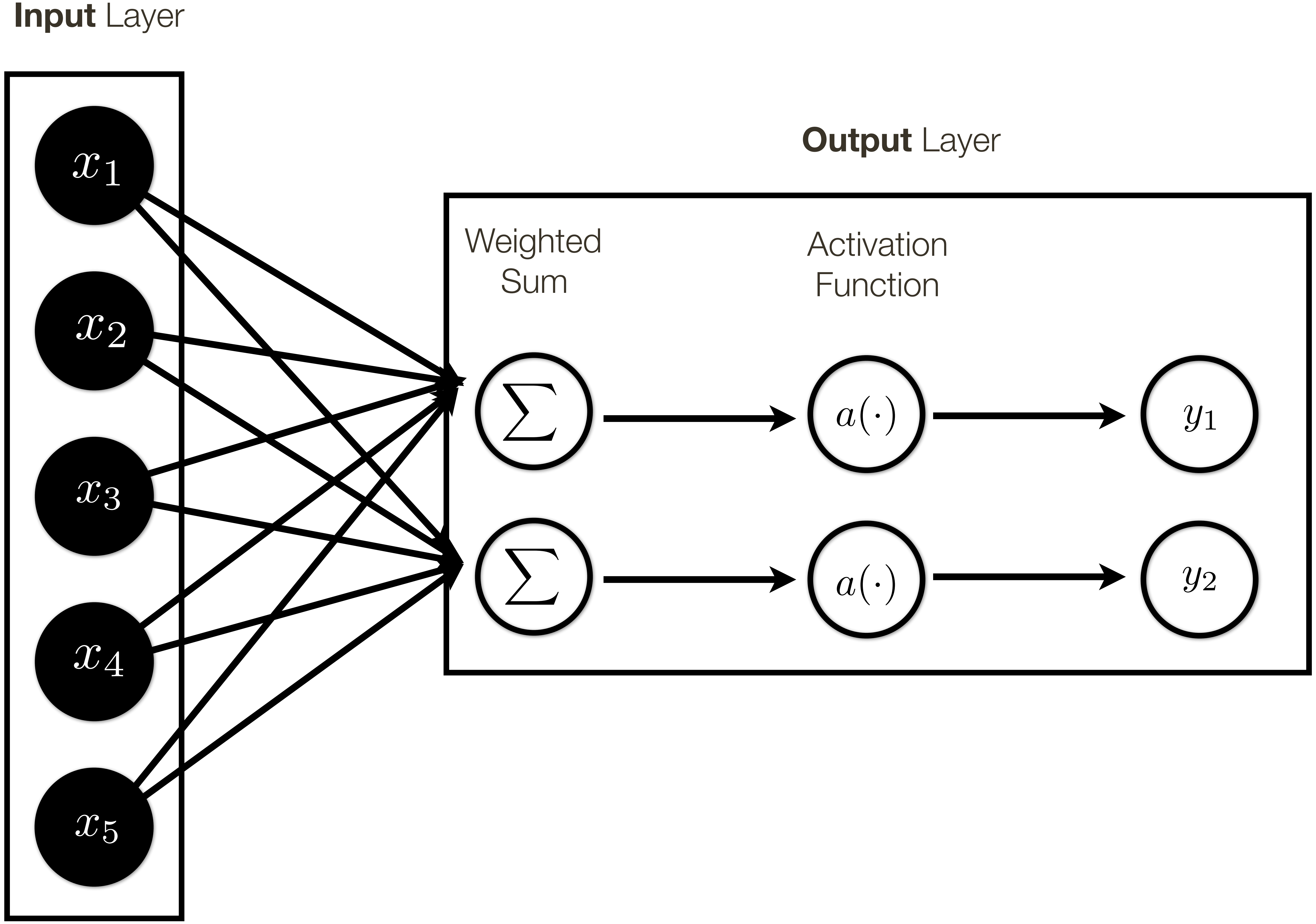
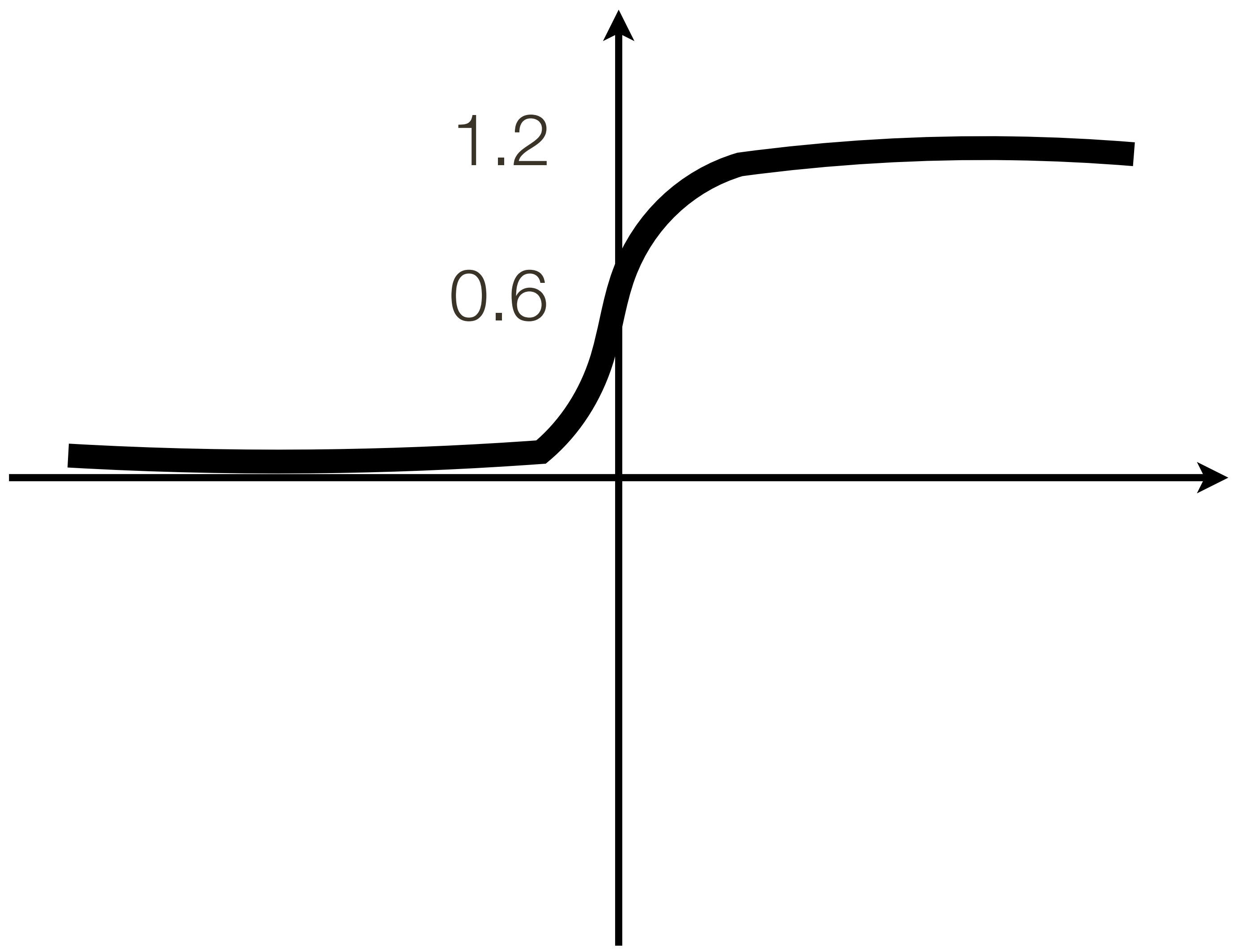


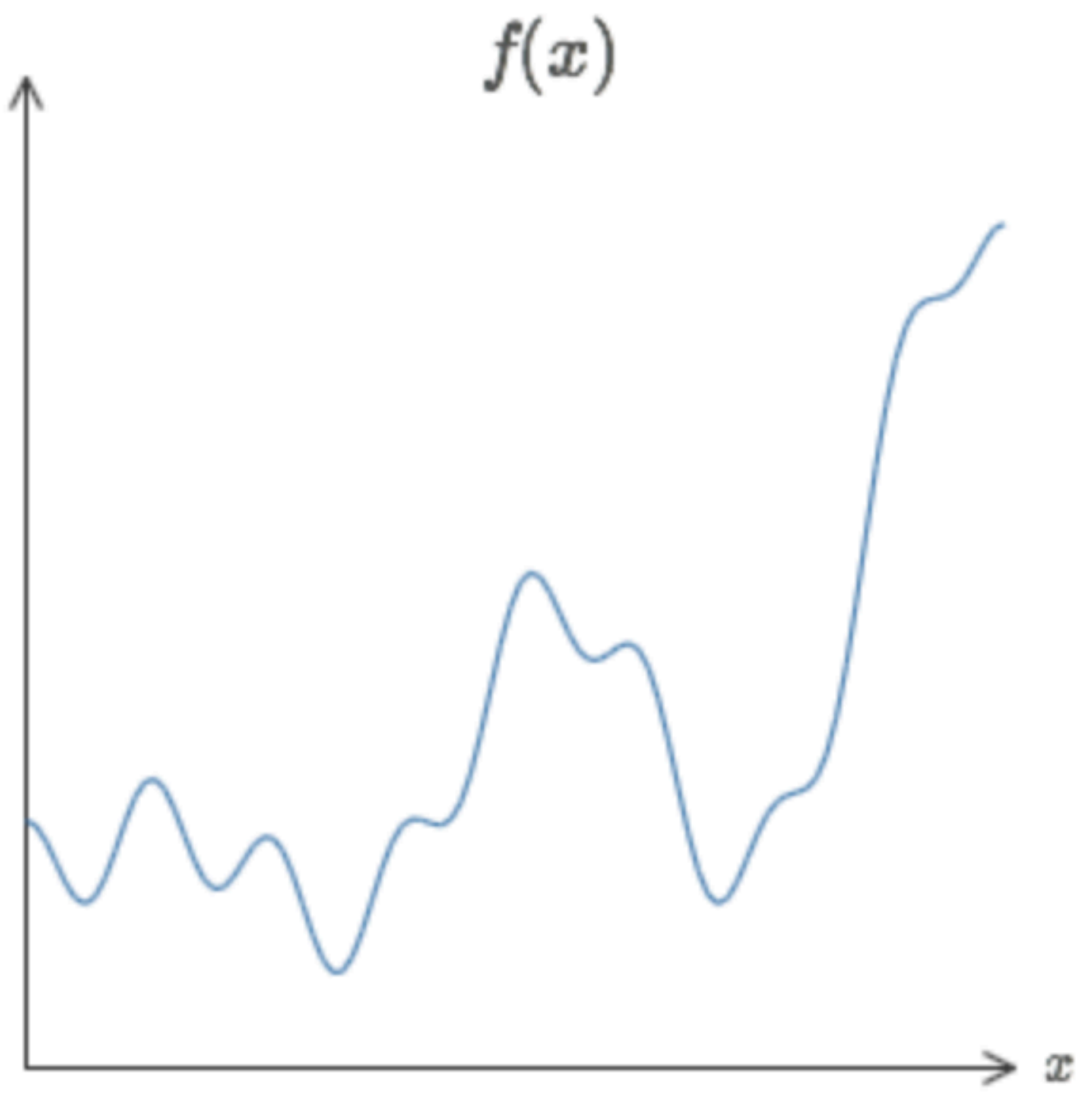
$$a(x) = \mathbf{sigmoid}(x) = \frac{1}{1+e^{-x}}$$



Sigmoid Activation

Light Theory: Neural Network as Universal Approximator

Neural network can arbitrarily approximate *any* continuous function for every value of possible inputs



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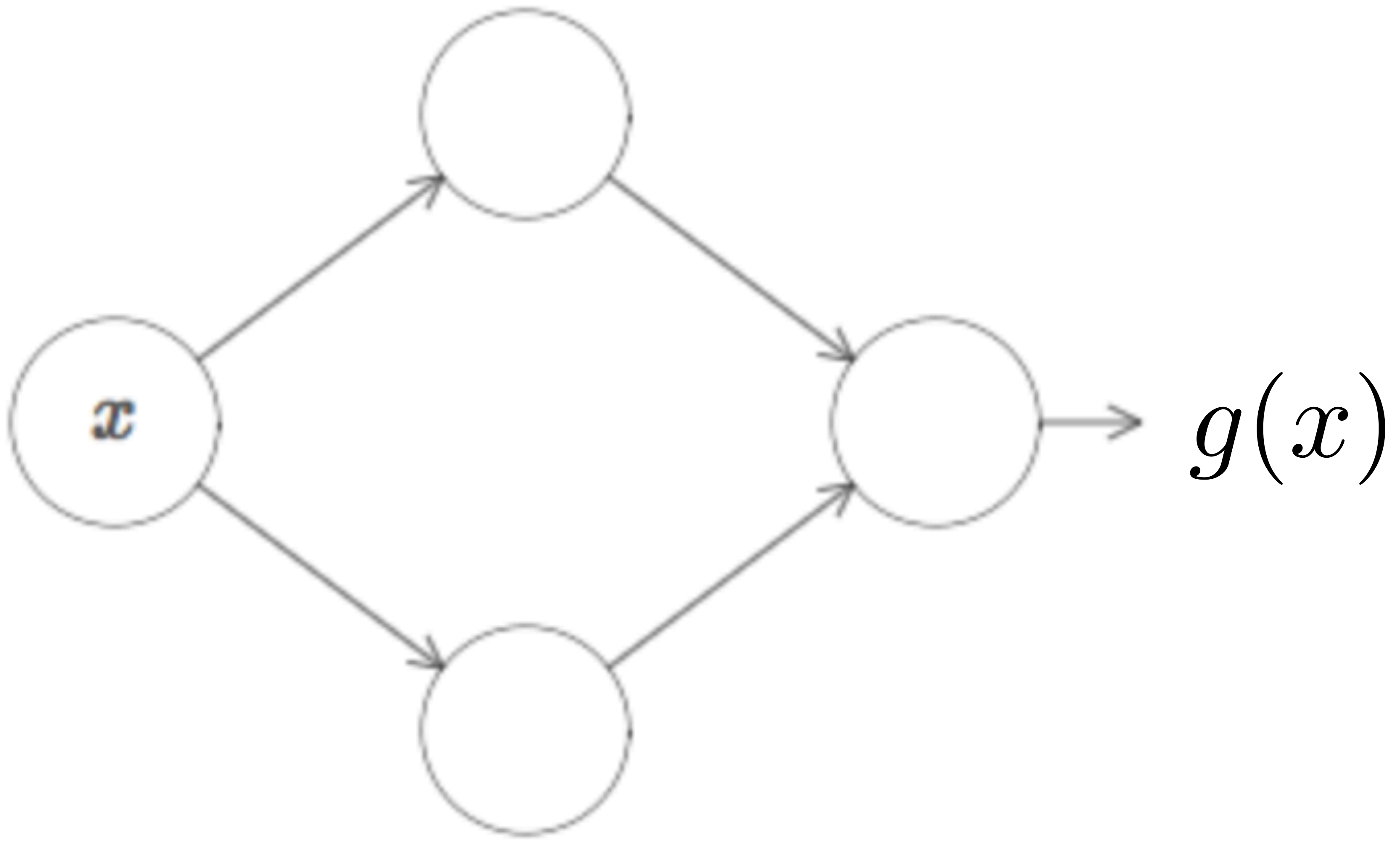

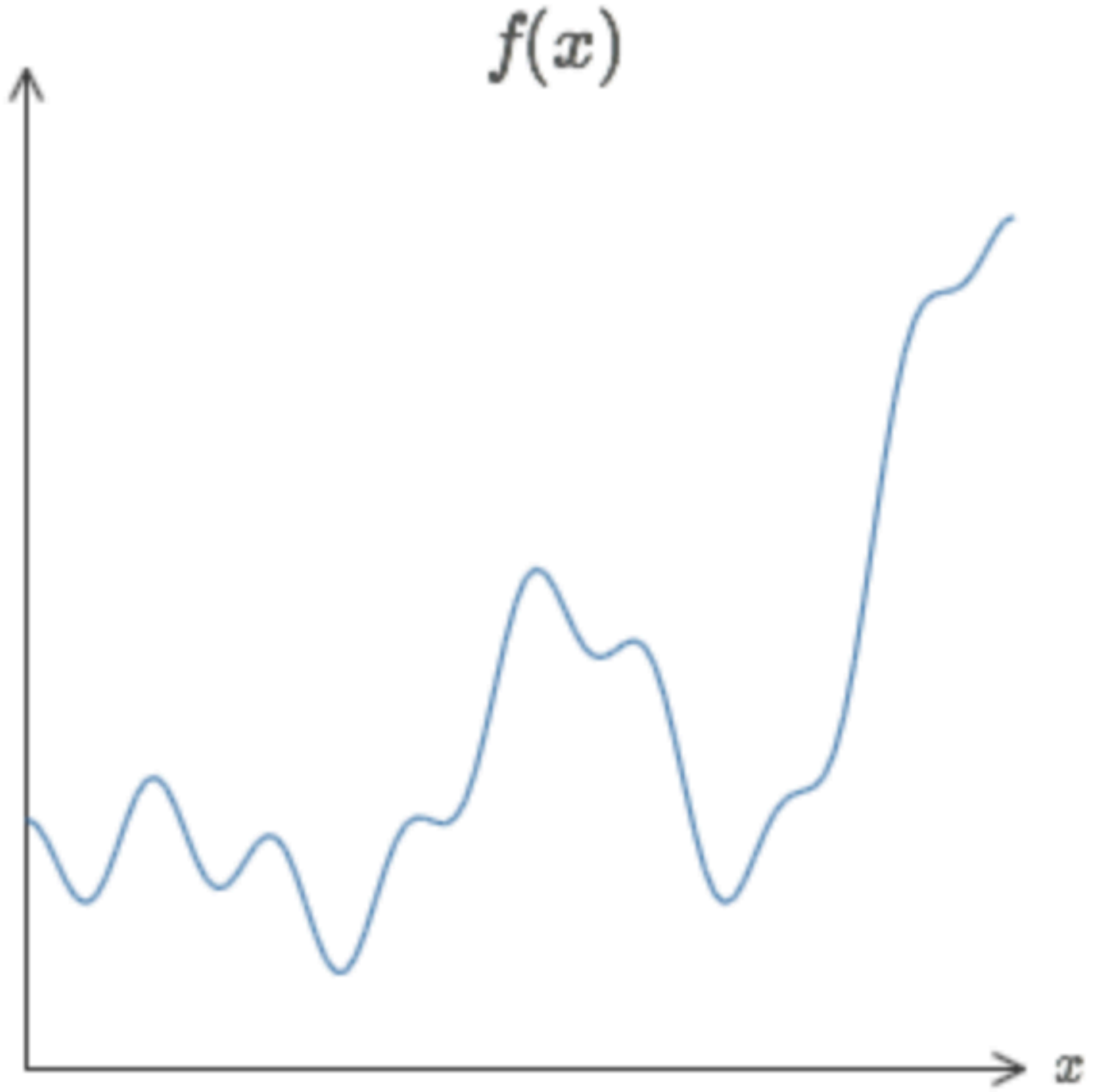

The guarantee is that by using enough hidden neurons we can always find a neural network whose output $g(x)$ satisfies $|g(x) - f(x)| < \epsilon$ for an arbitrarily small ϵ

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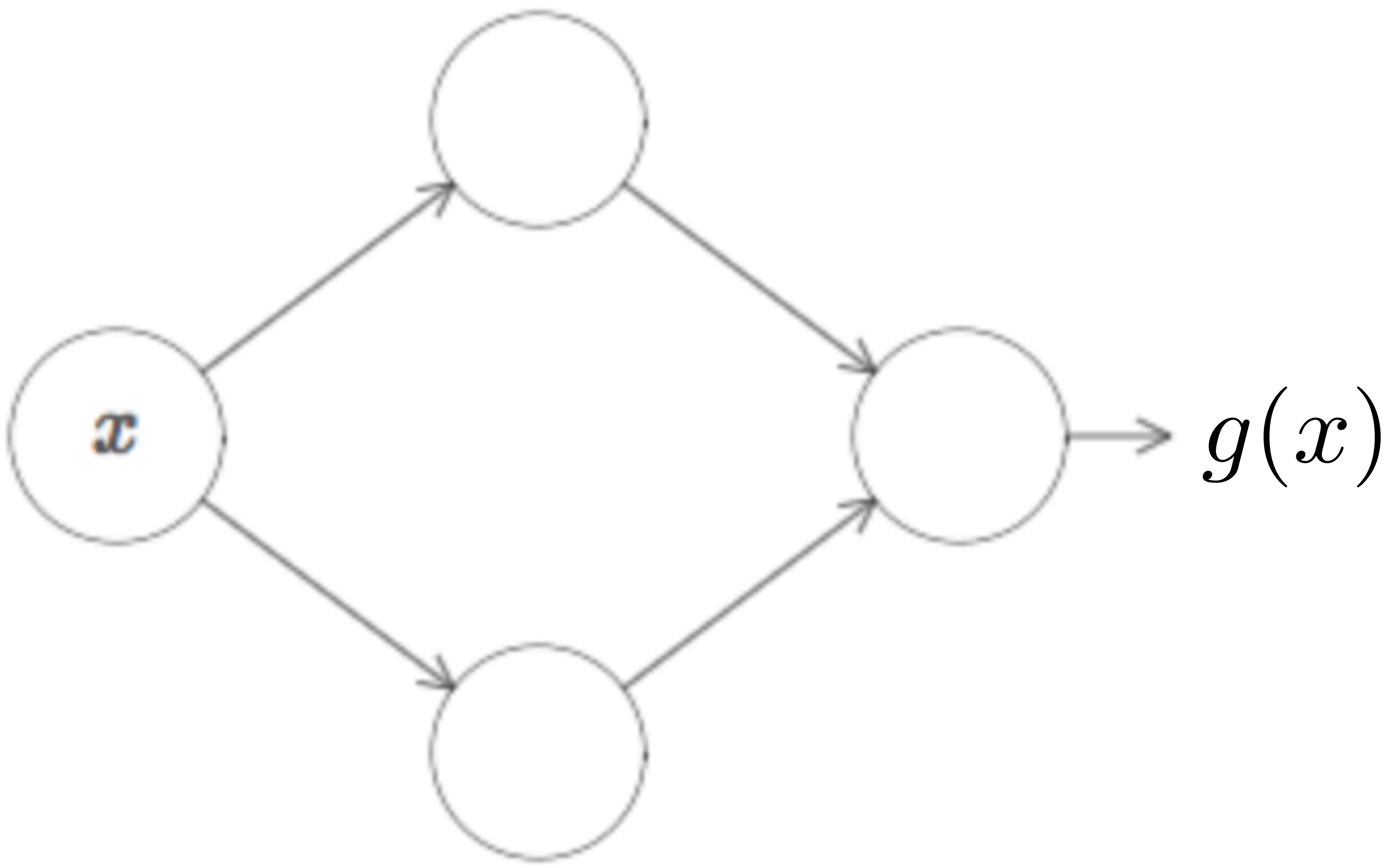
Light Theory: Neural Network as Universal Approximator

Lets start with a simple network: one hidden layer with two hidden neurons and a single output layer with one neuron (with sigmoid activations)



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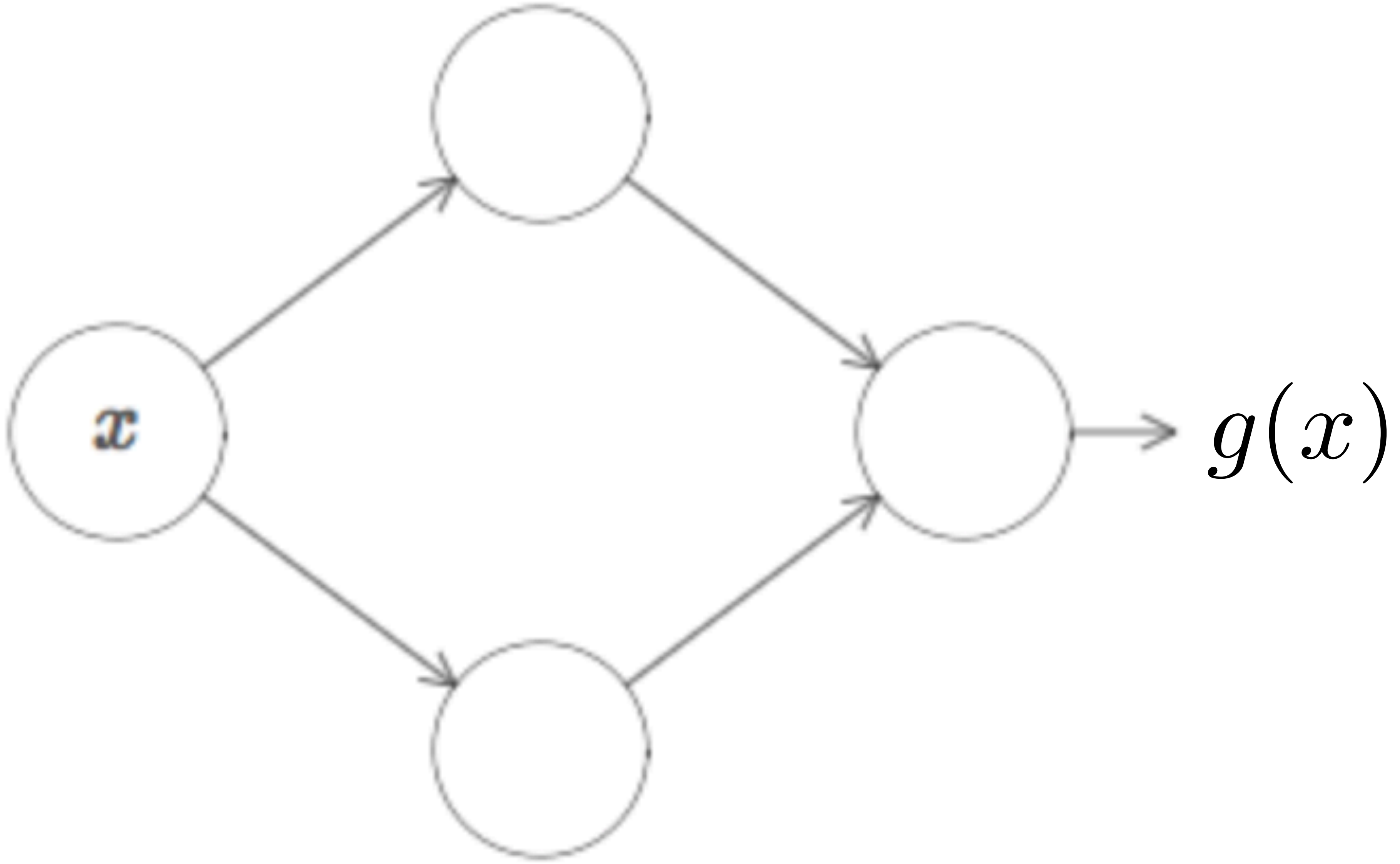
Let's look at output of this (hidden) neuron as a function of parameters (weight, bias)



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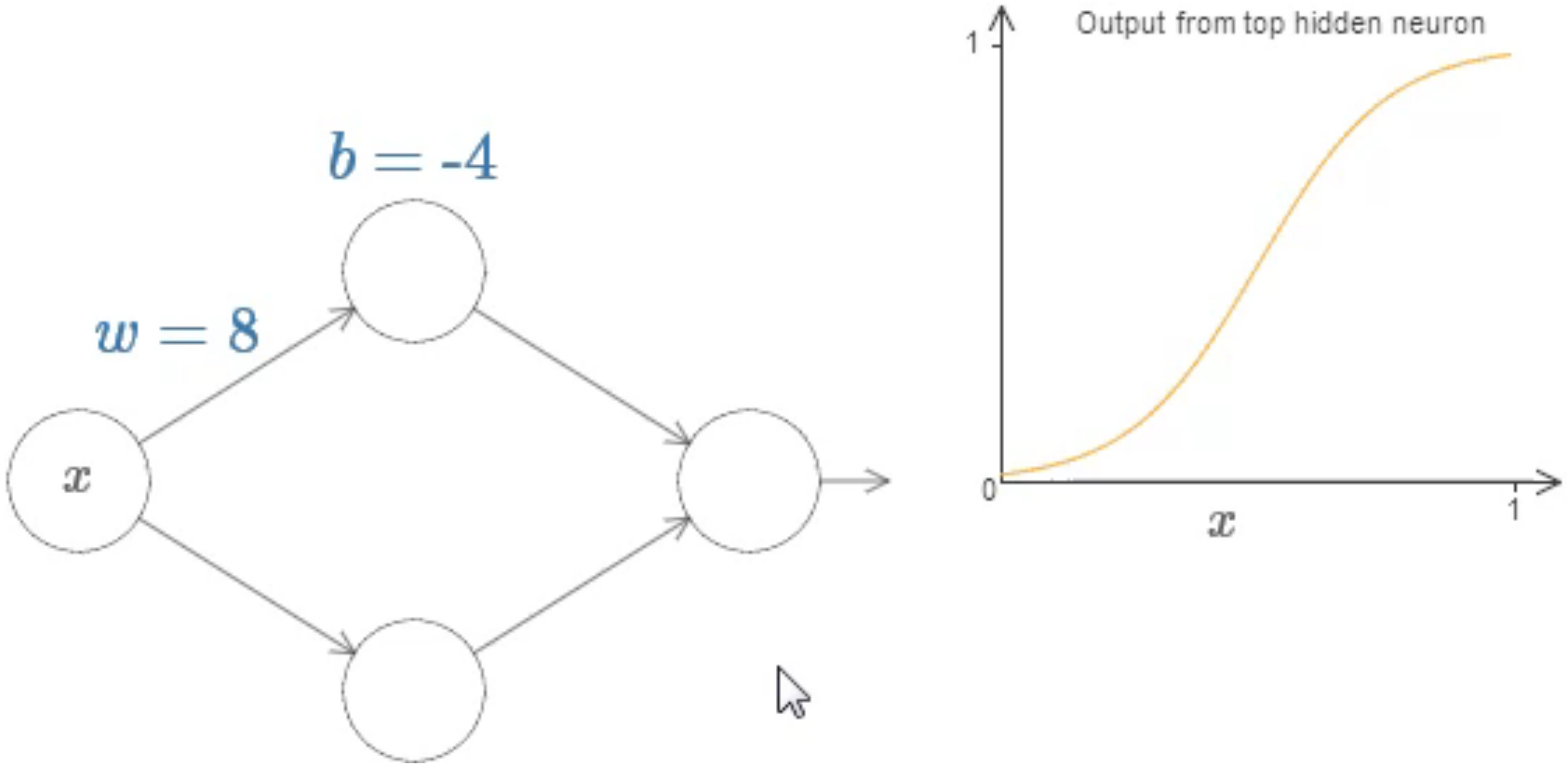

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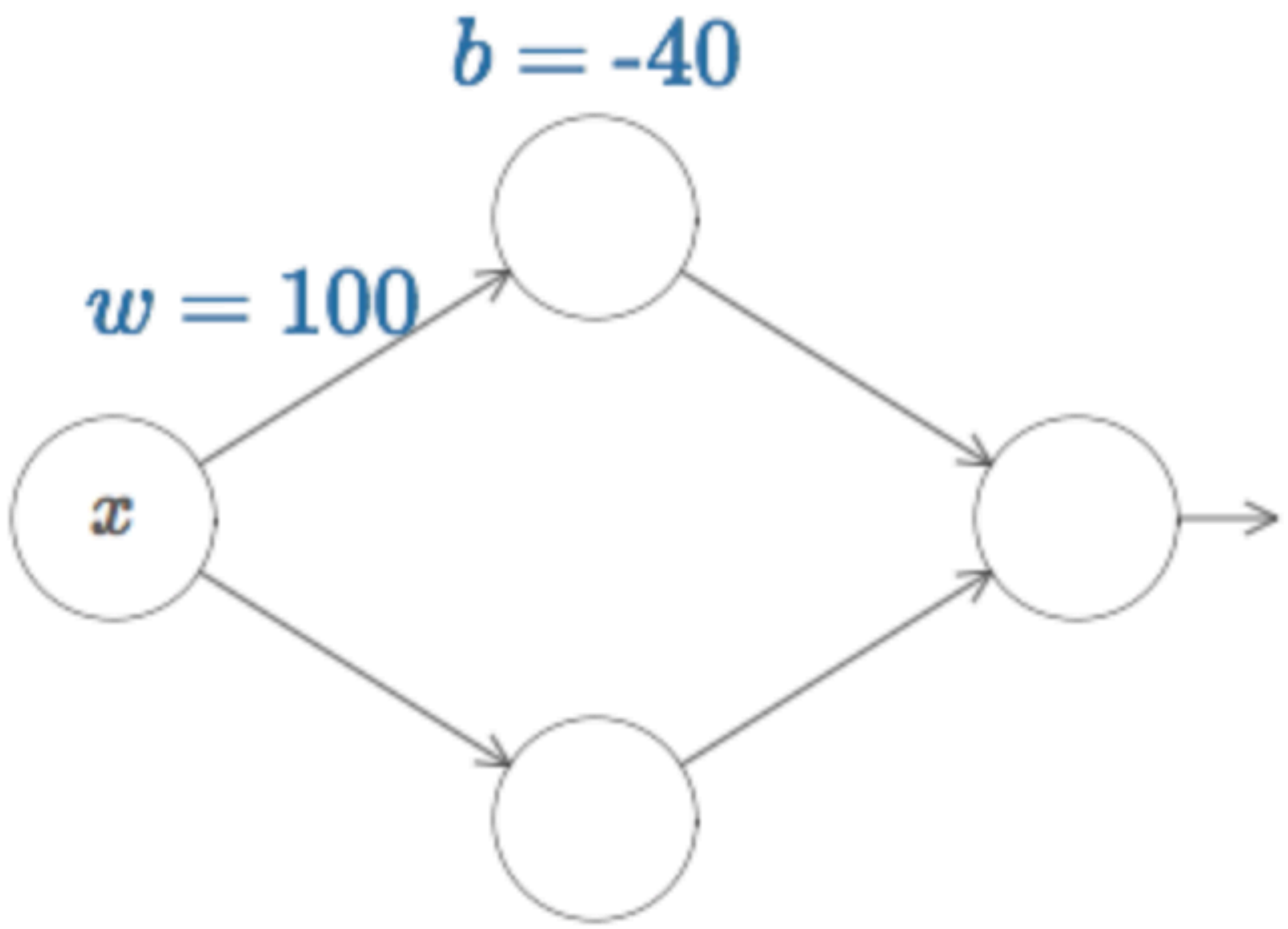
Light Theory: Neural Network as Universal Approximator

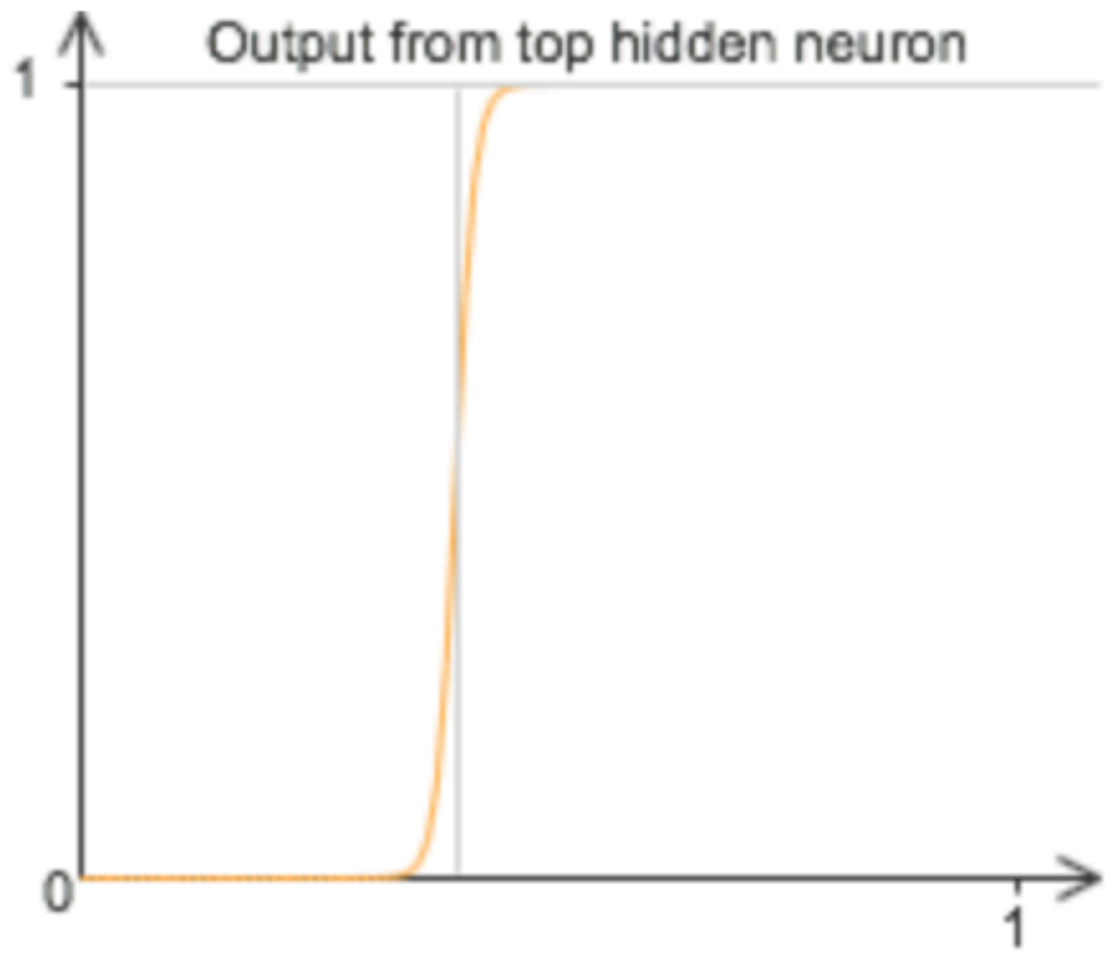
By dialing up the weight (e.g. $w = 999$) we can actually create a “step” function

It is easier to work with sums of step functions, so we can assume that every neuron outputs a step function.

Location of the step?

$$s = -\frac{b}{w}$$





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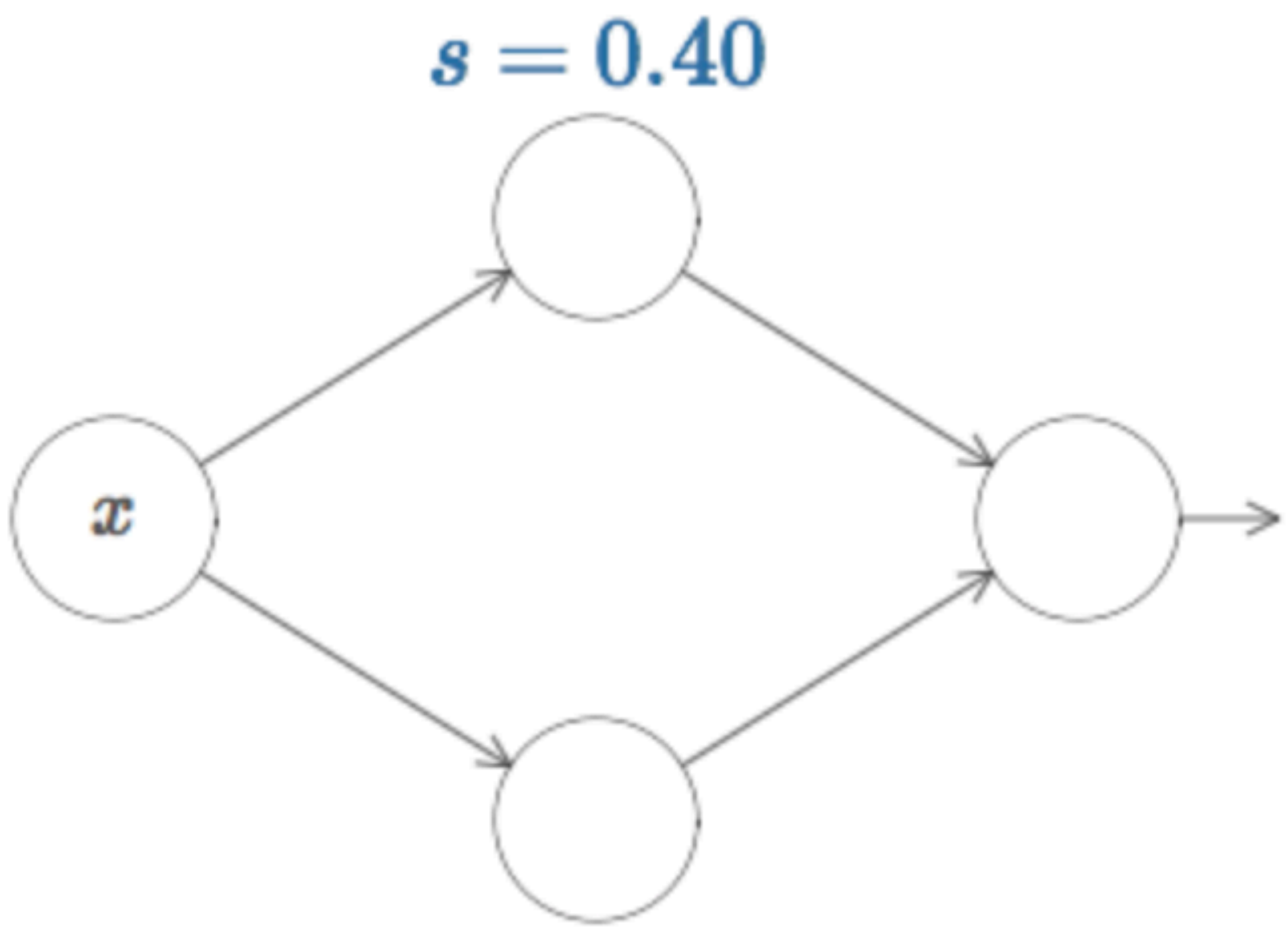

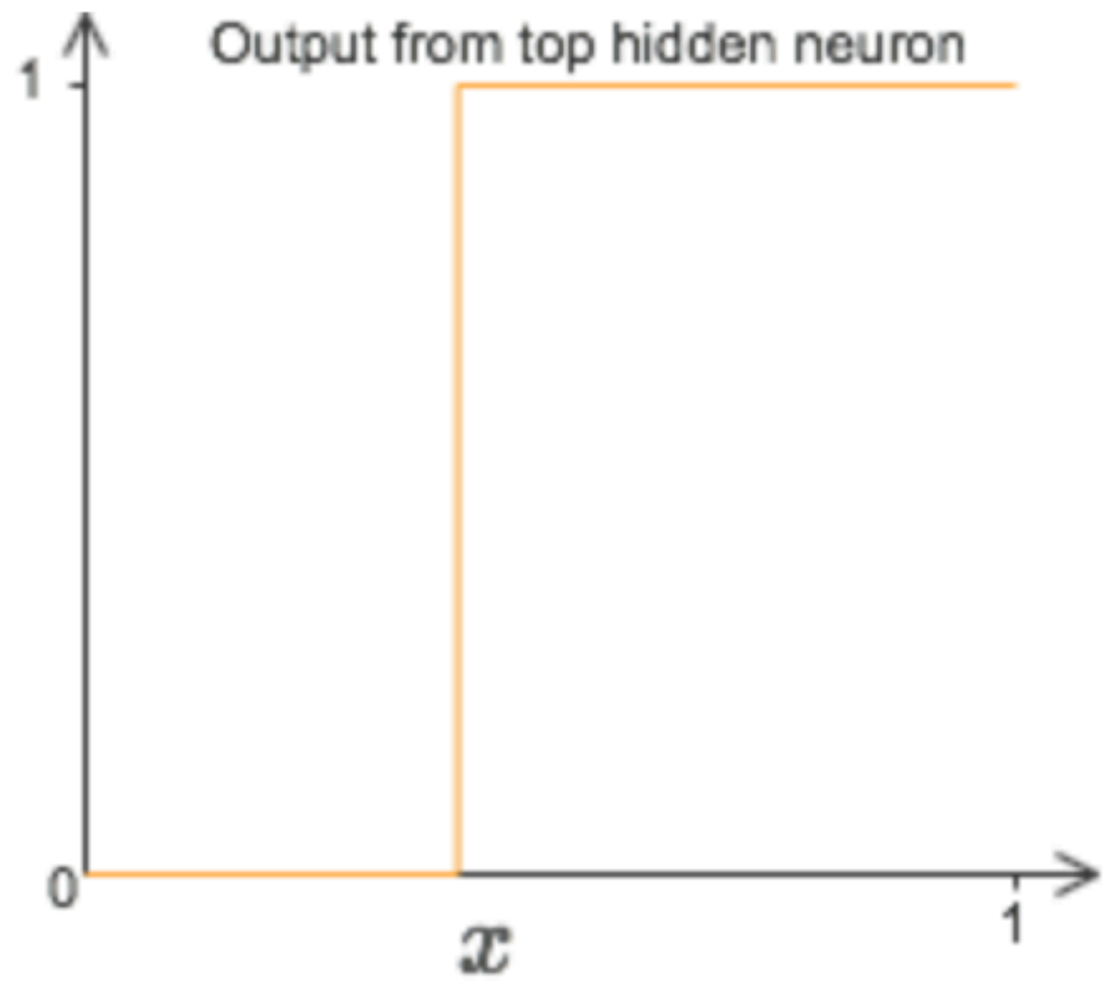

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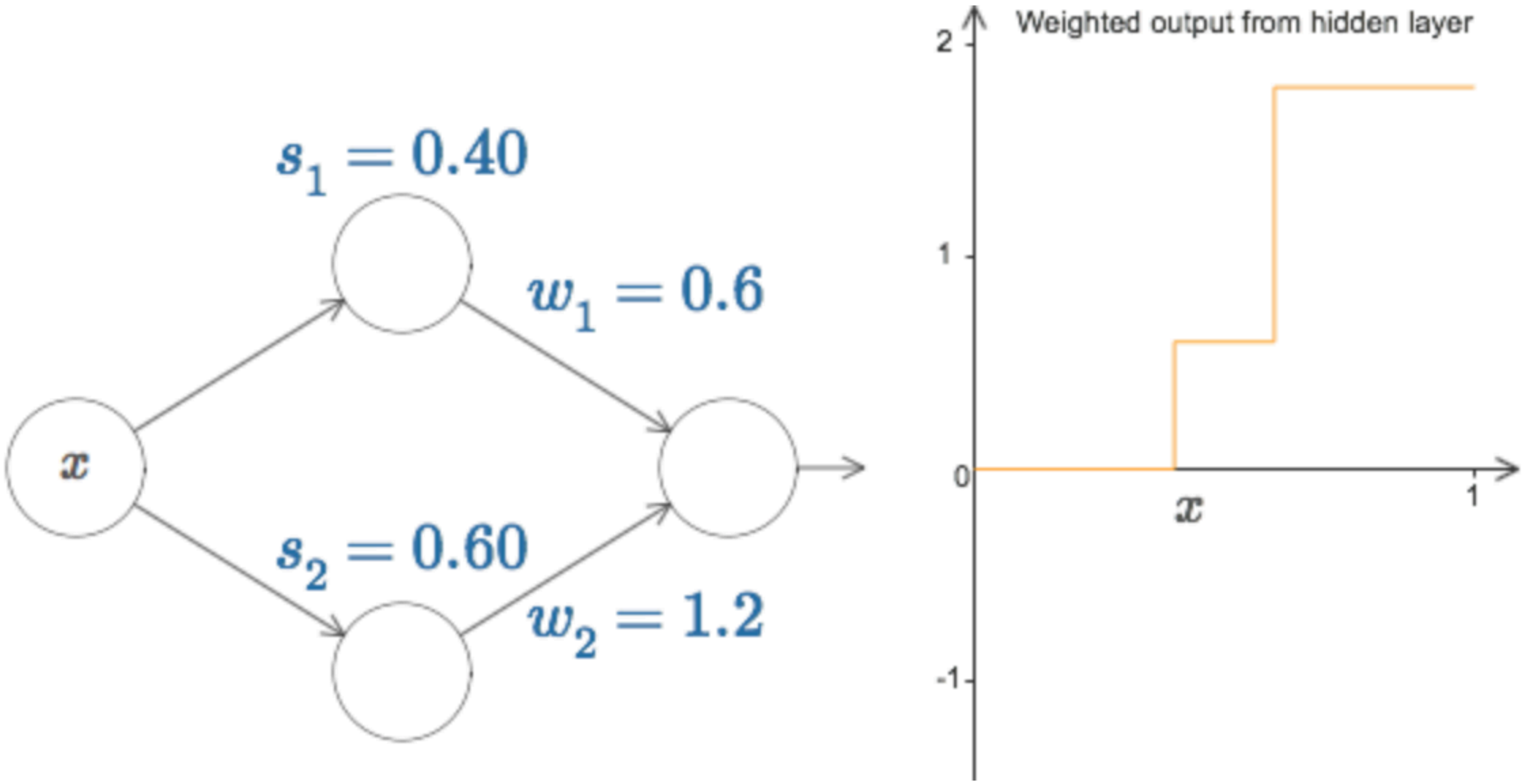
Light Theory: Neural Network as Universal Approximator

The output neuron is a **weighted combination of step functions** (assuming bias for that layer is 0)



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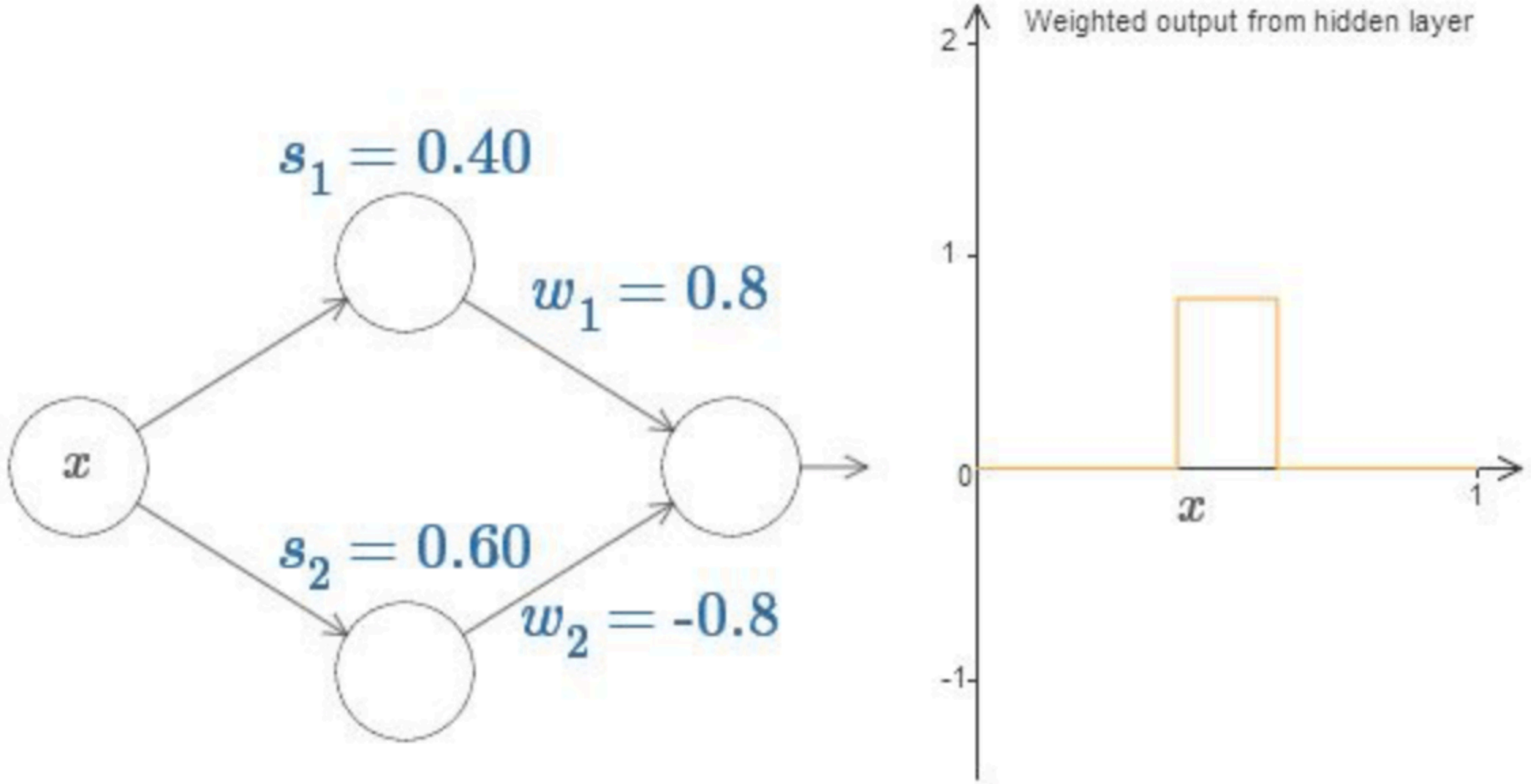

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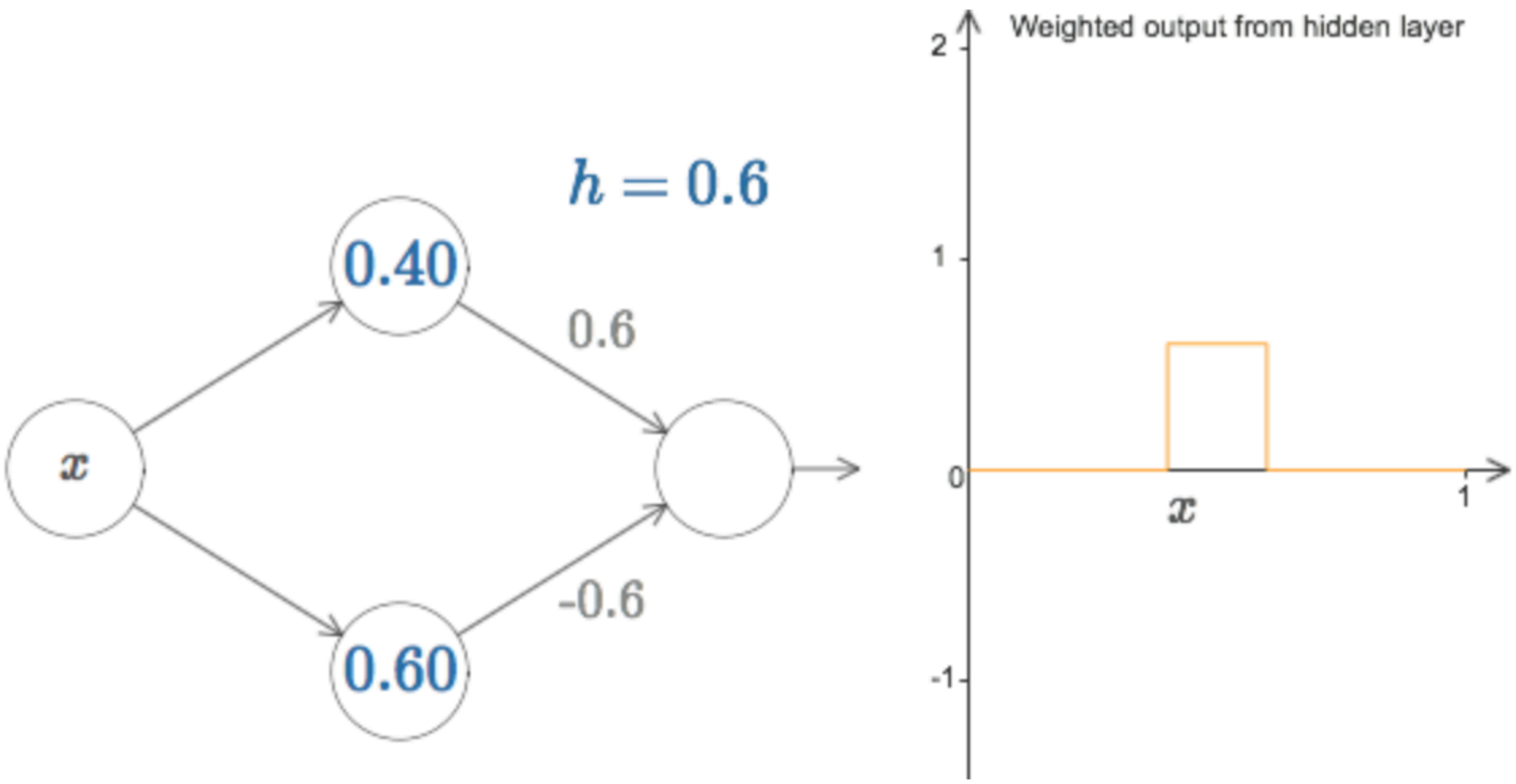

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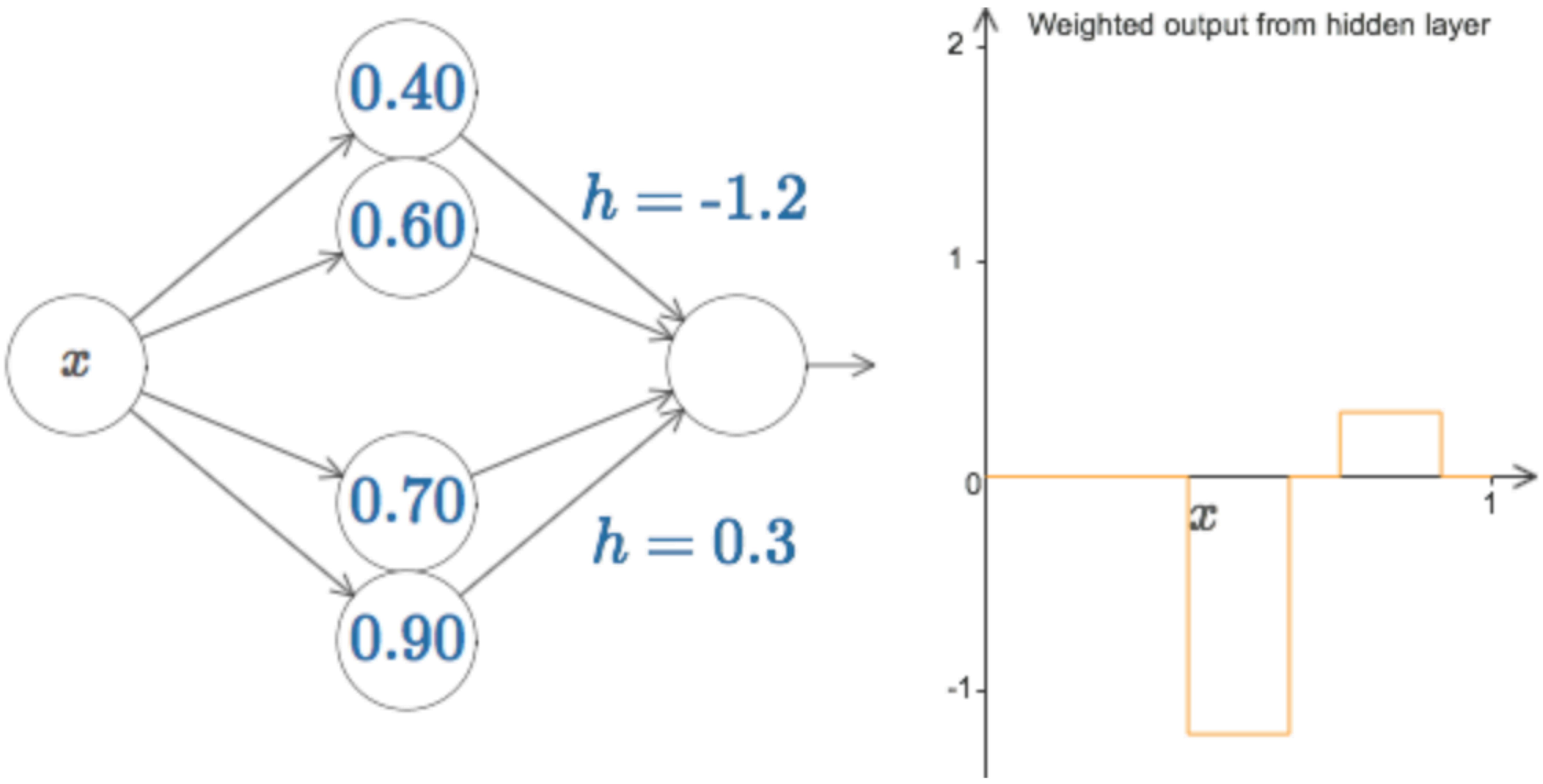

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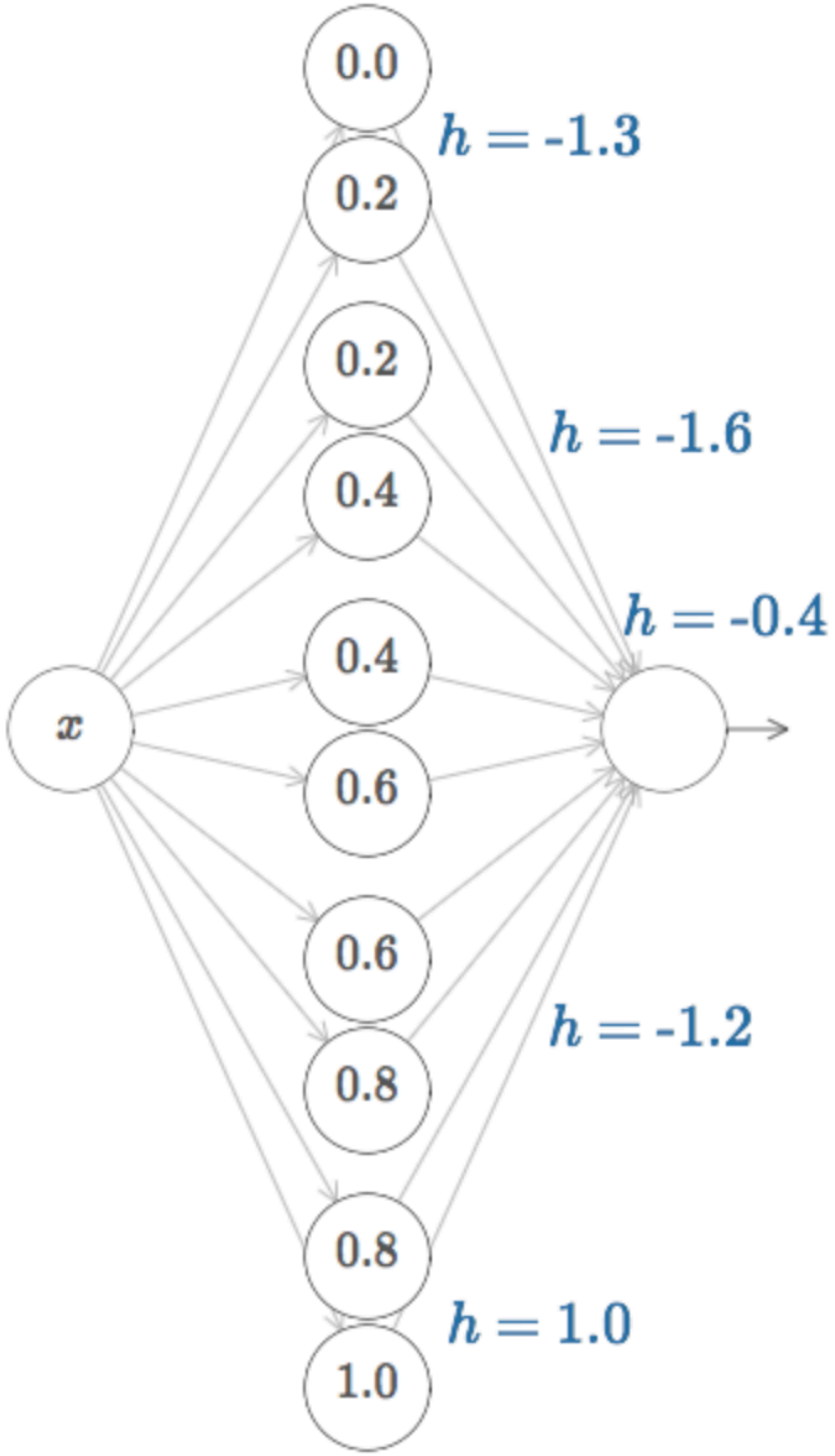

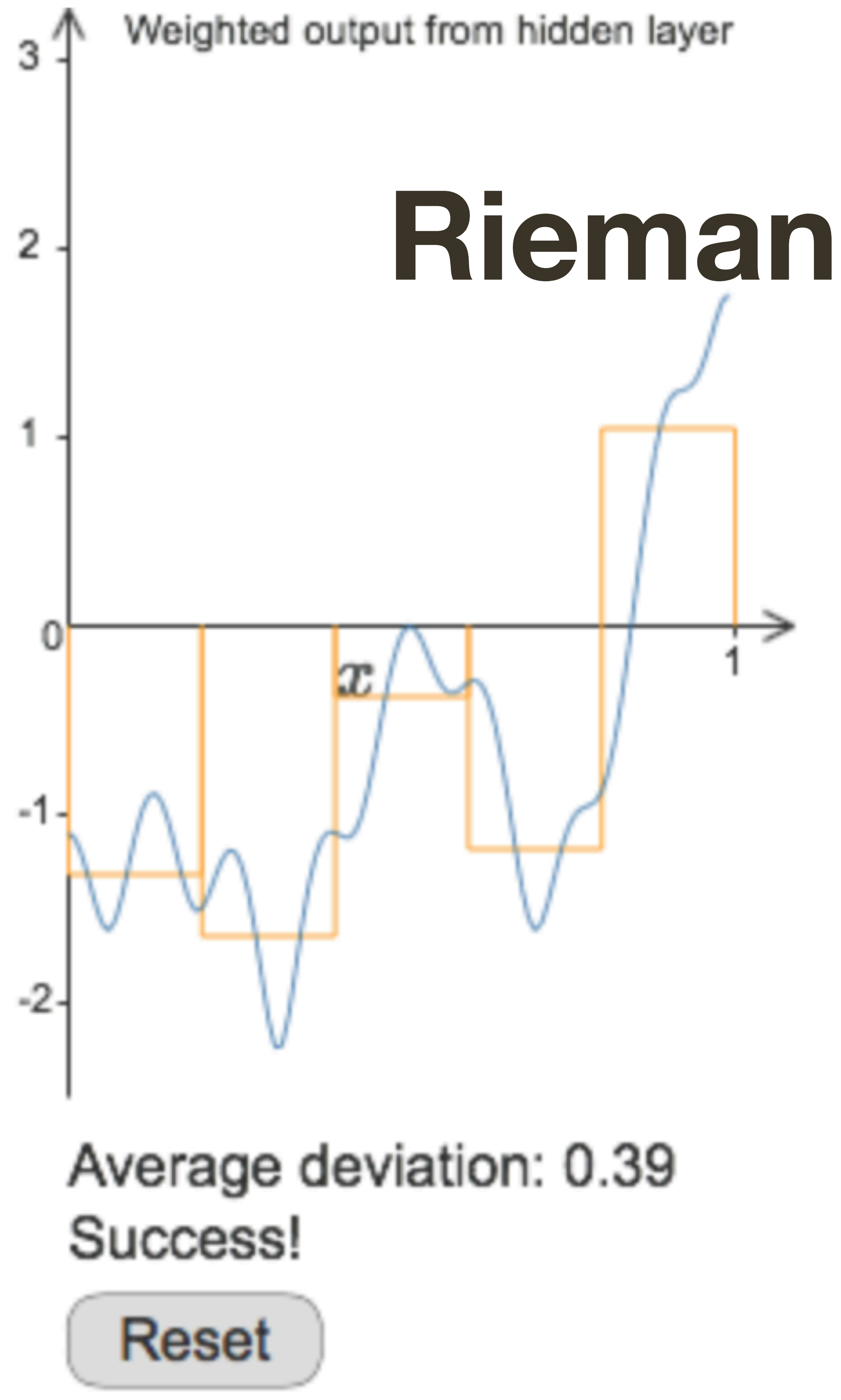

Riemann sum approximation

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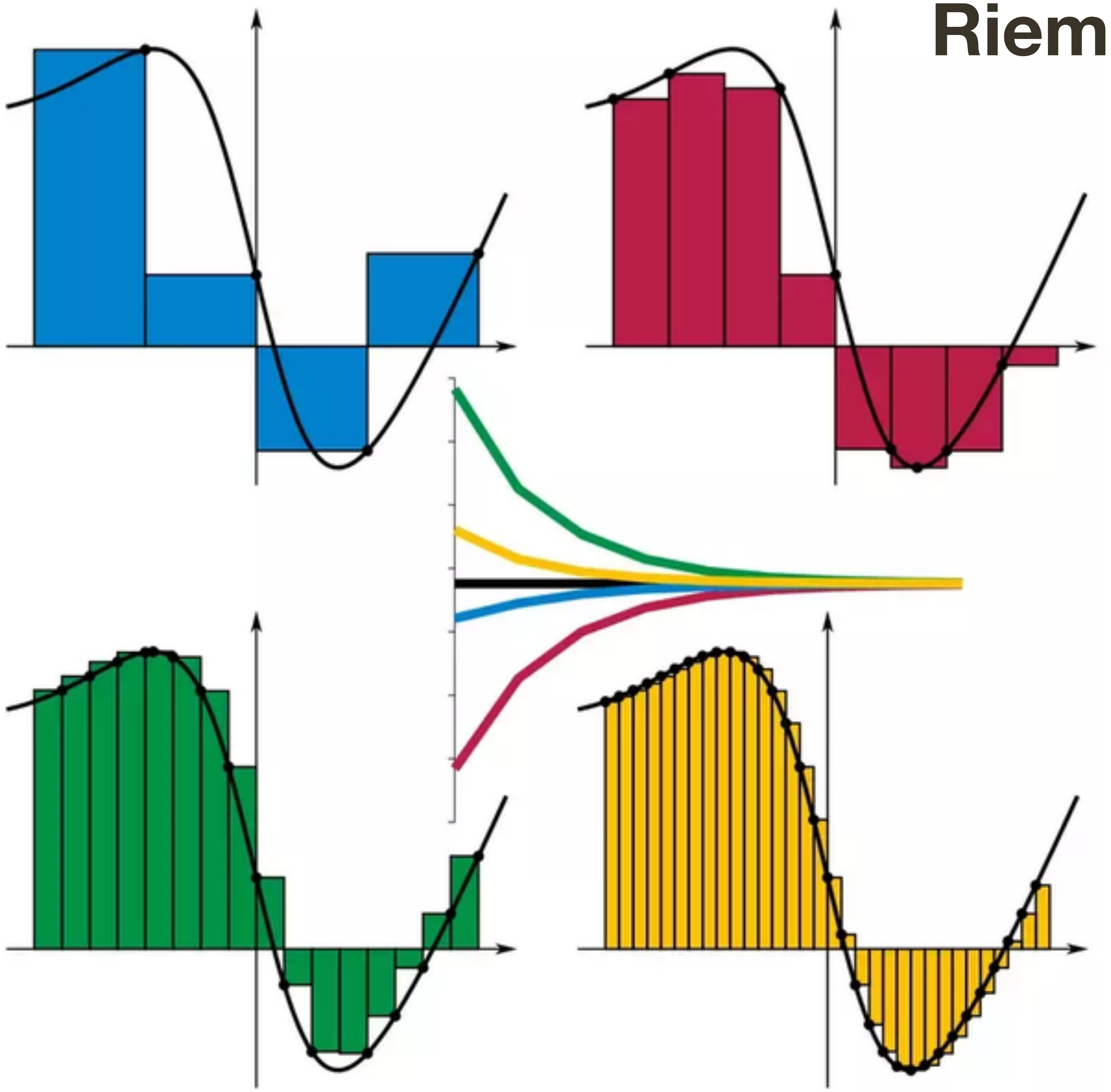

Riemann sum approximation

Light Theory: Neural Network as Universal Approximator

Conditions needed for proof to hold: Activation function needs to be well defined

$$\lim_{x \to \infty} a(x) = A$$

$$\lim_{x \to -\infty} a(x) = B$$

$$A \neq B$$

*slide adopted from http://neuralnetworksanddeeplearning.com/chap4.html

Light Theory: Neural Network as Universal Approximator

Universal Approximation Theorem: Single hidden layer can approximate any continuous function with compact support to arbitrary accuracy, when the width goes to infinity.

[Hornik *et al*., 1989]

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Universal Approximation Theorem (revised): A network of infinite depth with a hidden layer of size $d+1$ neurons, where d is the dimension of the input space, can approximate any continuous function.

[Lu *et al*., NIPS 2017]

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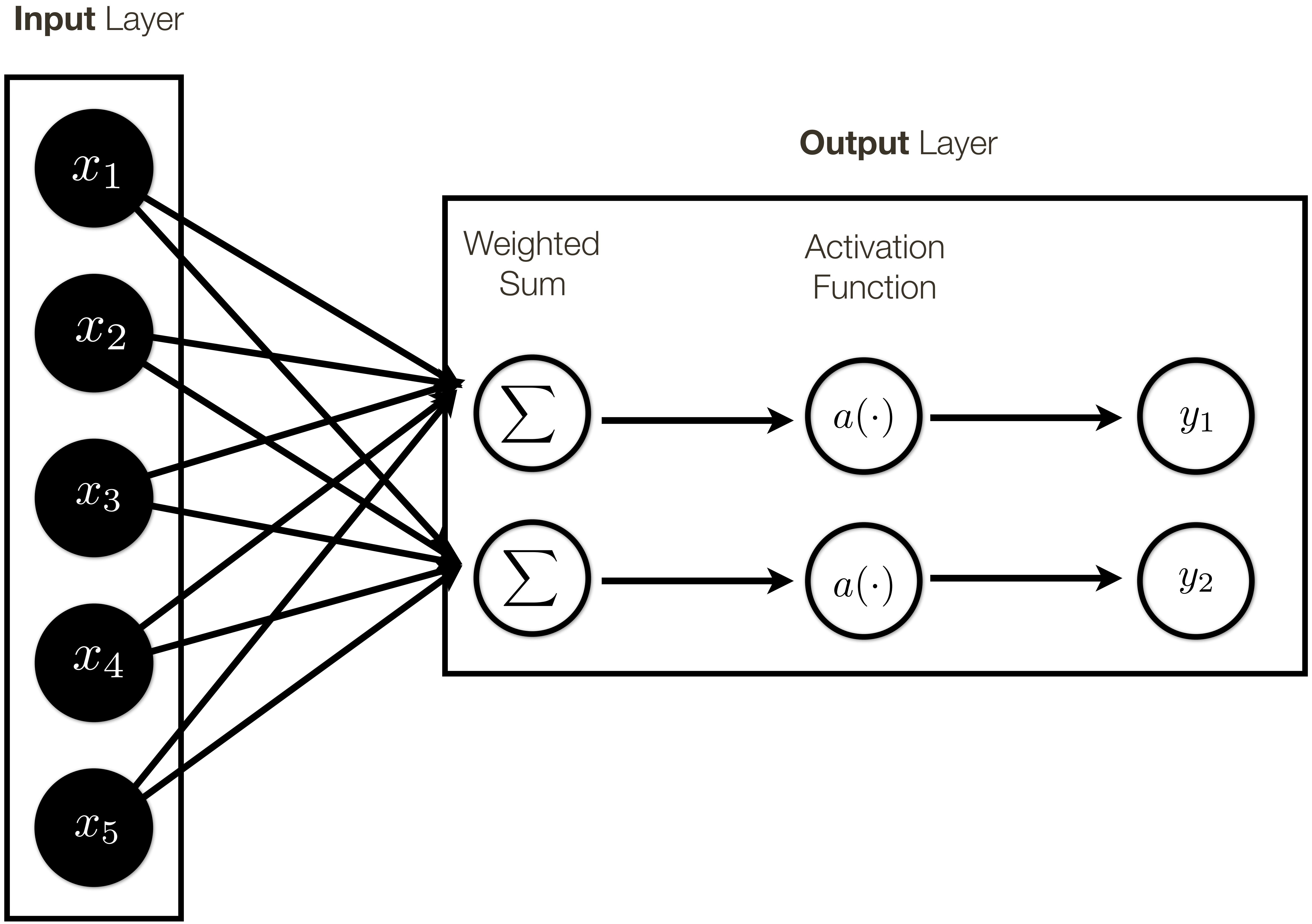
[Lu *et al*., NIPS 2017]

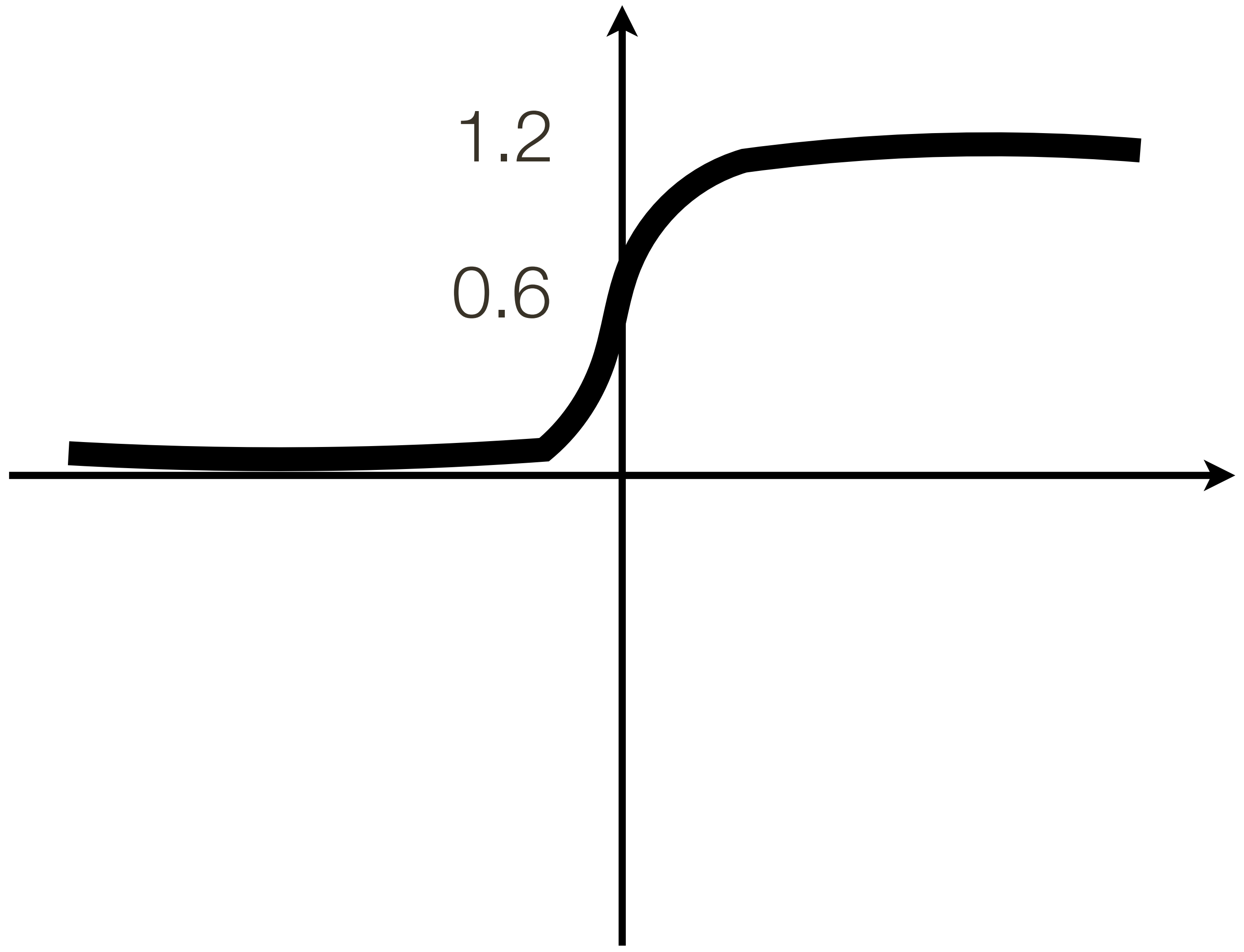
Universal Approximation Theorem (further revised): ResNet with a single hidden unit and infinite depth can approximate any continuous function.

[Lin and Jegelka, NIPS 2018]

One-layer **Neural Network**



$$a(x) = \mathbf{sigmoid}(x) = \frac{1}{1+e^{-x}}$$



Sigmoid Activation

Learning Parameters of One-layer Neural Network

$$\mathcal{L}(\mathbf{W}, \mathbf{b}) = \sum_{d=1}^{|D_{train}|} \left(\textbf{sigmoid}\left(\mathbf{W}^T \mathbf{x}^{(d)} + \mathbf{b} \right) - \mathbf{y}^{(d)} \right)^2$$

$$\mathbf{W}^*, \mathbf{b}^* = \arg\min \mathcal{L}(\mathbf{W}, \mathbf{b})$$

Solution:

$$\frac{\partial \mathcal{L}(\mathbf{W}, \mathbf{b})}{\partial w_{ji}} = \frac{\partial}{\partial w_{ji}} \sum_{d=1}^{|D_{train}|} \left(\textbf{sigmoid}\left(\mathbf{W}^T \mathbf{x}^{(d)} + \mathbf{b} \right) - \mathbf{y}^{(d)} \right)^2$$

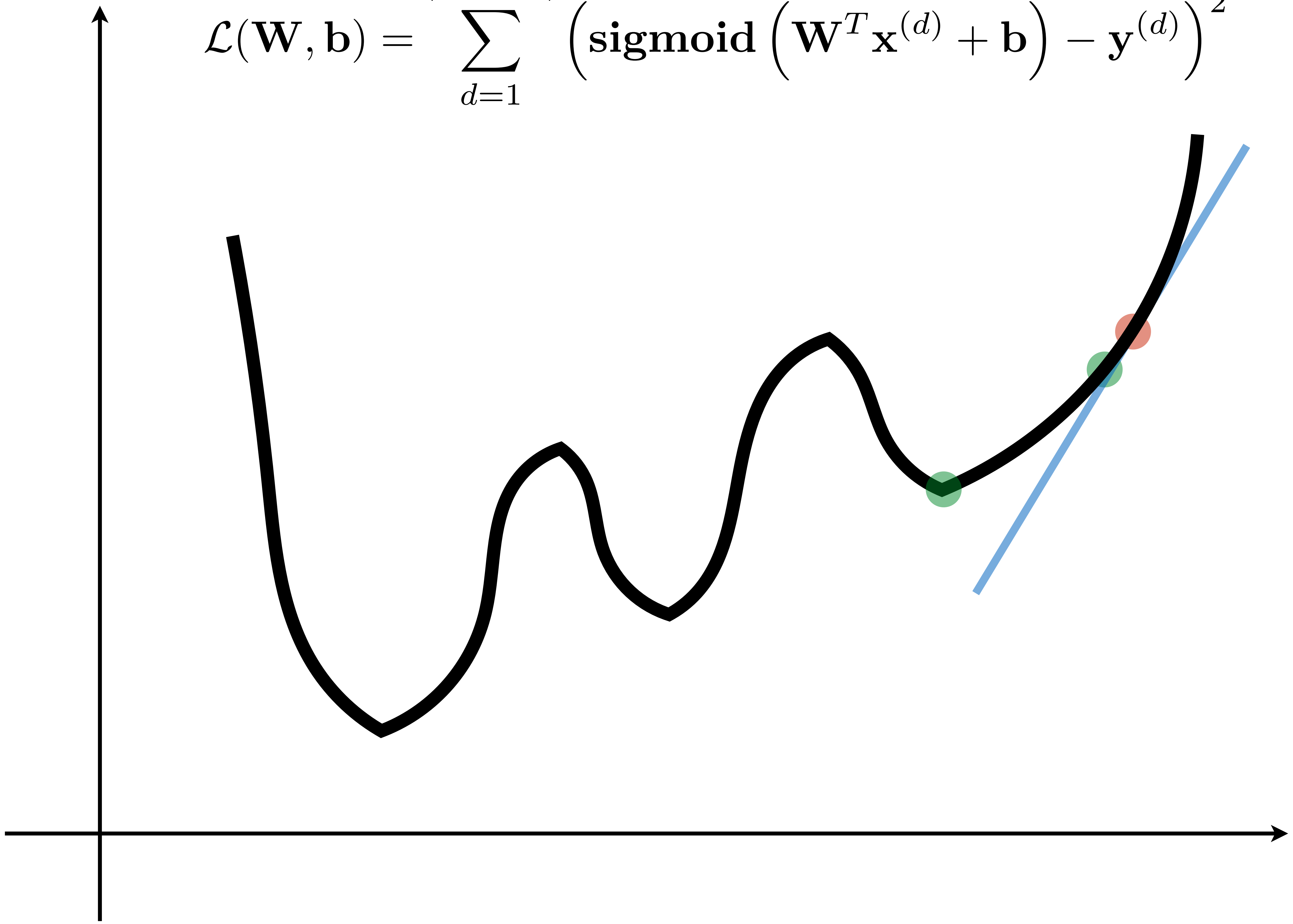
$$\frac{\partial \mathcal{L}(\mathbf{W}, \mathbf{b})}{\partial w_{ji}} = \frac{\partial}{\partial w_{ji}} \sum_{d=1}^{|D_{train}|} \left(\textbf{sigmoid}\left(\mathbf{W}^T \mathbf{x}^{(d)} + \mathbf{b} \right) - \mathbf{y}^{(d)} \right)^2 = 0$$

Problem: No closed form solution $\frac{\partial \mathcal{L}(\mathbf{W}, \mathbf{b})}{\partial w_{ji}} = 0$

*slide adopted from V. Ordonex

Gradient Descent (review)

$$\mathcal{L}(\mathbf{W},\mathbf{b}) = \sum_{d=1}^{|D_{train}|} \left(\textbf{sigmoid}\left(\mathbf{W}^T\mathbf{x}^{(d)}+\mathbf{b}\right) - \mathbf{y}^{(d)}\right)^2$$



1. Start from random value of $\boxed{\mathbf{W}_0, \mathbf{b}_0}$

For $k=0$ to max number of iterations

2. Compute gradient of the loss with respect to previous (initial) parameters:

$$\nabla\, \mathcal{L}(\mathbf{W},\mathbf{b})\big|_{\mathbf{W}=\mathbf{W}_k,\mathbf{b}=\mathbf{b}_k}$$

3. Re-estimate the parameters

$$\mathbf{W}_{k+1} = \mathbf{W}_k - \underline{\lambda} \left.\frac{\partial \mathcal{L}(\mathbf{W},\mathbf{b})}{\partial \mathbf{W}}\right|_{\mathbf{W}=\mathbf{W}_k,\mathbf{b}=\mathbf{b}_k}$$

$$\mathbf{b}_{k+1} = \mathbf{b}_k - \underline{\lambda} \left.\frac{\partial \mathcal{L}(\mathbf{W},\mathbf{b})}{\partial \mathbf{b}}\right|_{\mathbf{W}=\mathbf{W}_k,\mathbf{b}=\mathbf{b}_k}$$

λ - is the learning rate

*slide adopted from V. Ordonex

Stochastic Gradient Descent (review)

$$\frac{\partial \mathcal{L}(\mathbf{W}, \mathbf{b})}{\partial w_{ji}} = \frac{\partial}{\partial w_{ji}} \boxed{\sum_{d=1}^{|D_{train}|}} \left(\mathbf{sigmoid} \left(\mathbf{W}^T \mathbf{x}^{(d)} + \mathbf{b} \right) - \mathbf{y}^{(d)} \right)^2$$

Problem: For large datasets computing sum is expensive

Solution: Compute approximate gradient with mini-batches of much smaller size (as little as 1-example sometimes)

Problem: How do we compute the actual gradient?

Numerical Differentiation

$\mathbf{1}_i$ - Vector of all zeros, except for one 1 in i-th location

We can approximate the gradient numerically, using:

$$\frac{\partial f(\mathbf{x})}{\partial x_i} \approx \lim_{h \to 0} \frac{f(\mathbf{x} + h\mathbf{1}_i) - f(\mathbf{x})}{h}$$

*slide adopted from T. Chen, H. Shen, A. Krishnamurthy CSE 599G1 lecture at UWashington

Numerical Differentiation

$\mathbf{1}_i$ - Vector of all zeros, except for one 1 in i-th location

$\mathbf{1}_{ij}$ - Matrix of all zeros, except for one 1 in (i,j)-th location

We can approximate the gradient numerically, using:

$$\frac{\partial \mathcal{L}(\mathbf{W}, \mathbf{b})}{\partial w_{ij}} \approx \lim_{h \to 0} \frac{\mathcal{L}(\mathbf{W} + h\mathbf{1}_{ij}, \mathbf{b}) - \mathcal{L}(\mathbf{W}, \mathbf{b})}{h} \qquad \frac{\partial \mathcal{L}(\mathbf{W}, \mathbf{b})}{\partial b_j} \approx \lim_{h \to 0} \frac{\mathcal{L}(\mathbf{W}, \mathbf{b} + h\mathbf{1}_j) - \mathcal{L}(\mathbf{W}, \mathbf{b})}{h}$$

Even better, we can use central differencing:

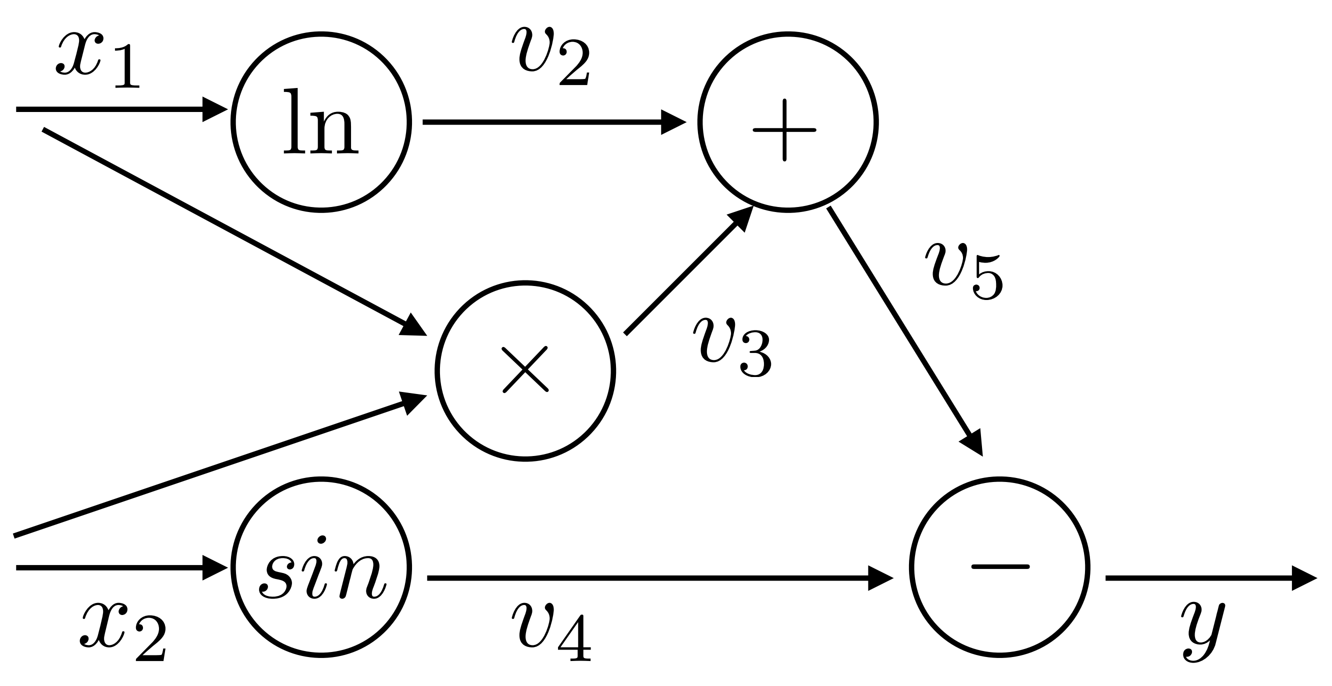
$$\frac{\partial \mathcal{L}(\mathbf{W}, \mathbf{b})}{\partial w_{ij}} \approx \lim_{h \to 0} \frac{\mathcal{L}(\mathbf{W} + h\mathbf{1}_{ij}, \mathbf{b}) - \mathcal{L}(\mathbf{W} + h\mathbf{1}_{ij}, \mathbf{b})}{2h} \qquad \frac{\partial \mathcal{L}(\mathbf{W}, \mathbf{b})}{\partial b_j} \approx \lim_{h \to 0} \frac{\mathcal{L}(\mathbf{W}, \mathbf{b} + h\mathbf{1}_j) - \mathcal{L}(\mathbf{W}, \mathbf{b} + h\mathbf{1}_j)}{2h}$$

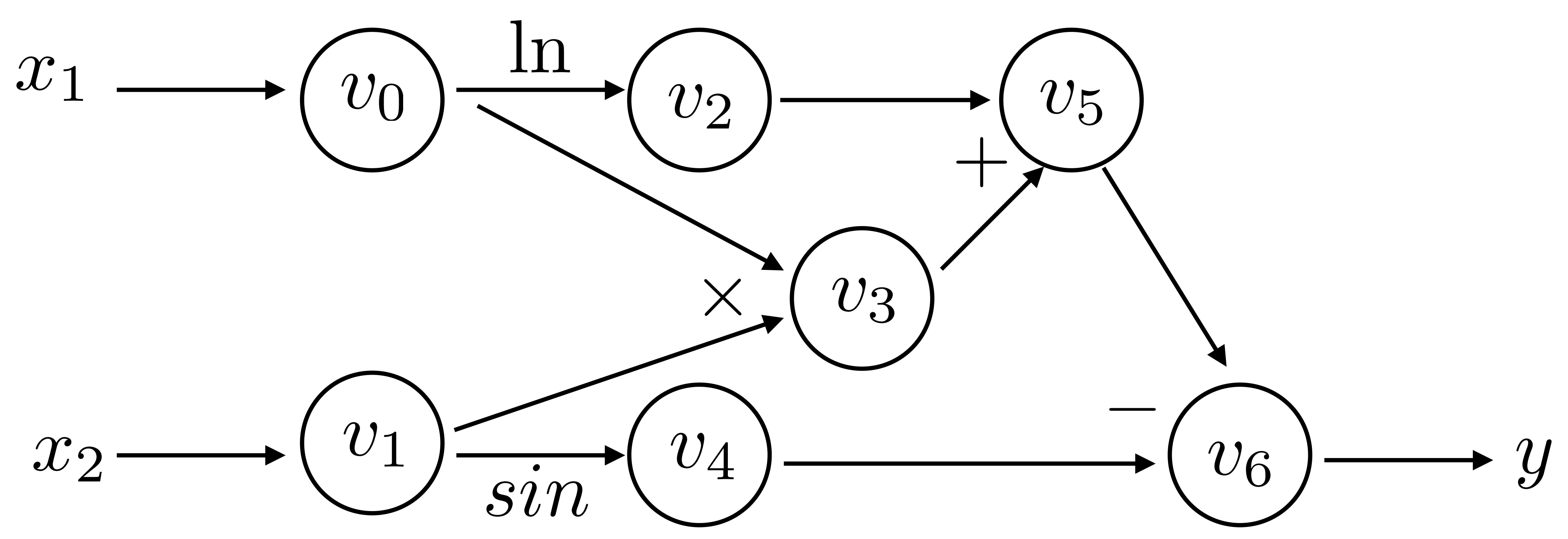
However, both of theses suffer from rounding errors and are not good enough for learning (they are very good tools for checking the correctness of implementation though, e.g., use $h = 0.000001$).

Symbolic Differentiation

$$y = f(x_1, x_2) = \ln(x_1) + x_1 x_2 - sin(x_2)$$

Input function is represented as **computational graph** (a symbolic tree)





Implements differentiation rules for composite functions:

Sum Rule

$$\frac{\mathrm{d}\,(f(x) + g(x))}{\mathrm{d}x} = \frac{\mathrm{d}f(x)}{\mathrm{d}x} + \frac{\mathrm{d}g(x)}{\mathrm{d}x}$$

Product Rule

$$\frac{\mathrm{d}\,(f(x) \cdot g(x))}{\mathrm{d}x} = \frac{\mathrm{d}f(x)}{\mathrm{d}x} g(x) + f(x) \frac{\mathrm{d}g(x)}{\mathrm{d}x}$$

Chain Rule

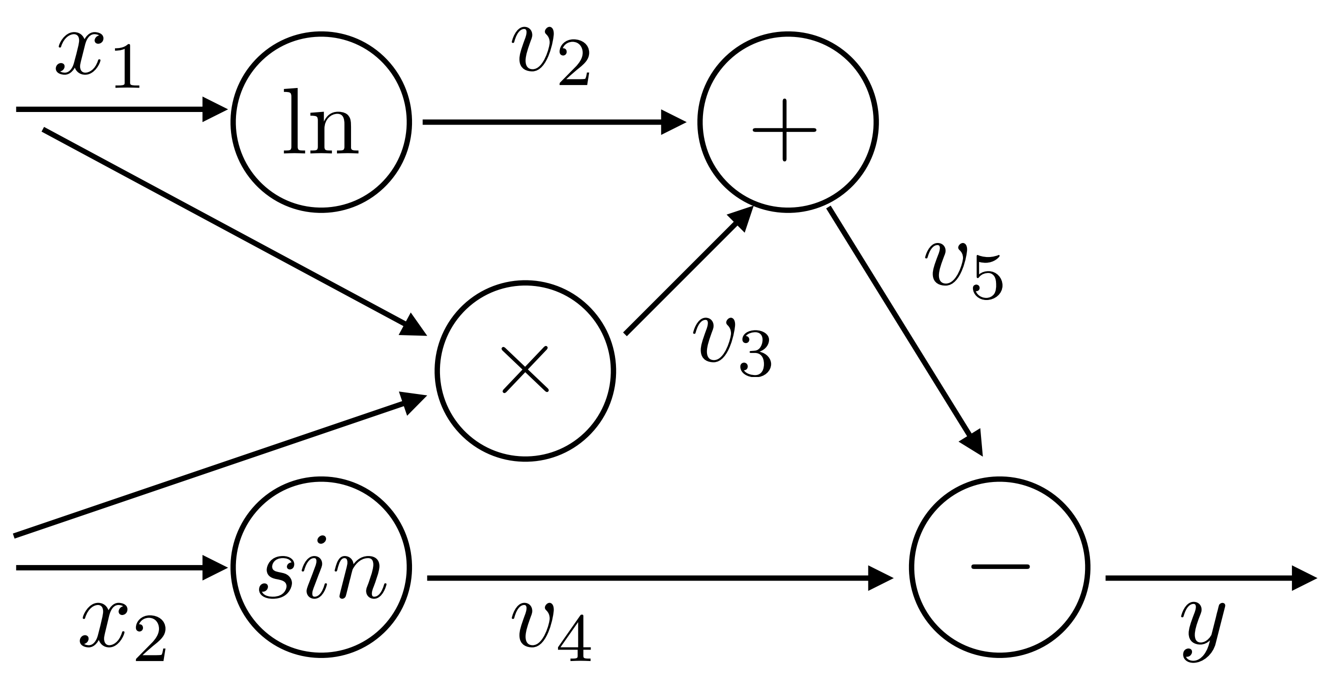
$$\frac{\mathrm{d}(f(g(x)))}{\mathrm{d}x} = \frac{\mathrm{d}f(g(x))}{\mathrm{d}x} \cdot \frac{\mathrm{d}g(x)}{\mathrm{d}x}$$

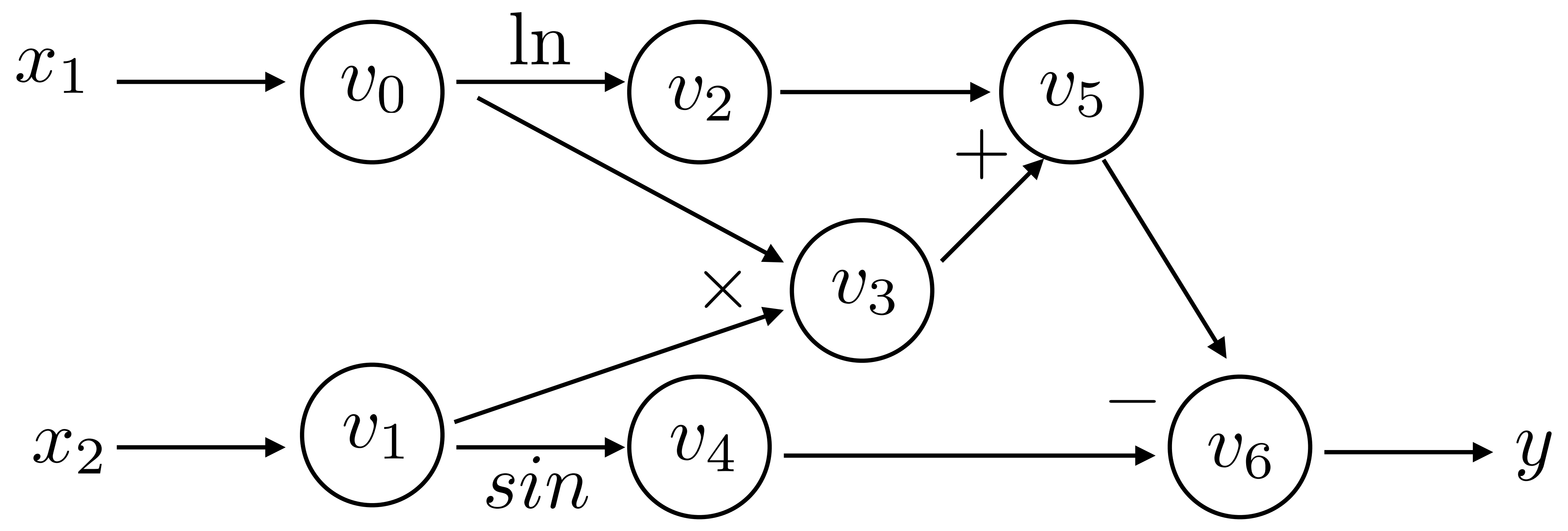
*slide adopted from T. Chen, H. Shen, A. Krishnamurthy CSE 599G1 lecture at UWashington

Symbolic Differentiation

$$y = f(x_1, x_2) = \ln(x_1) + x_1 x_2 - sin(x_2)$$

Input function is represented as **computational graph** (a symbolic tree)





Implements differentiation rules for composite functions:

Sum Rule	**Product** Rule	**Chain** Rule
$\frac{\mathrm{d}\,(f(x)+g(x))}{\mathrm{d}x} = \frac{\mathrm{d}f(x)}{\mathrm{d}x} + \frac{\mathrm{d}g(x)}{\mathrm{d}x}$	$\frac{\mathrm{d}\,(f(x)\cdot g(x))}{\mathrm{d}x} = \frac{\mathrm{d}f(x)}{\mathrm{d}x}g(x) + f(x)\frac{\mathrm{d}g(x)}{\mathrm{d}x}$	$\frac{\mathrm{d}(f(g(x)))}{\mathrm{d}x} = \frac{\mathrm{d}f(g(x))}{\mathrm{d}x} \cdot \frac{\mathrm{d}g(x)}{\mathrm{d}x}$

Problem: For complex functions, expressions can be exponentially large; also difficult to deal with piece-wise functions (creates many symbolic cases)

*slide adopted from T. Chen, H. Shen, A. Krishnamurthy CSE 599G1 lecture at UWashington

Automatic Differentiation (AutoDiff)

$$y = f(x_1, x_2) = \ln(x_1) + x_1 x_2 - sin(x_2)$$

Intuition: Interleave symbolic differentiation and simplification

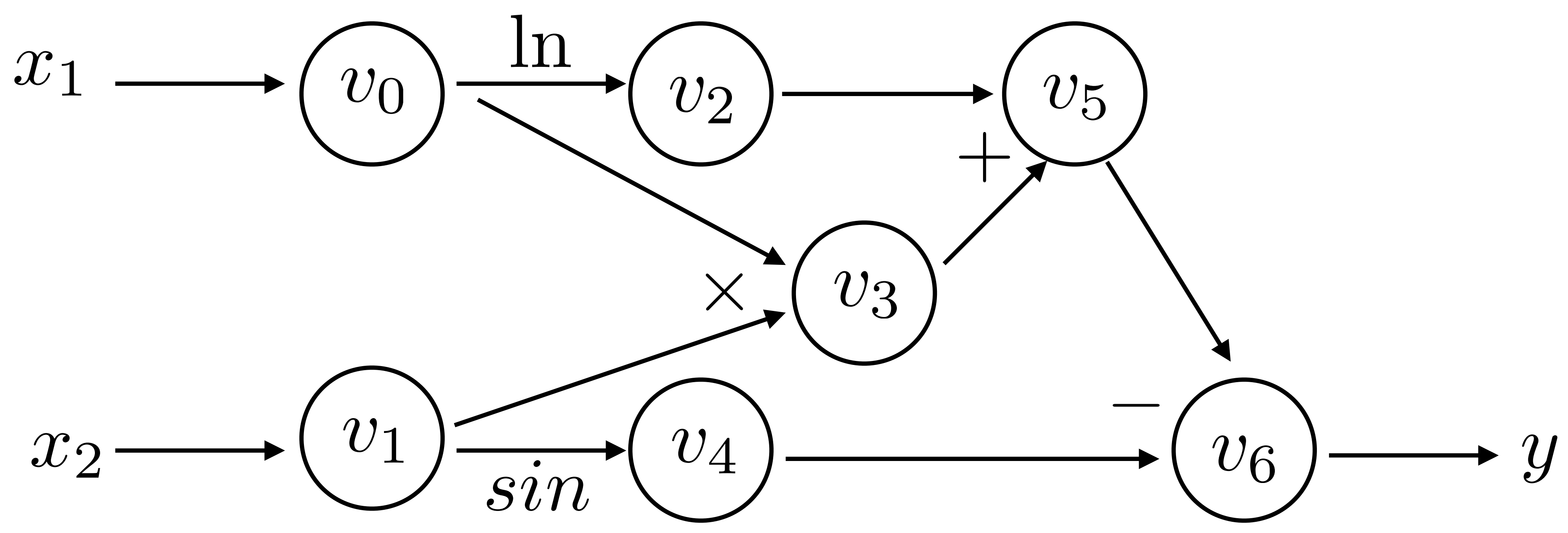
Key Idea: apply symbolic differentiation at the elementary operation level, evaluate and keep intermediate results

Success of **deep learning** owes A LOT to success of AutoDiff algorithms
(also to advances in parallel architectures, and large datasets, …)

*slide adopted from T. Chen, H. Shen, A. Krishnamurthy CSE 599G1 lecture at UWashington

Automatic Differentiation (AutoDiff)

$$y = f(x_1, x_2) = \ln(x_1) + x_1 x_2 - sin(x_2)$$

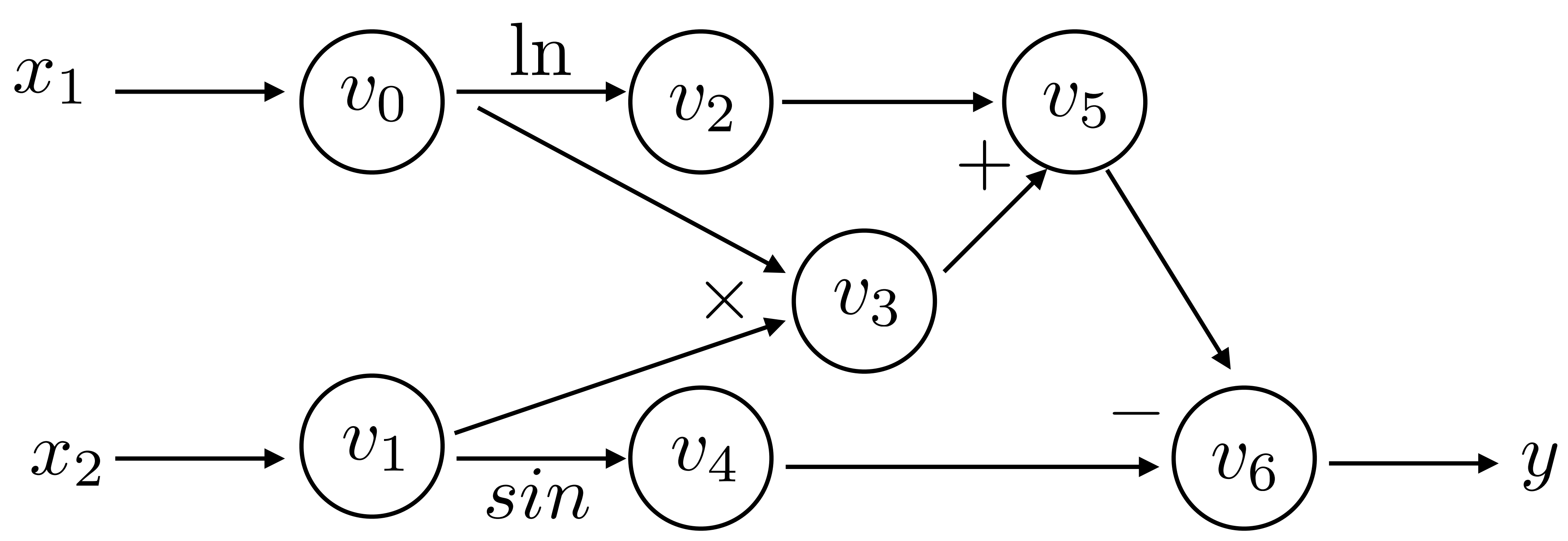


Each **node** is an input, intermediate, or output variable

Computational graph (a DAG) with variable ordering from topological sort.

Automatic Differentiation (AutoDiff)

$$y = f(x_1, x_2) = \ln(x_1) + x_1 x_2 - sin(x_2)$$



Lets see how we can **evaluate a function** using computational graph (DNN inferences)

Each **node** is an input, intermediate, or output variable

Computational graph (a DAG) with variable ordering from topological sort.

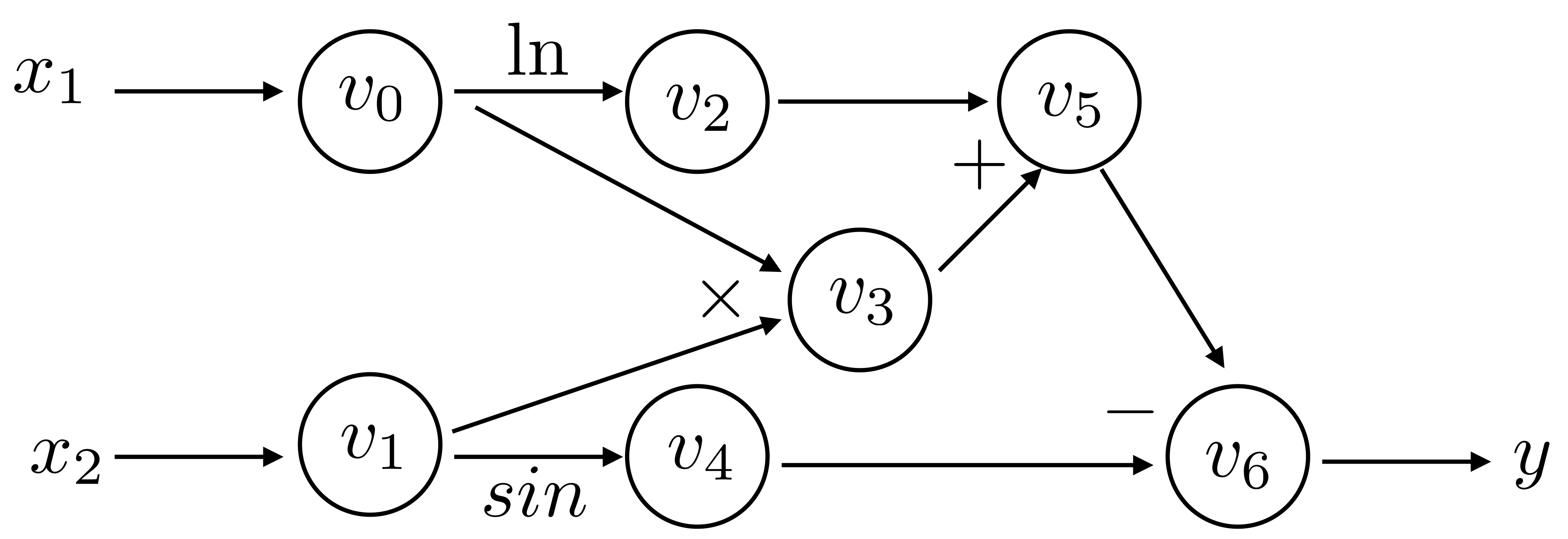
Computational graph is governed by these equations

$$\begin{aligned}
v_0 &= x_1 \\
v_1 &= x_2 \\
v_2 &= \ln(v_0) \\
v_3 &= v_0 \cdot v_1 \\
v_4 &= sin(v_1) \\
v_5 &= v_2 + v_3 \\
v_6 &= v_5 - v_4 \\
y &= v_6
\end{aligned}$$

*slide adopted from T. Chen, H. Shen, A. Krishnamurthy CSE 599G1 lecture at UWashington

Automatic Differentiation (AutoDiff)

$$y = f(x_1, x_2) = \ln(x_1) + x_1 x_2 - sin(x_2)$$



Each **node** is an input, intermediate, or output variable

Computational graph (a DAG) with variable ordering from topological sort.

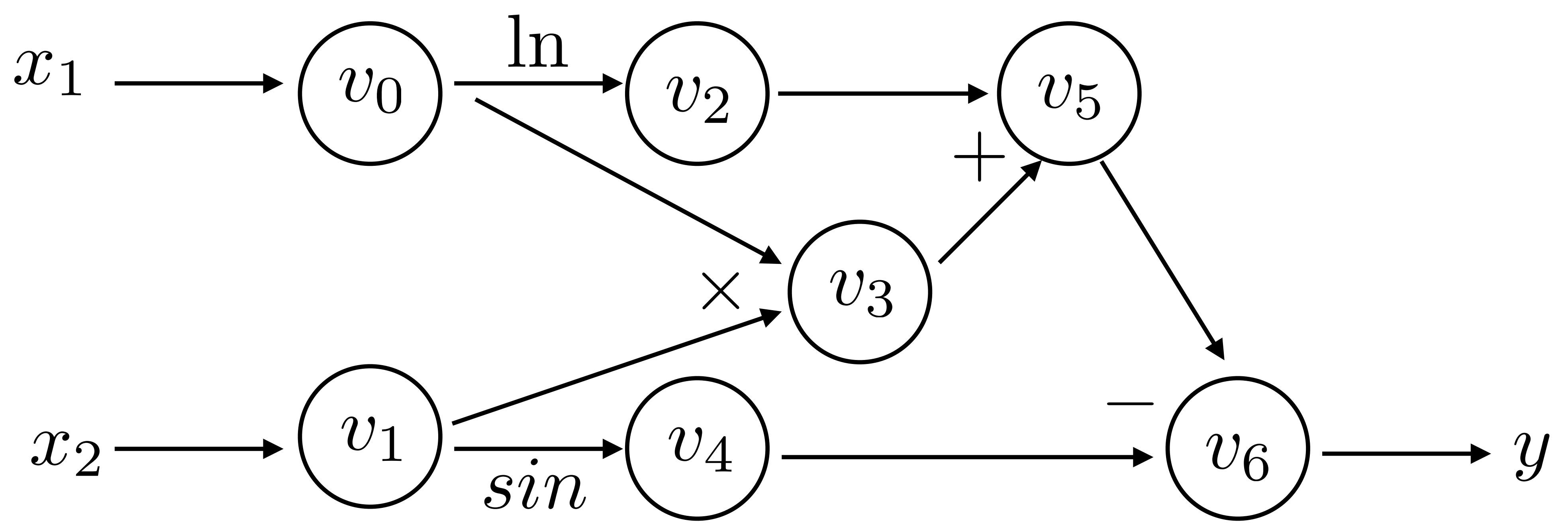
Lets see how we can **evaluate a function** using computational graph (DNN inferences)

Forward Evaluation Trace:

	$f(2,5)$
$v_0 = x_1$	
$v_1 = x_2$	
$v_2 = \ln(v_0)$	
$v_3 = v_0 \cdot v_1$	
$v_4 = sin(v_1)$	
$v_5 = v_2 + v_3$	
$v_6 = v_5 - v_4$	
$y = v_6$	

Automatic Differentiation (AutoDiff)

$$y = f(x_1, x_2) = \ln(x_1) + x_1 x_2 - sin(x_2)$$



Lets see how we can **evaluate a function** using computational graph (DNN inferences)

Each **node** is an input, intermediate, or output variable

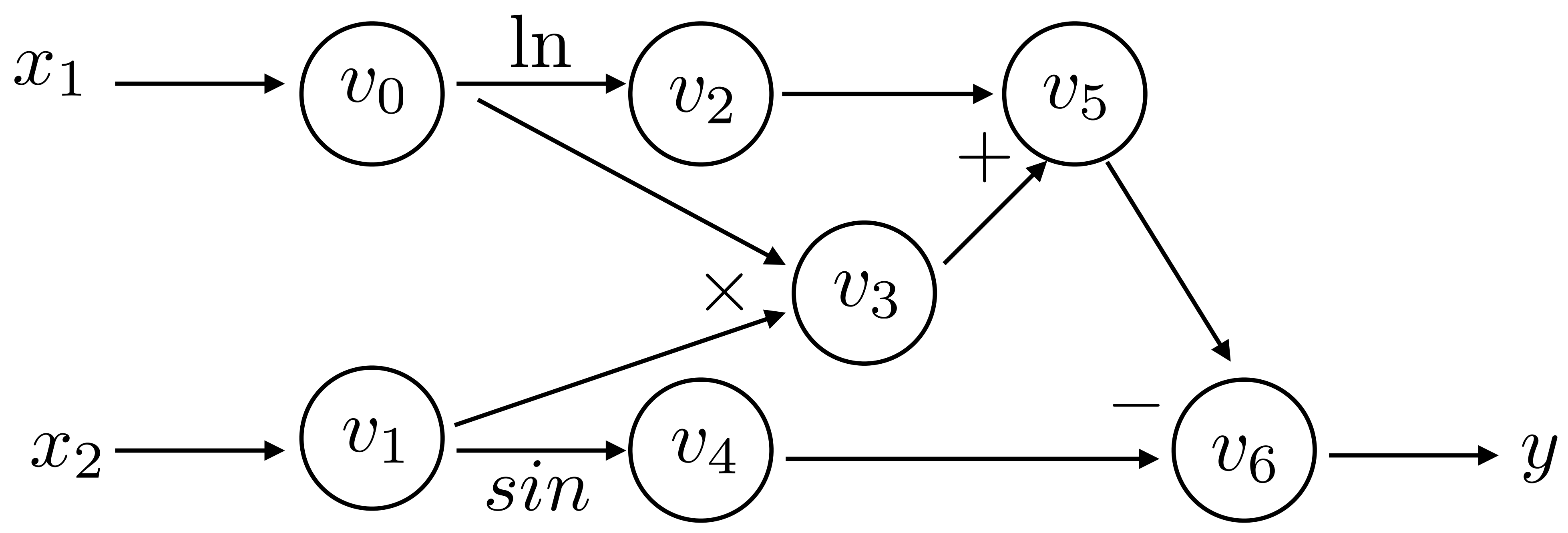
Computational graph (a DAG) with variable ordering from topological sort.

Forward Evaluation Trace:

	$f(2,5)$
$v_0 = x_1$	2
$v_1 = x_2$	
$v_2 = \ln(v_0)$	
$v_3 = v_0 \cdot v_1$	
$v_4 = sin(v_1)$	
$v_5 = v_2 + v_3$	
$v_6 = v_5 - v_4$	
$y = v_6$	

Automatic Differentiation (AutoDiff)

$$y = f(x_1, x_2) = \ln(x_1) + x_1 x_2 - sin(x_2)$$



Each **node** is an input, intermediate, or output variable

Computational graph (a DAG) with variable ordering from topological sort.

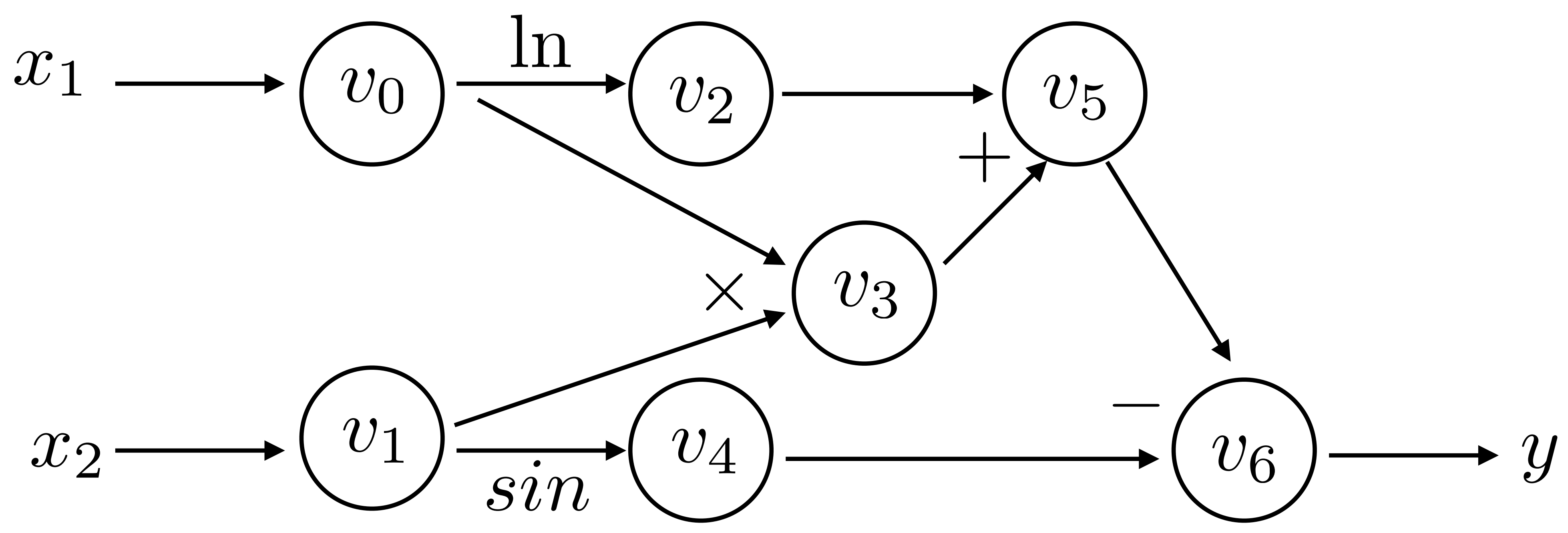
Lets see how we can **evaluate a function** using computational graph (DNN inferences)

Forward Evaluation Trace:

	$f(2,5)$
$v_0 = x_1$	2
$v_1 = x_2$	5
$v_2 = \ln(v_0)$	
$v_3 = v_0 \cdot v_1$	
$v_4 = sin(v_1)$	
$v_5 = v_2 + v_3$	
$v_6 = v_5 - v_4$	
$y = v_6$	

Automatic Differentiation (AutoDiff)

$$y = f(x_1, x_2) = \ln(x_1) + x_1 x_2 - sin(x_2)$$



Lets see how we can **evaluate a function** using computational graph (DNN inferences)

Each **node** is an input, intermediate, or output variable

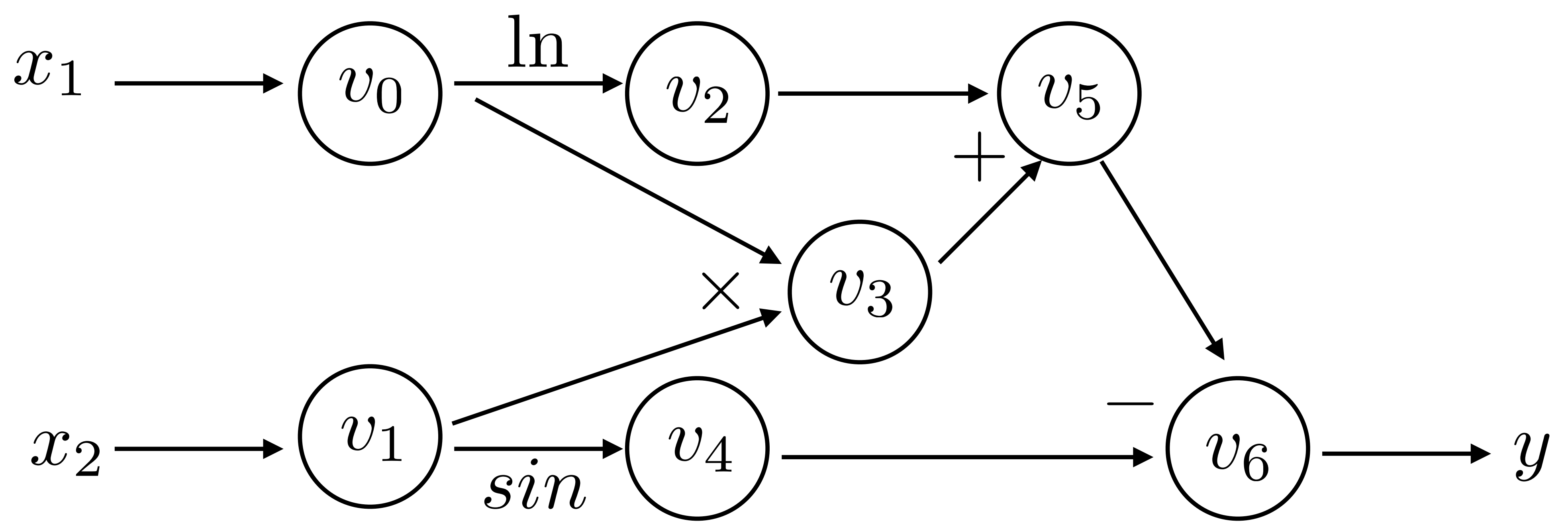
Computational graph (a DAG) with variable ordering from topological sort.

Forward Evaluation Trace:

	$f(2,5)$
$v_0 = x_1$	2
$v_1 = x_2$	5
$v_2 = \ln(v_0)$	ln(2) = 0.693
$v_3 = v_0 \cdot v_1$	
$v_4 = sin(v_1)$	
$v_5 = v_2 + v_3$	
$v_6 = v_5 - v_4$	
$y = v_6$	

Automatic Differentiation (AutoDiff)

$$y = f(x_1, x_2) = \ln(x_1) + x_1 x_2 - sin(x_2)$$



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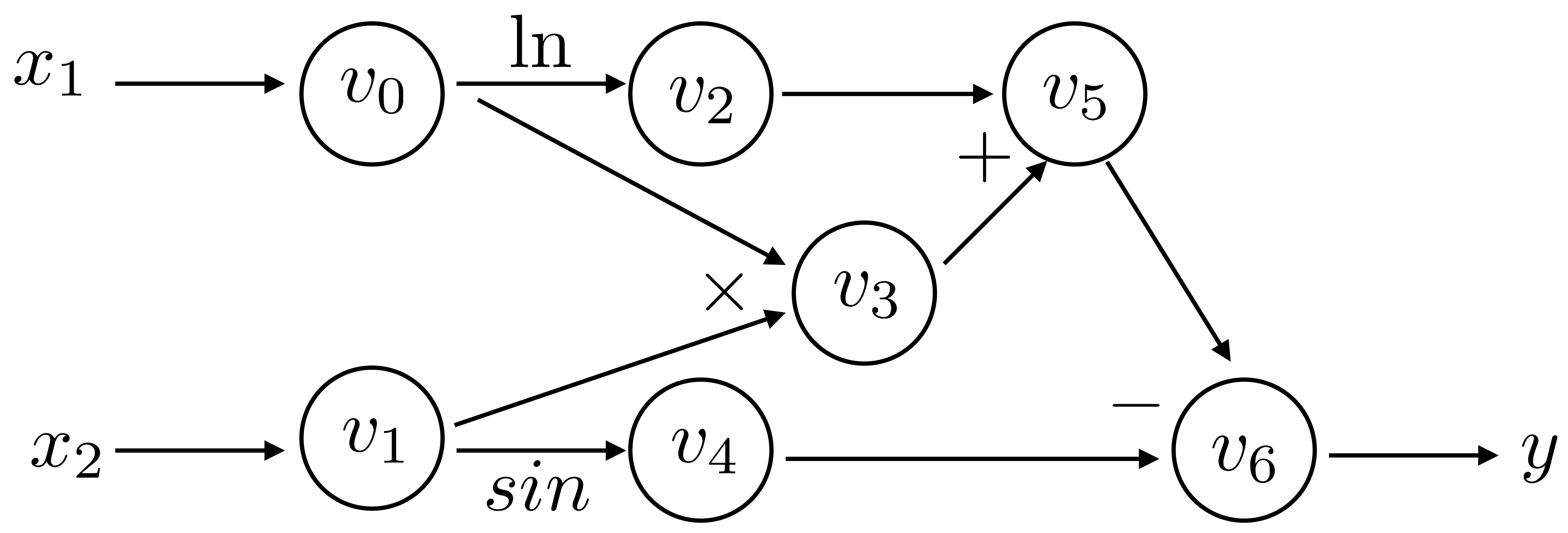
Lets see how we can **evaluate a function** using computational graph (DNN inferences)

Forward Evaluation Trace:

	$f(2,5)$
$v_0 = x_1$	2
$v_1 = x_2$	5
$v_2 = \ln(v_0)$	ln(2) = 0.693
$v_3 = v_0 \cdot v_1$	2 x 5 = 10
$v_4 = sin(v_1)$	sin(5) = 0.959
$v_5 = v_2 + v_3$	0.693 + 10 = 10.693
$v_6 = v_5 - v_4$	10.693 + 0.959 = 11.652
$y = v_6$	11.652

Automatic Differentiation (AutoDiff)

$$y = f(x_1, x_2) = \ln(x_1) + x_1 x_2 - sin(x_2)$$



Lets see how we can **evaluate a function** using computational graph (DNN inferences)

Forward Evaluation Trace:

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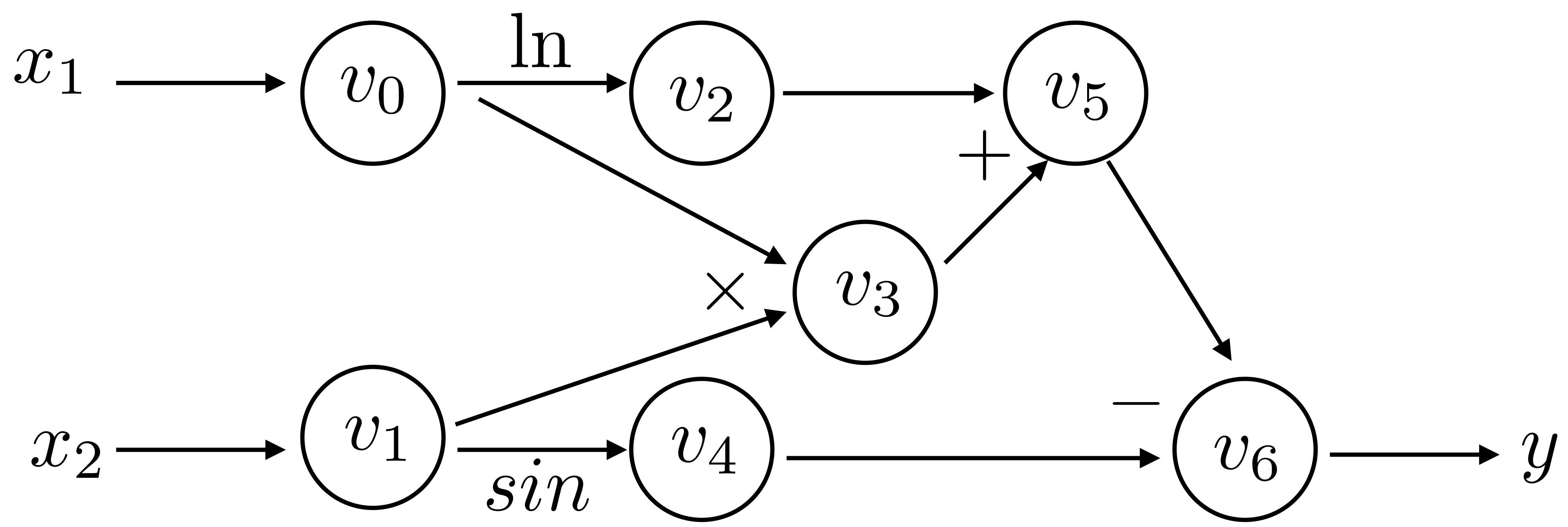
Each **node** is an input, intermediate, or output variable

Computational graph (a DAG) with variable ordering from topological sort.

AutoDiff - **Forward Mode**

$$y = f(x_1, x_2) = \ln(x_1) + x_1 x_2 - sin(x_2)$$



Lets see how we can **evaluate a derivative** using computational graph (DNN learning)

$$\left.\frac{\partial f(x_1, x_2)}{\partial x_1}\right|_{(x_1=2, x_2=5)}$$

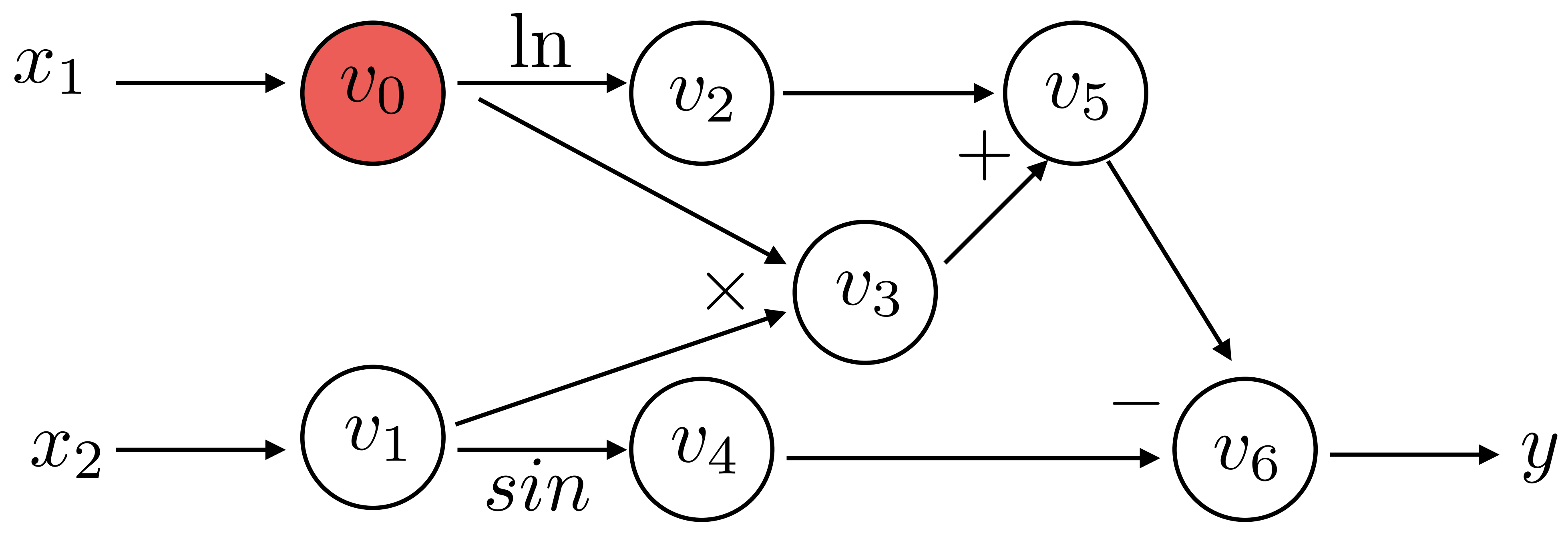
Forward Evaluation Trace:

	$f(2,5)$
$v_0 = x_1$	2
$v_1 = x_2$	5
$v_2 = \ln(v_0)$	ln(2) = 0.693
$v_3 = v_0 \cdot v_1$	2 x 5 = 10
$v_4 = sin(v_1)$	sin(5) = 0.959
$v_5 = v_2 + v_3$	0.693 + 10 = 10.693
$v_6 = v_5 - v_4$	10.693 + 0.959 = 11.652
$y = v_6$	11.652

We will do this with **forward mode** first, by introducing a derivative of each variable node with respect to the input variable.

AutoDiff - **Forward Mode**

$$y = f(x_1, x_2) = \ln(x_1) + x_1 x_2 - sin(x_2)$$



Forward Evaluation Trace:

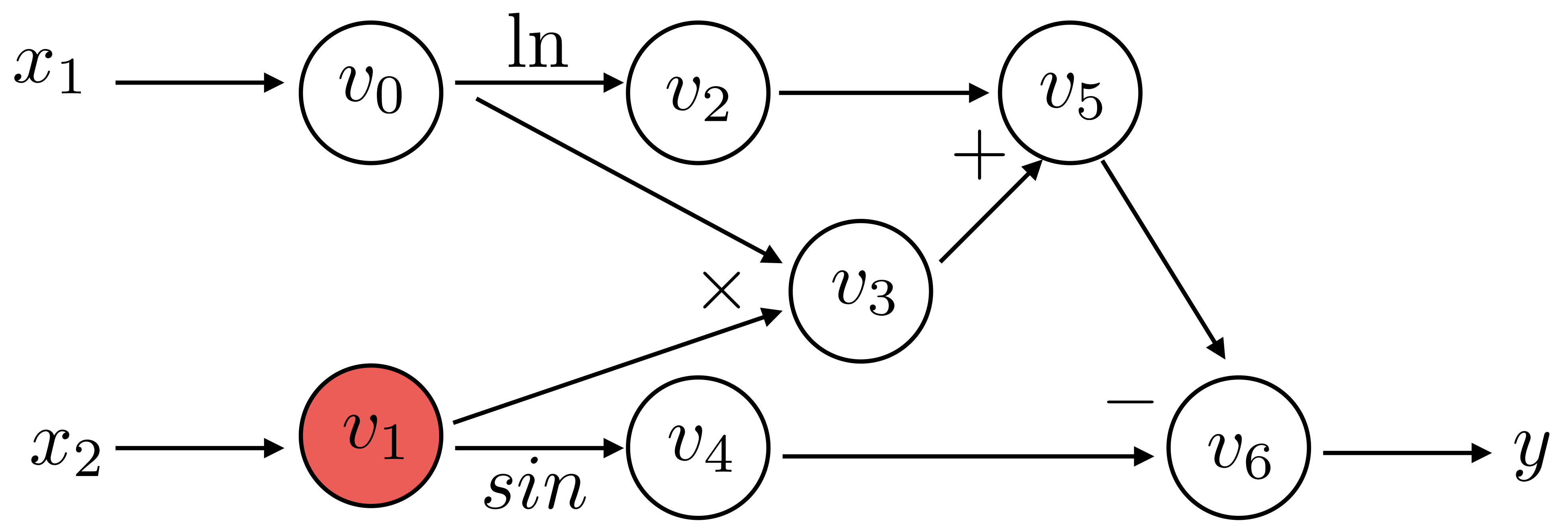
	$f(2,5)$
$v_0 = x_1$	2
$v_1 = x_2$	5
$v_2 = \ln(v_0)$	ln(2) = 0.693
$v_3 = v_0 \cdot v_1$	2 x 5 = 10
$v_4 = sin(v_1)$	sin(5) = 0.959
$v_5 = v_2 + v_3$	0.693 + 10 = 10.693
$v_6 = v_5 - v_4$	10.693 + 0.959 = 11.652
$y = v_6$	11.652

Forward Derivative Trace:

	$\left.\frac{\partial f(x_1, x_2)}{\partial x_1}\right\|_{(x_1=2, x_2=5)}$
$\frac{\partial v_0}{\partial x_1}$	1

AutoDiff - **Forward Mode**

$$y = f(x_1, x_2) = \ln(x_1) + x_1 x_2 - sin(x_2)$$



Forward Evaluation Trace:

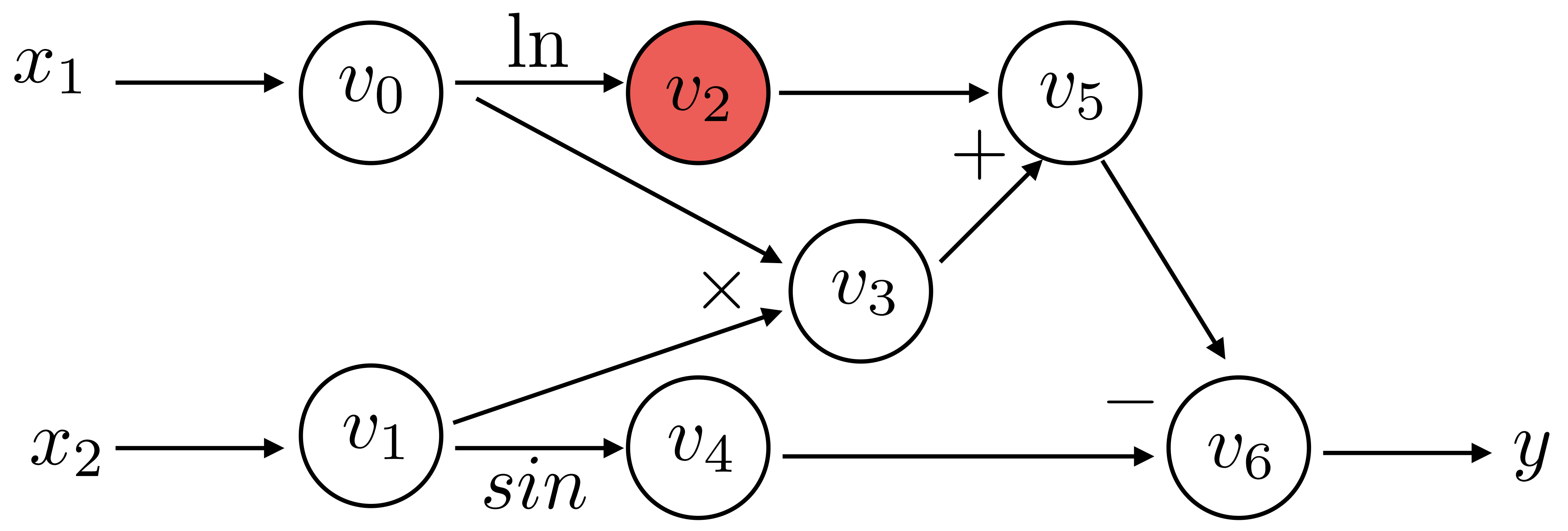
	$f(2,5)$
$v_0 = x_1$	2
$v_1 = x_2$	5
$v_2 = \ln(v_0)$	ln(2) = 0.693
$v_3 = v_0 \cdot v_1$	2 x 5 = 10
$v_4 = sin(v_1)$	sin(5) = 0.959
$v_5 = v_2 + v_3$	0.693 + 10 = 10.693
$v_6 = v_5 - v_4$	10.693 + 0.959 = 11.652
$y = v_6$	11.652

Forward Derivative Trace:

	$\left.\frac{\partial f(x_1,x_2)}{\partial x_1}\right\vert_{(x_1=2, x_2=5)}$
$\frac{\partial v_0}{\partial x_1}$	1
$\frac{\partial v_1}{\partial x_1}$	0

AutoDiff - **Forward Mode**

$$y = f(x_1, x_2) = \ln(x_1) + x_1 x_2 - sin(x_2)$$



Forward Evaluation Trace:

	$f(2,5)$
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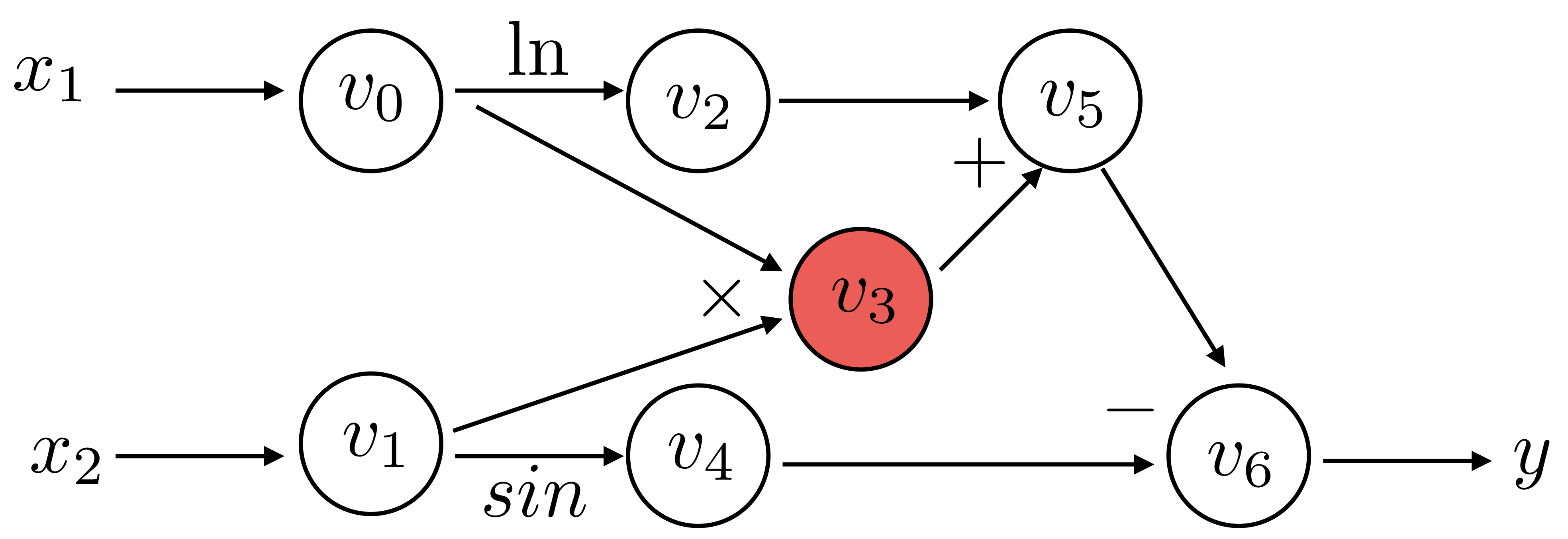
$v_6 = v_5 - v_4$	10.693 + 0.959 = 11.652
$y = v_6$	11.652

Forward Derivative Trace:

	$\left.\frac{\partial f(x_1,x_2)}{\partial x_1}\right\|_{(x_1=2,x_2=5)}$
$\frac{\partial v_0}{\partial x_1}$	1
$\frac{\partial v_1}{\partial x_1}$	0
$\frac{\partial v_2}{\partial x_1} = \frac{1}{v_0}\frac{\partial v_0}{\partial x_1}$ **Chain** Rule	1/2 * 1 = 0.5

AutoDiff - **Forward Mode**

$$y = f(x_1, x_2) = \ln(x_1) + x_1 x_2 - sin(x_2)$$



Forward Evaluation Trace:

	$f(2,5)$
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$v_2 = \ln(v_0)$	ln(2) = 0.693
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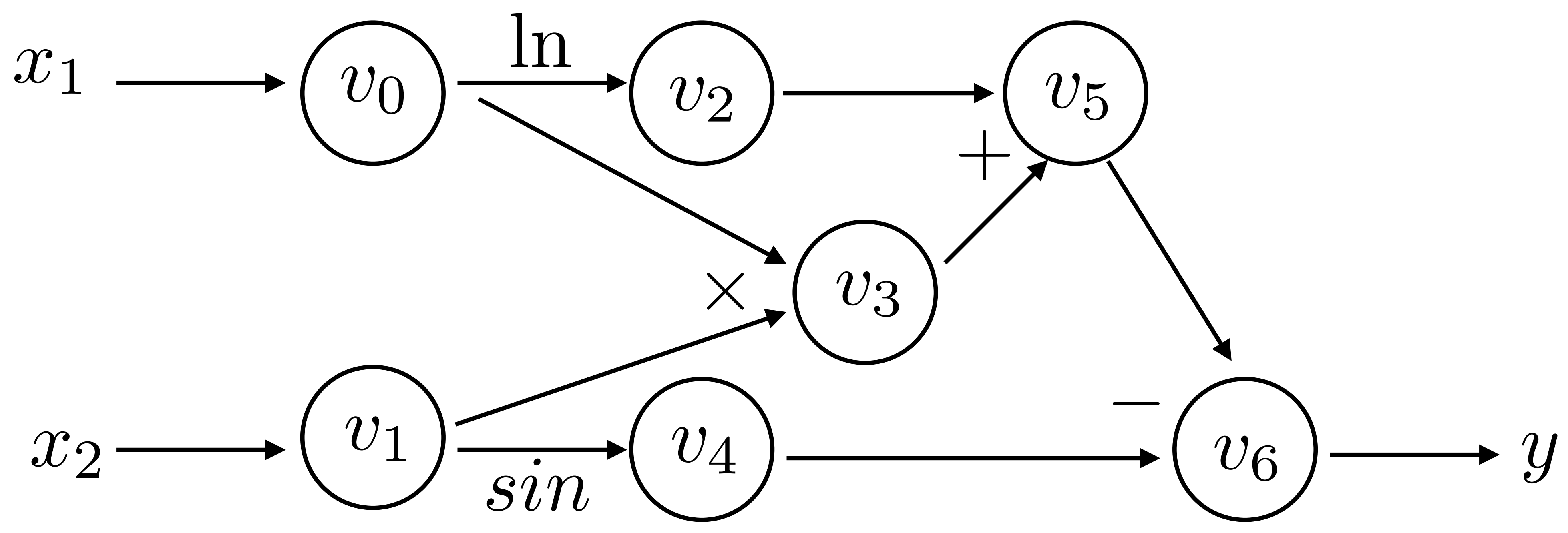
$v_5 = v_2 + v_3$	0.693 + 10 = 10.693
$v_6 = v_5 - v_4$	10.693 + 0.959 = 11.652
$y = v_6$	11.652

Forward Derivative Trace:

	$\left.\frac{\partial f(x_1,x_2)}{\partial x_1}\right\|_{(x_1=2,x_2=5)}$
$\frac{\partial v_0}{\partial x_1}$	1
$\frac{\partial v_1}{\partial x_1}$	0
$\frac{\partial v_2}{\partial x_1} = \frac{1}{v_0}\frac{\partial v_0}{\partial x_1}$	1/2 * 1 = 0.5
$\frac{\partial v_3}{\partial x_1} = \frac{\partial v_0}{\partial x_1} \cdot v_1 + v_0 \cdot \frac{\partial v_1}{\partial x_1}$ **Product** Rule	1*5 + 2*0 = 5

AutoDiff - **Forward Mode**

$$y = f(x_1, x_2) = \ln(x_1) + x_1 x_2 - sin(x_2)$$



Forward Evaluation Trace:

	$f(2,5)$
$v_0 = x_1$	2
$v_1 = x_2$	5
$v_2 = \ln(v_0)$	ln(2) = 0.693
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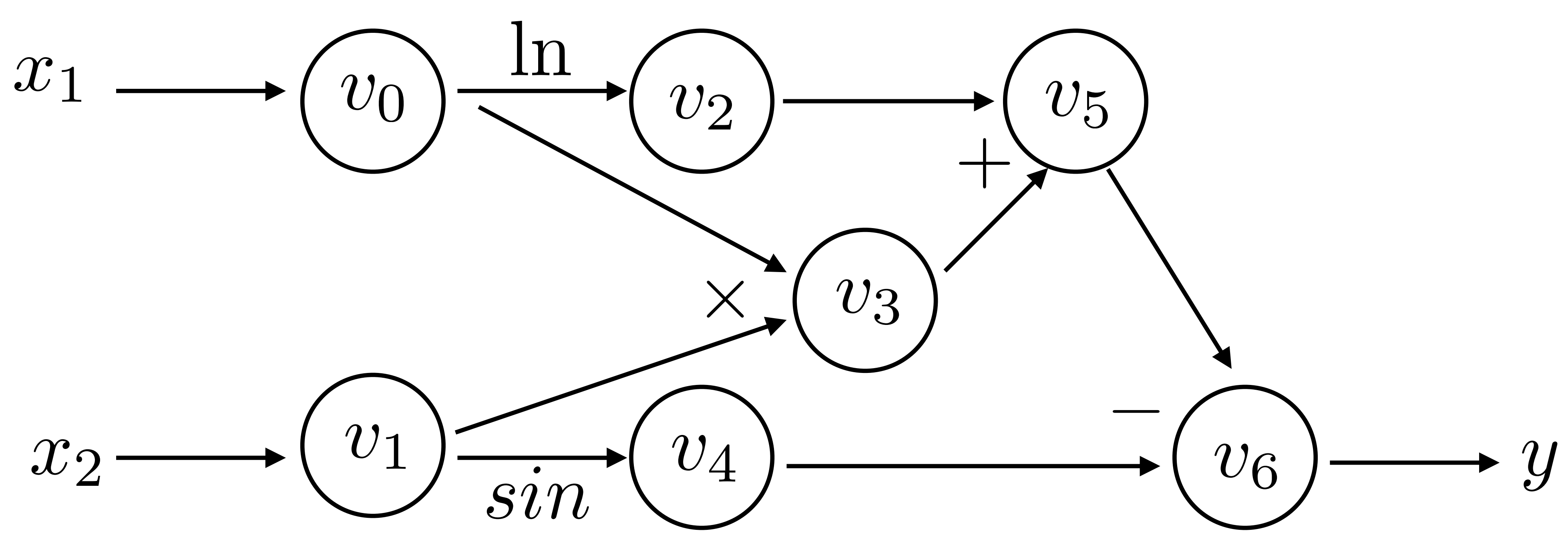
$v_6 = v_5 - v_4$	10.693 + 0.959 = 11.652
$y = v_6$	11.652

Forward Derivative Trace:

	$\left.\frac{\partial f(x_1, x_2)}{\partial x_1}\right\vert_{(x_1=2, x_2=5)}$
$\frac{\partial v_0}{\partial x_1}$	1
$\frac{\partial v_1}{\partial x_1}$	0
$\frac{\partial v_2}{\partial x_1} = \frac{1}{v_0}\frac{\partial v_0}{\partial x_1}$	1/2 * 1 = 0.5
$\frac{\partial v_3}{\partial x_1} = \frac{\partial v_0}{\partial x_1} \cdot v_1 + v_0 \cdot \frac{\partial v_1}{\partial x_1}$	1*5 + 2*0 = 5
$\frac{\partial v_4}{\partial x_1} = \frac{\partial v_1}{\partial x_1} cos(v_1)$	0 * cos(5) = 0
$\frac{\partial v_5}{\partial x_1} = \frac{\partial v_2}{\partial x_1} + \frac{\partial v_3}{\partial x_1}$	0.5 + 5 = 5.5
$\frac{\partial v_6}{\partial x_1} = \frac{\partial v_5}{\partial x_1} - \frac{\partial v_4}{\partial x_1}$	5.5 - 0 = 5.5
$\frac{\partial y}{\partial x_1} = \frac{\partial v_6}{\partial x_1}$	5.5

AutoDiff - **Forward Mode**

$$y = f(x_1, x_2) = \ln(x_1) + x_1 x_2 - sin(x_2)$$



We now have:

$$\left.\frac{\partial f(x_1, x_2)}{\partial x_1}\right|_{(x_1=2, x_2=5)} = 5.5$$

Still need:

$$\left.\frac{\partial f(x_1, x_2)}{\partial x_2}\right|_{(x_1=2, x_2=5)}$$

Forward Derivative Trace:

	$\left.\frac{\partial f(x_1, x_2)}{\partial x_1}\right|_{(x_1=2, x_2=5)}$
$\frac{\partial v_0}{\partial x_1}$	1
$\frac{\partial v_1}{\partial x_1}$	0
$\frac{\partial v_2}{\partial x_1} = \frac{1}{v_0} \frac{\partial v_0}{\partial x_1}$	1/2 * 1 = 0.5
$\frac{\partial v_3}{\partial x_1} = \frac{\partial v_0}{\partial x_1} \cdot v_1 + v_0 \cdot \frac{\partial v_1}{\partial x_1}$	1*5 + 2*0 = 5
$\frac{\partial v_4}{\partial x_1} = \frac{\partial v_1}{\partial x_1} cos(v_1)$	0 * cos(5) = 0
$\frac{\partial v_5}{\partial x_1} = \frac{\partial v_2}{\partial x_1} + \frac{\partial v_3}{\partial x_1}$	0.5 + 5 = 5.5
$\frac{\partial v_6}{\partial x_1} = \frac{\partial v_5}{\partial x_1} - \frac{\partial v_4}{\partial x_1}$	5.5 - 0 = 5.5
$\frac{\partial y}{\partial x_1} = \frac{\partial v_6}{\partial x_1}$	5.5

AutoDiff - **Forward Mode**

Forward mode needs m forward passes to get a full Jacobian (all gradients of output with respect to each input), where m is the number of inputs

$$\mathbf{y} = f(\mathbf{x}) : \mathbb{R}^m \to \mathbb{R}^n$$

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Problem: DNN typically has large number of inputs:

image as an input, plus all the weights and biases of layers = millions of inputs!

and very few outputs (many DNNs have $n = 1$)

Why?

*slide adopted from T. Chen, H. Shen, A. Krishnamurthy CSE 599G1 lecture at UWashington

AutoDiff - **Forward Mode**

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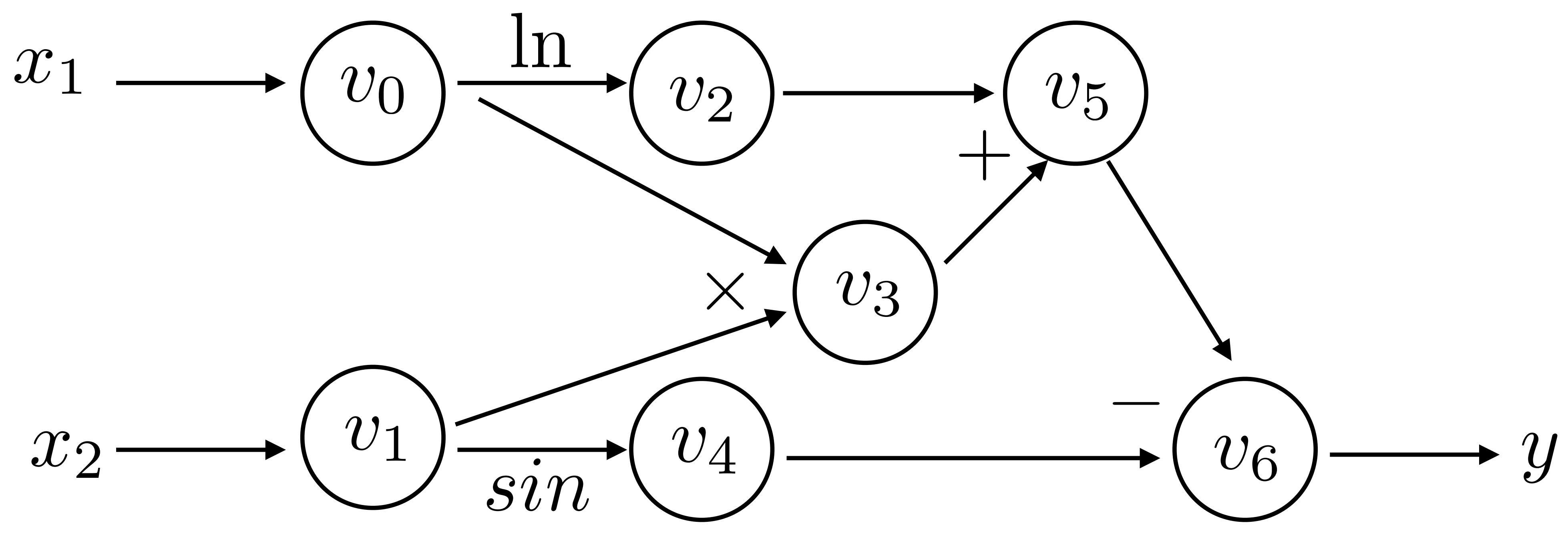
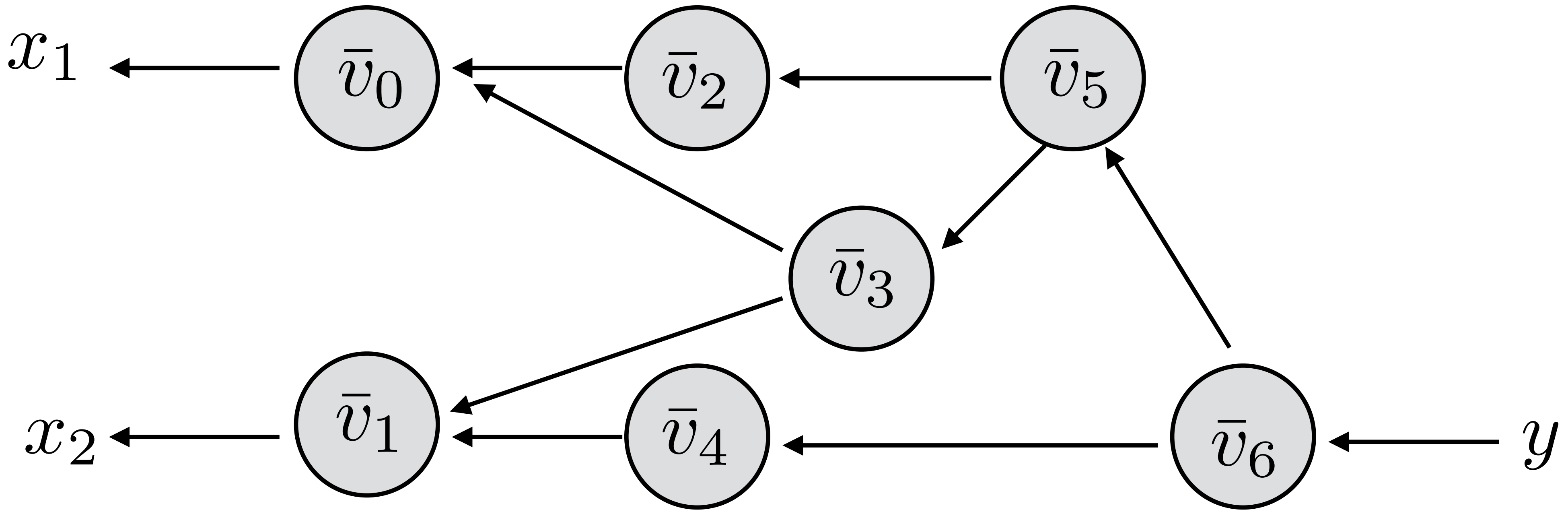
Automatic differentiation in **reverse mode** computes all gradients in n backwards passes (so for most DNNs in a single back pass — **back propagation**)

*slide adopted from T. Chen, H. Shen, A. Krishnamurthy CSE 599G1 lecture at UWashington

AutoDiff - **Reverse Mode**





Forward Evaluation Trace:

	$f(2,5)$
$v_0 = x_1$	2
$v_1 = x_2$	5
$v_2 = \ln(v_0)$	ln(2) = 0.693
$v_3 = v_0 \cdot v_1$	2 x 5 = 10
$v_4 = sin(v_1)$	sin(5) = 0.959
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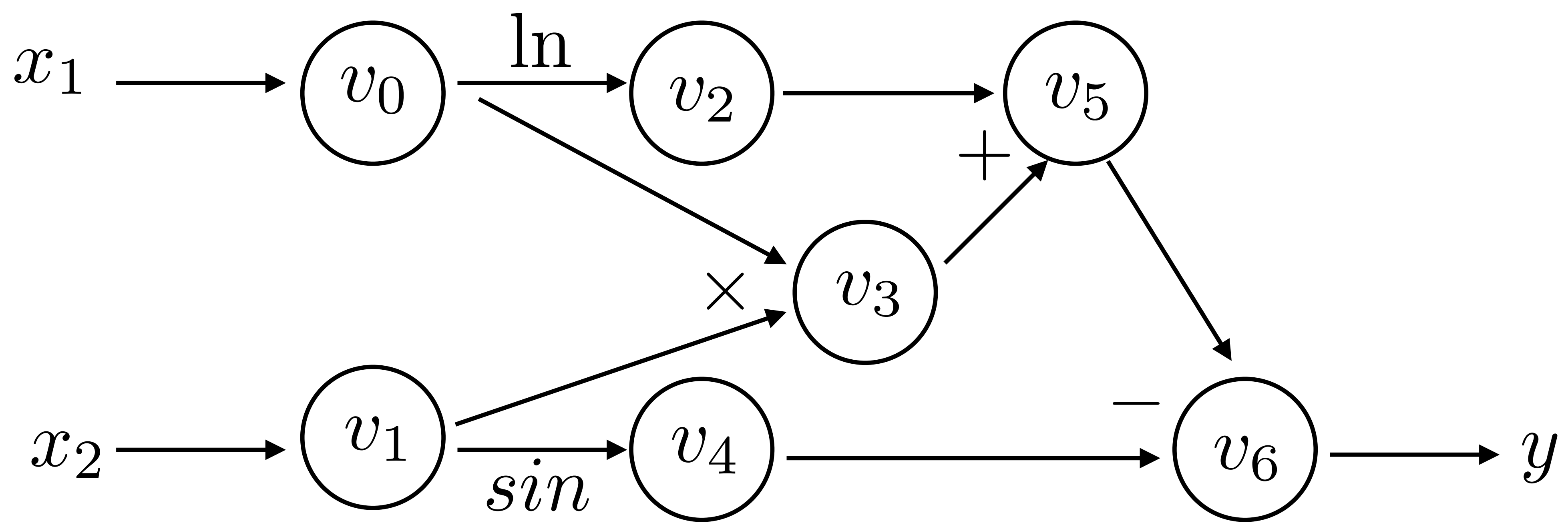
$y = v_6$	11.652

Traverse the original graph in the *reverse* topological order and for each node in the original graph introduce an **adjoint node**, which computes derivative of the output with respect to the local node (using Chain rule):

$$\bar{v}_i = \frac{\partial y_j}{\partial v_i} = \sum_{k \in \mathrm{pa}(i)} \frac{\partial v_k}{\partial v_i} \frac{\partial y_j}{\partial v_k} = \sum_{k \in \mathrm{pa}(i)} \boxed{\frac{\partial v_k}{\partial v_i}} \bar{v}_k$$

"**local**" derivative

AutoDiff - **Reverse Mode**



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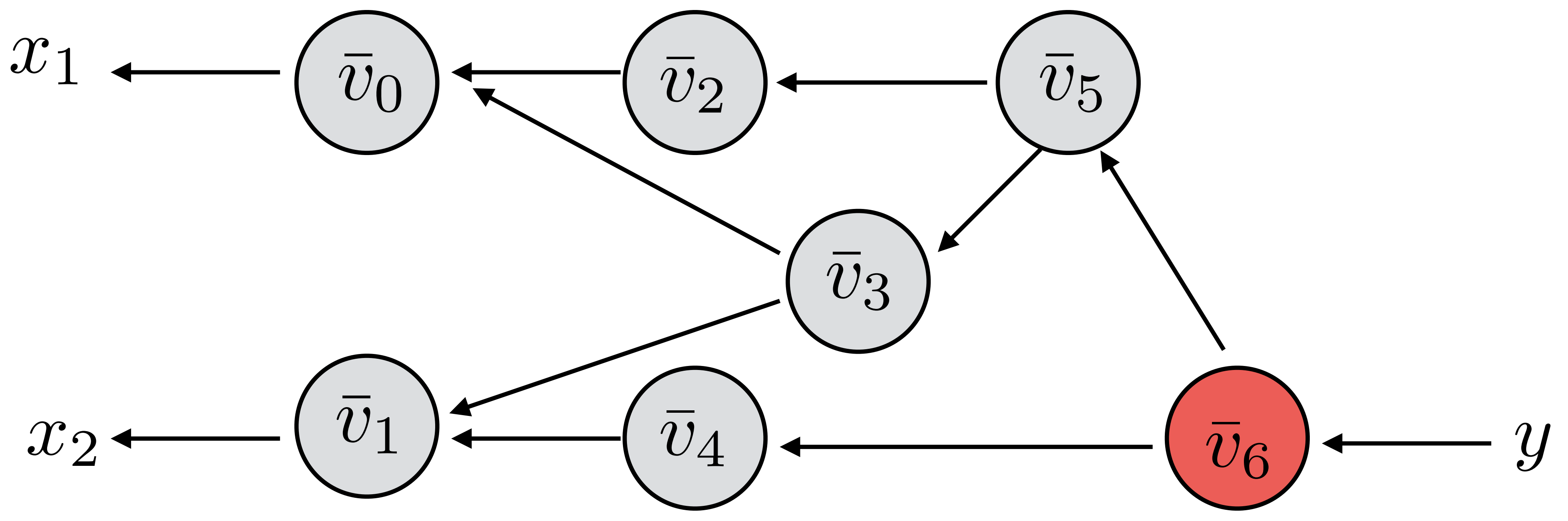
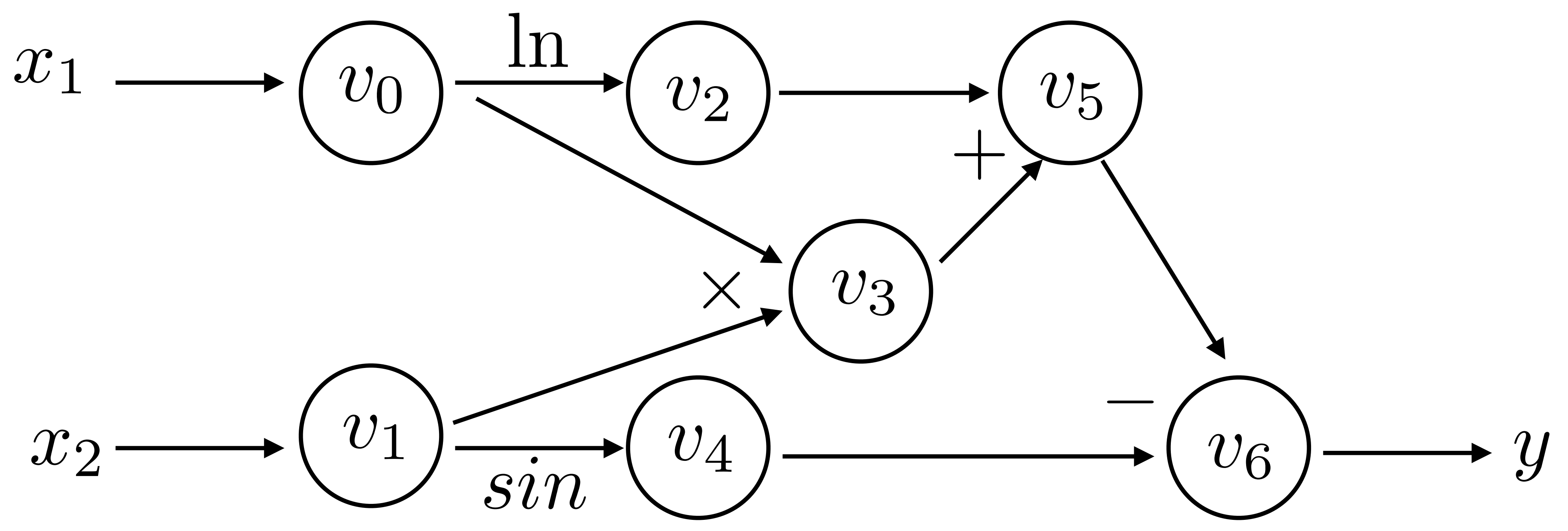
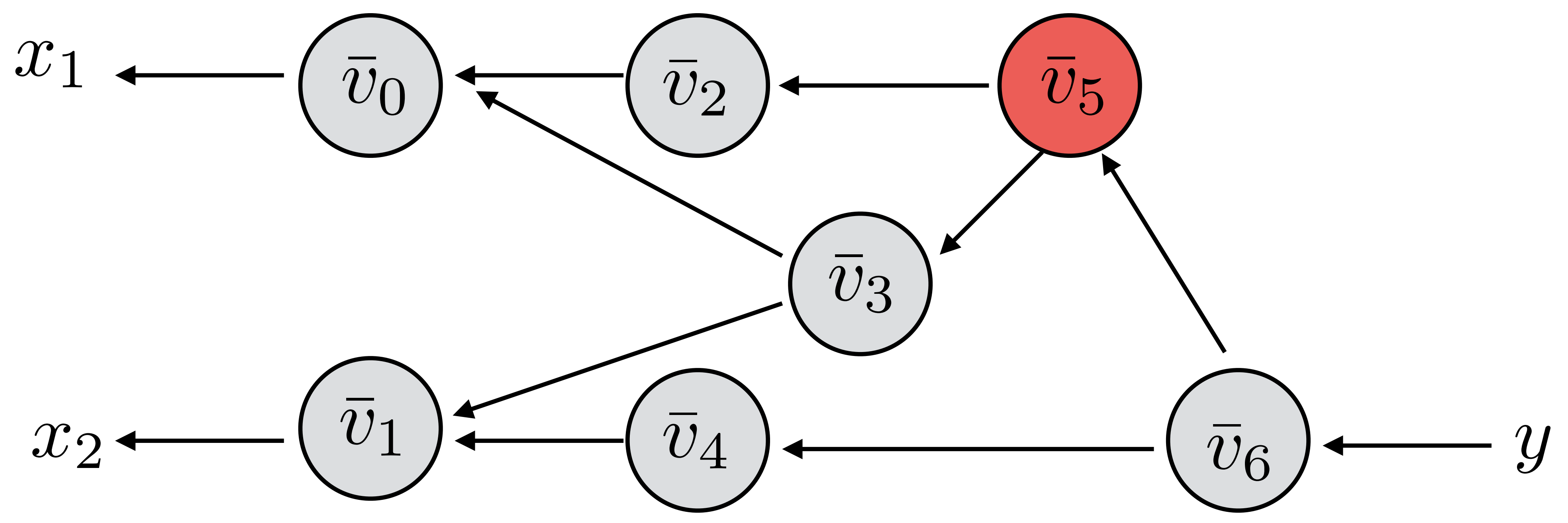


Backwards Derivative Trace:

$\bar{v}_6 = \dfrac{\partial y}{\partial v_6}$	1

AutoDiff - **Reverse Mode**





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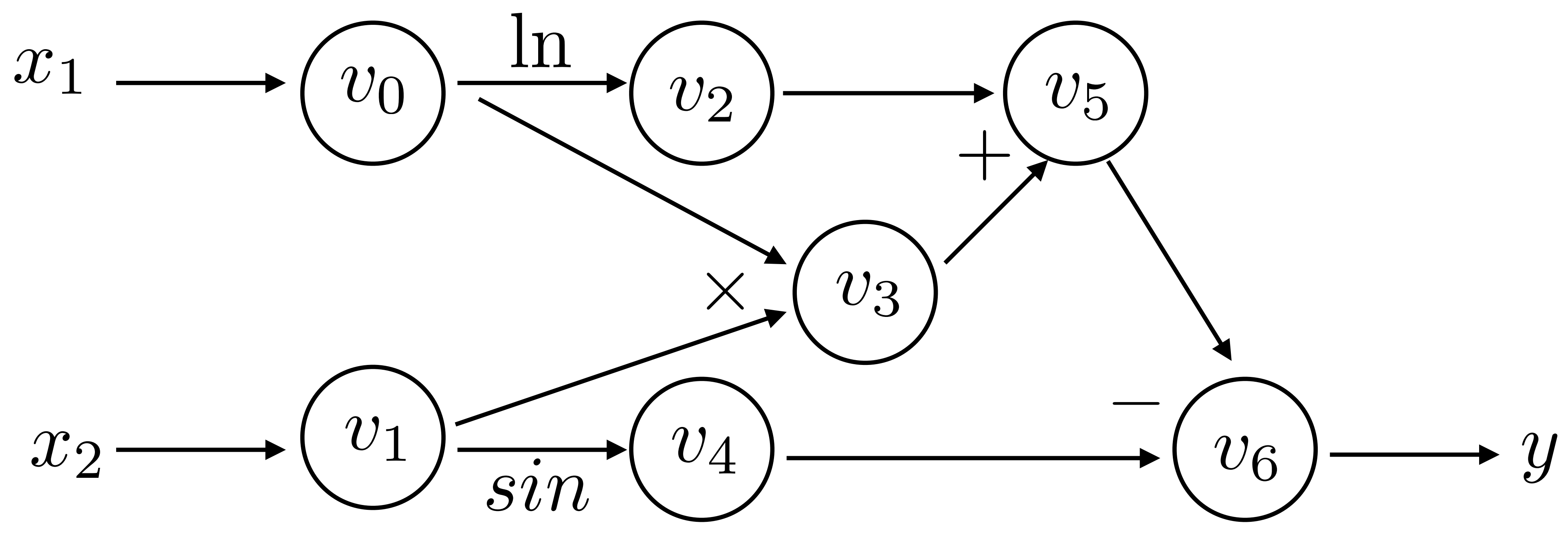
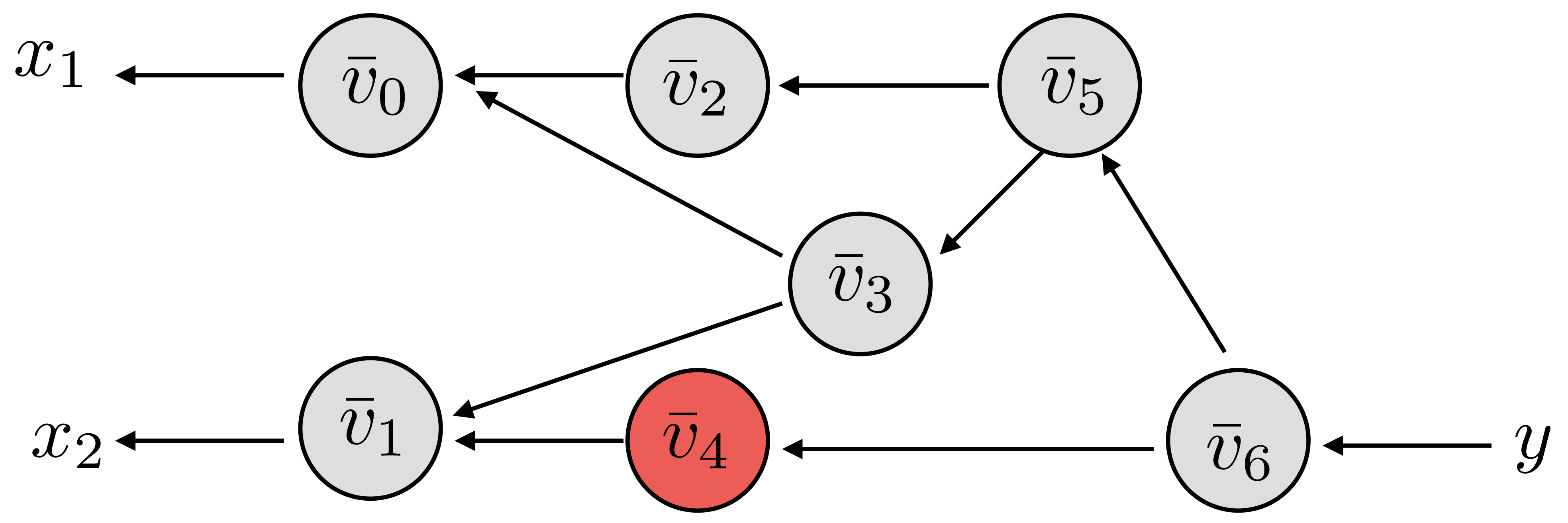
Backwards Derivative Trace:

$\bar{v}_5 = \bar{v}_6 \dfrac{\partial v_6}{\partial v_5} = \bar{v}_6 \cdot 1$	1x1 = 1
$\bar{v}_6 = \dfrac{\partial y}{\partial v_6}$	1

AutoDiff - **Reverse Mode**





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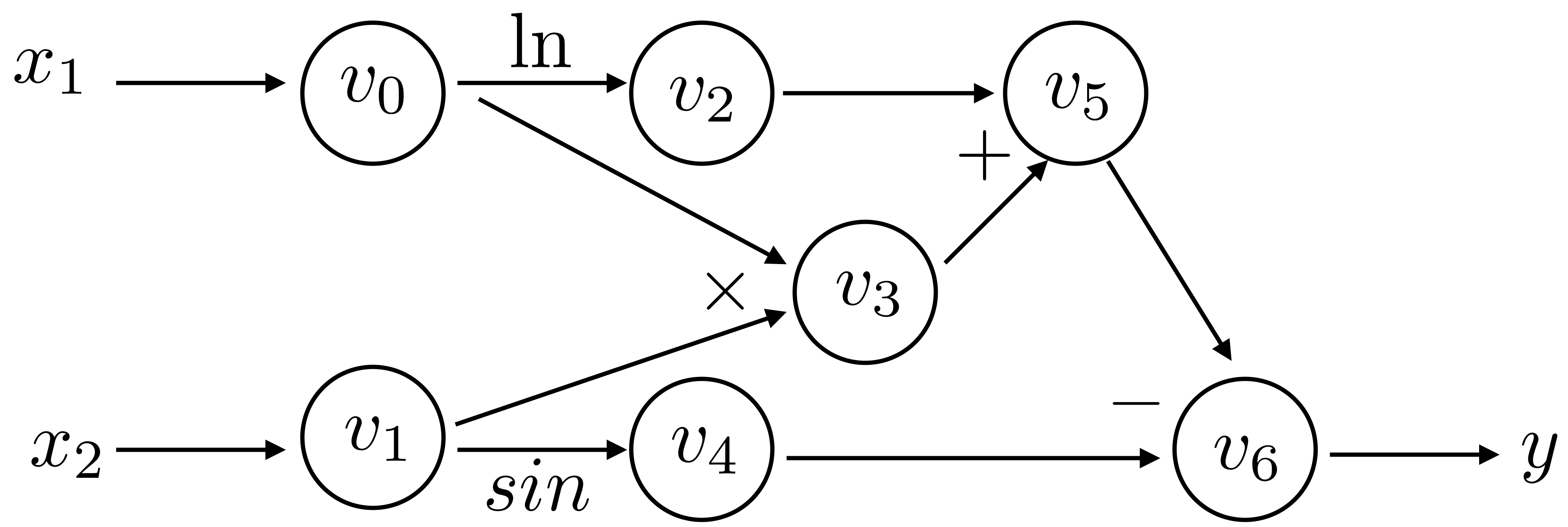
Backwards Derivative Trace:

$\bar{v}_4 = \bar{v}_6 \dfrac{\partial v_6}{\partial v_4} = \bar{v}_6 \cdot (-1)$	1x-1 = -1
$\bar{v}_5 = \bar{v}_6 \dfrac{\partial v_6}{\partial v_5} = \bar{v}_6 \cdot 1$	1x1 = 1
$\bar{v}_6 = \dfrac{\partial y}{\partial v_6}$	1

AutoDiff - **Reverse Mode**



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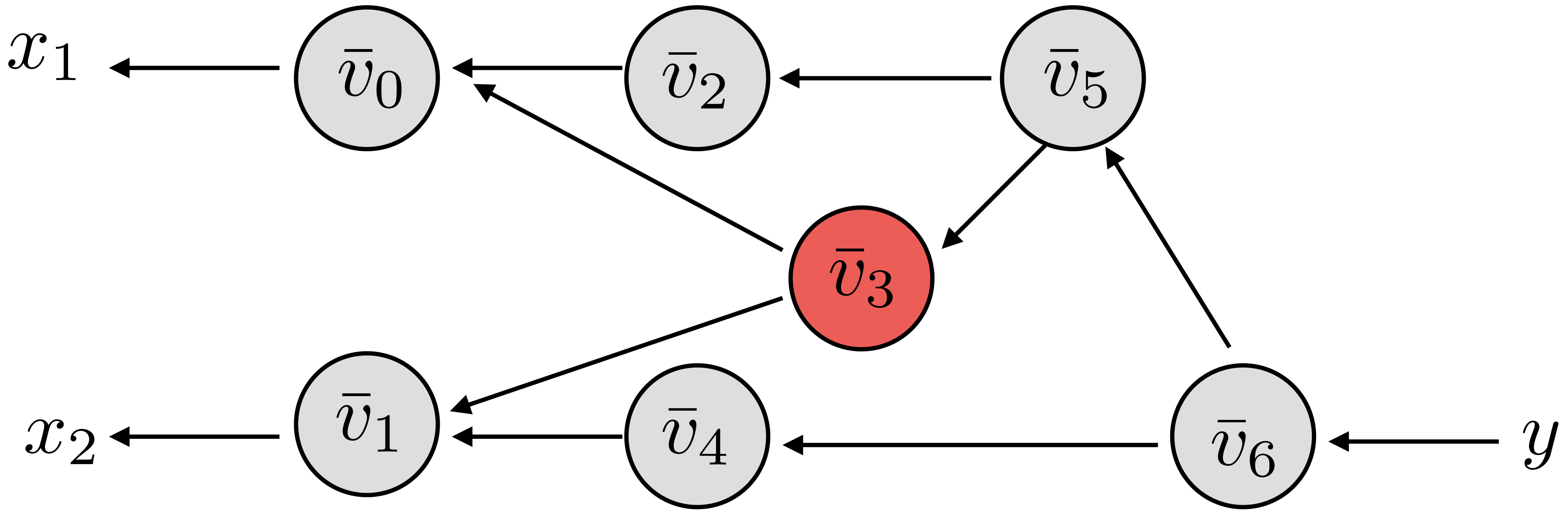

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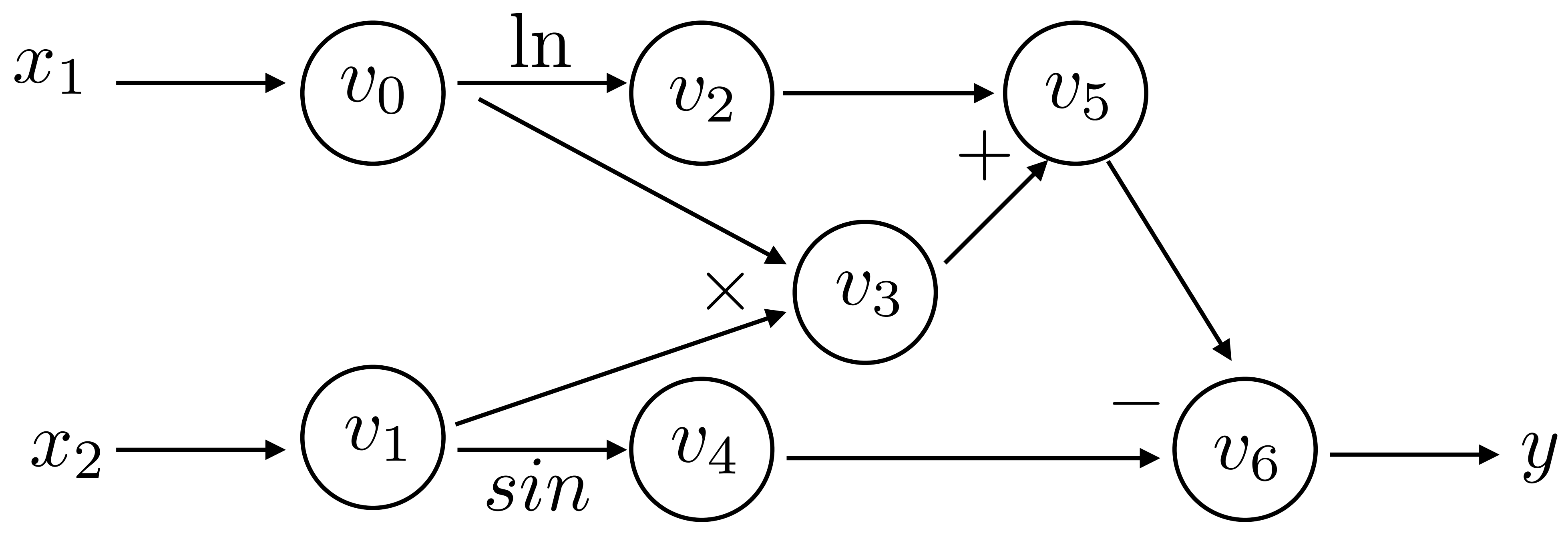
AutoDiff - **Reverse Mode**



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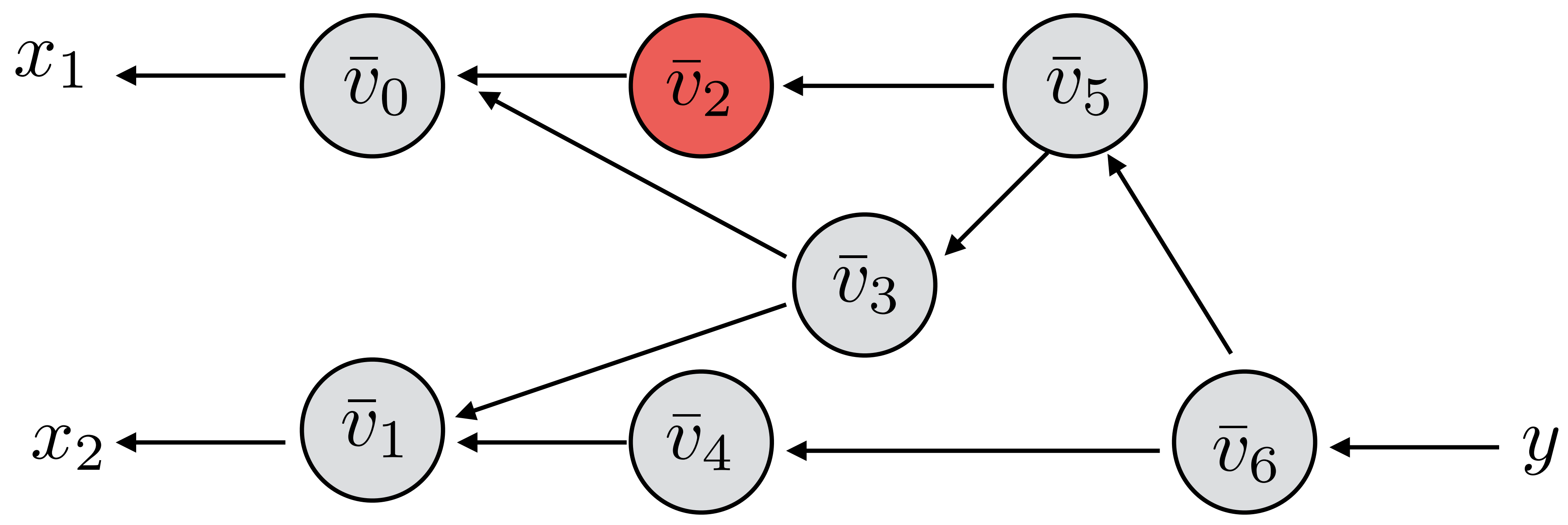

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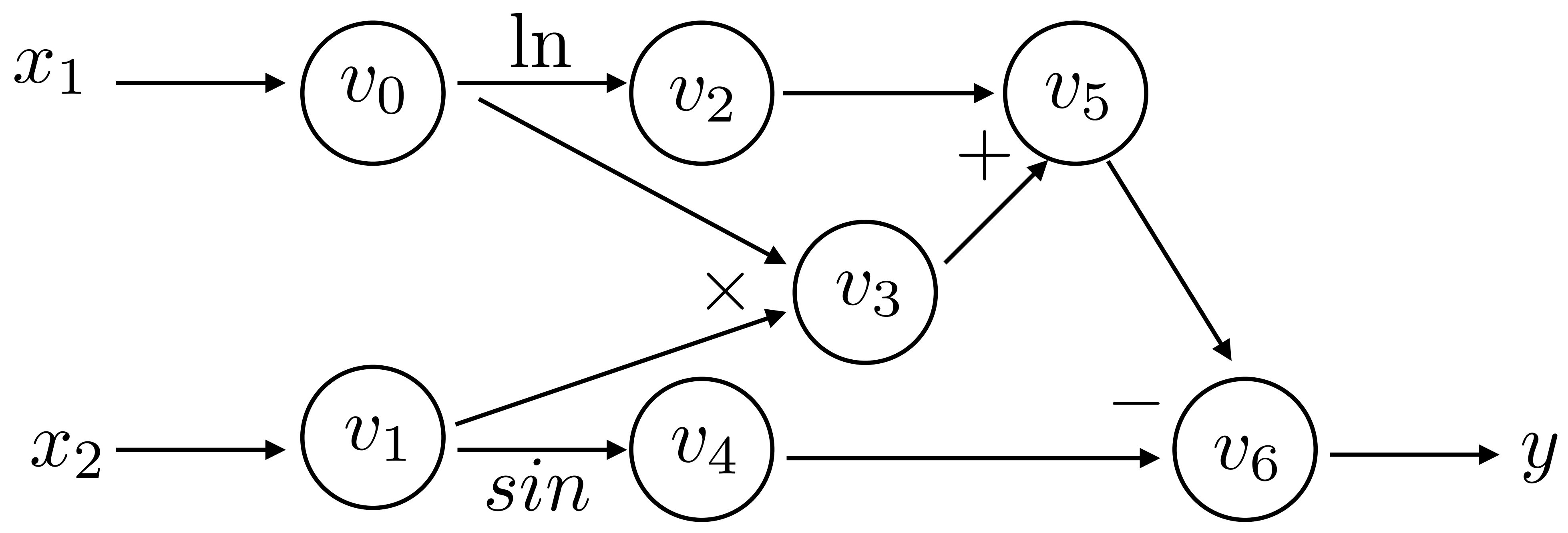
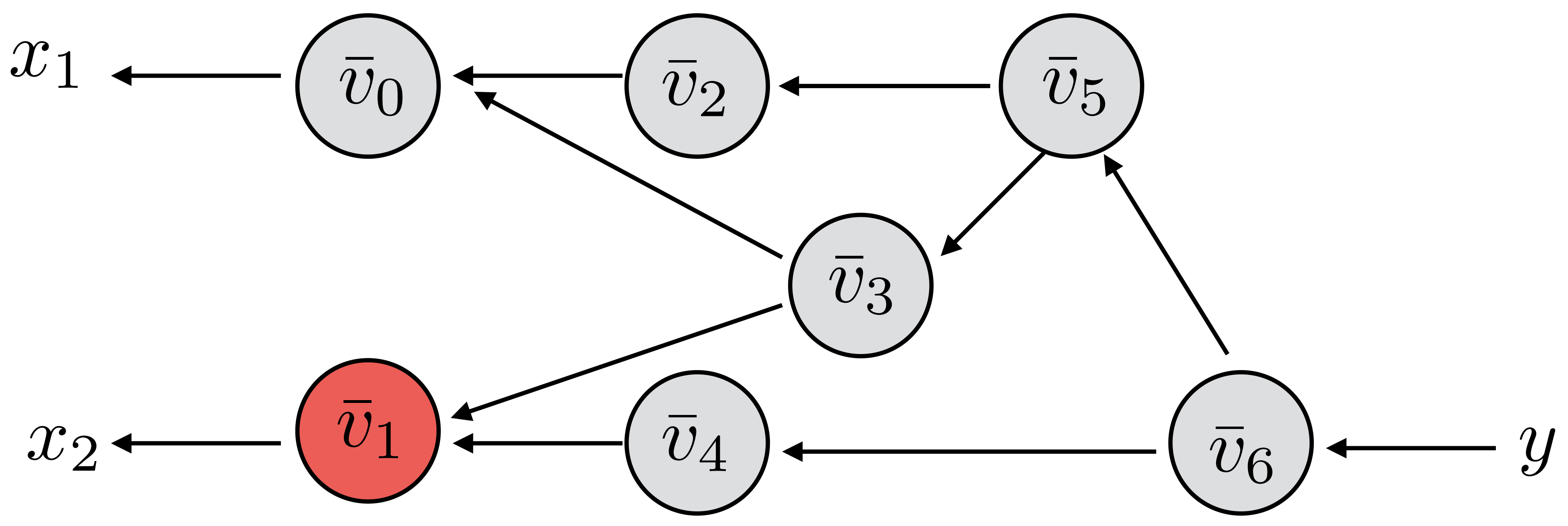
AutoDiff - **Reverse Mode**





Backwards Derivative Trace:

$\bar{v}_1 = \bar{v}_3 \frac{\partial v_3}{\partial v_1} + \bar{v}_4 \frac{\partial v_4}{\partial v_1} = \bar{v}_3 v_0 + \bar{v}_4 cos(v_1)$	1.716
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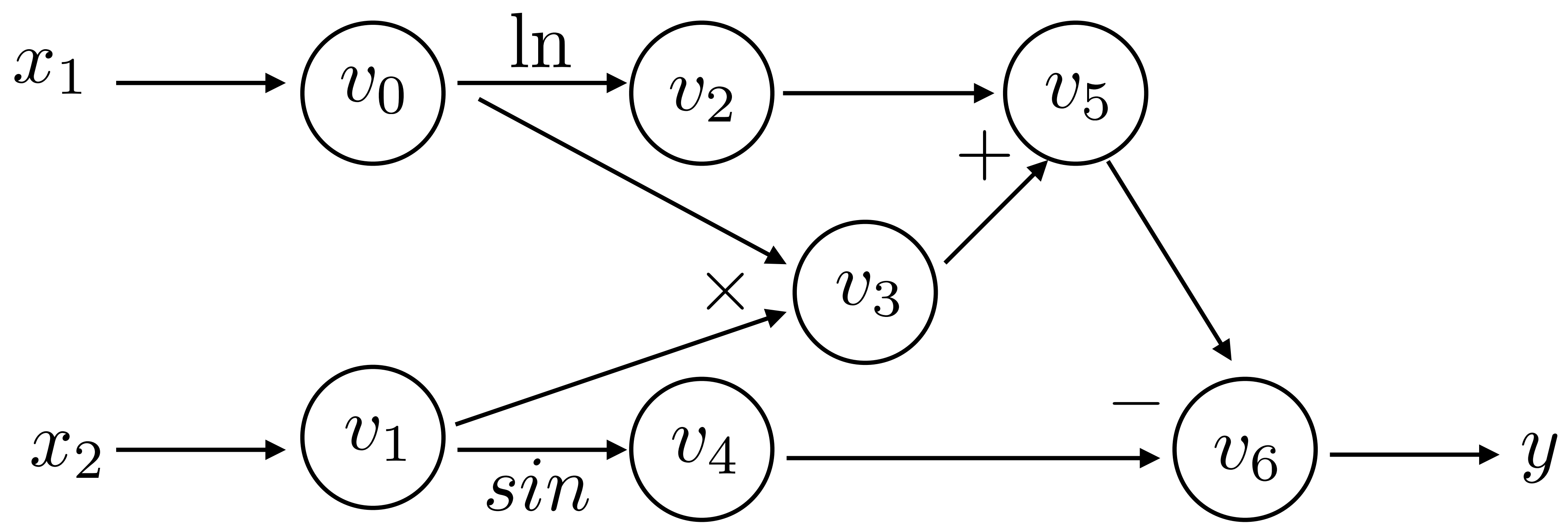

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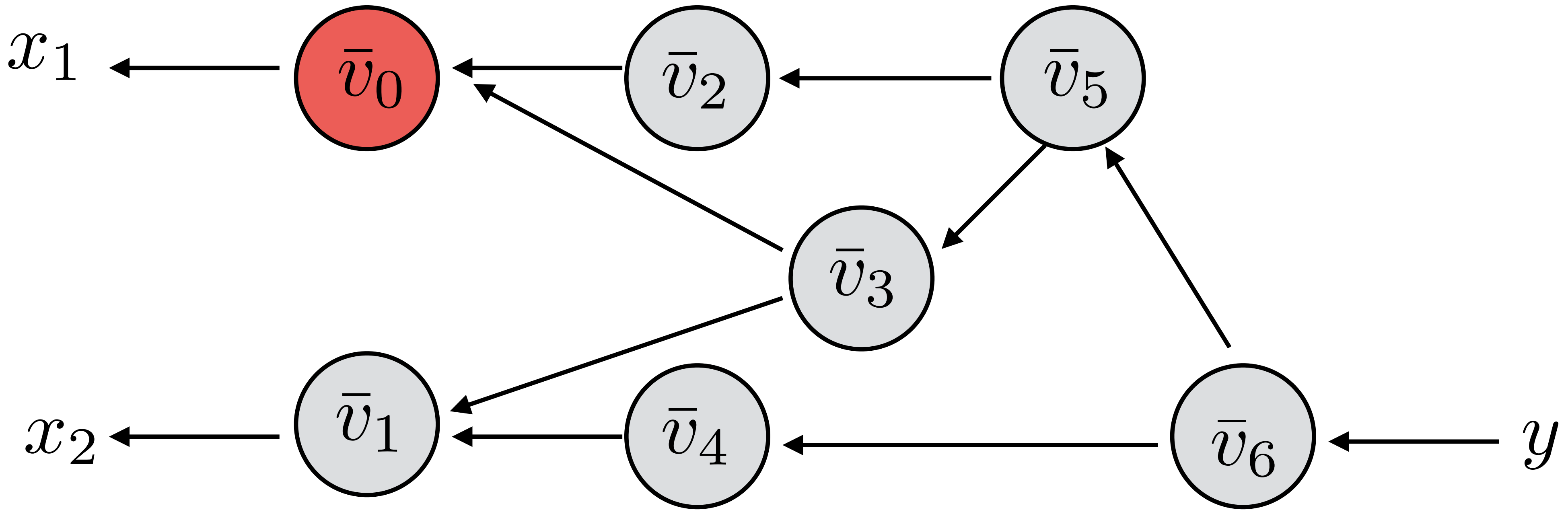

Backwards Derivative Trace:

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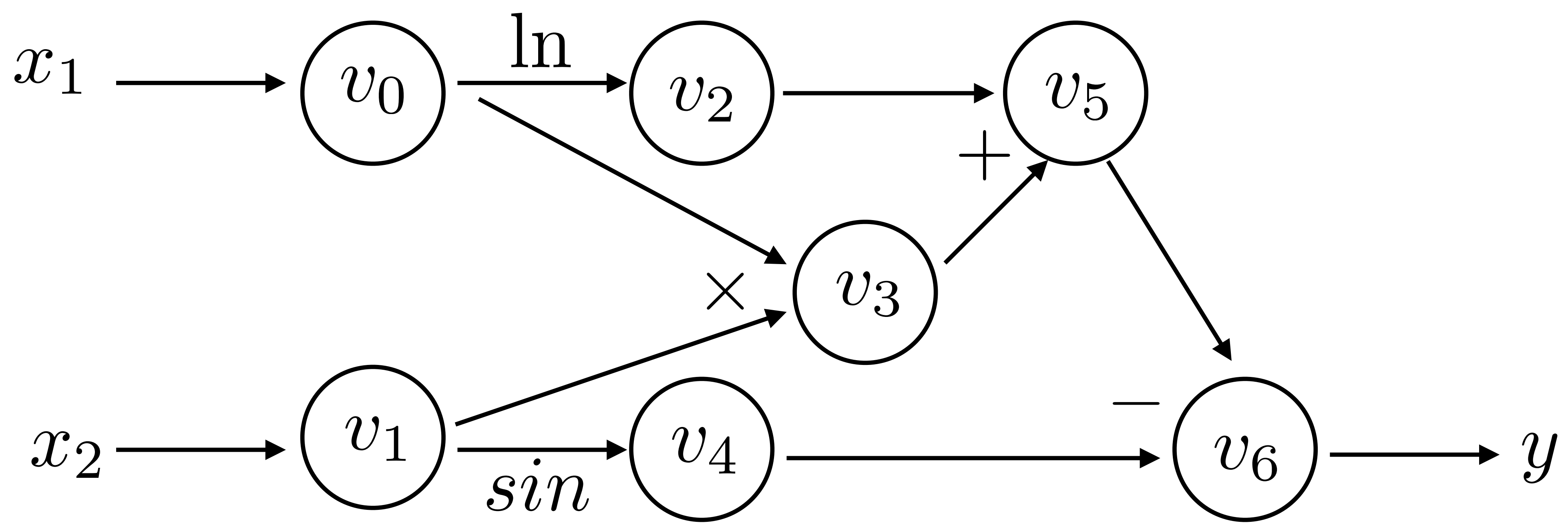
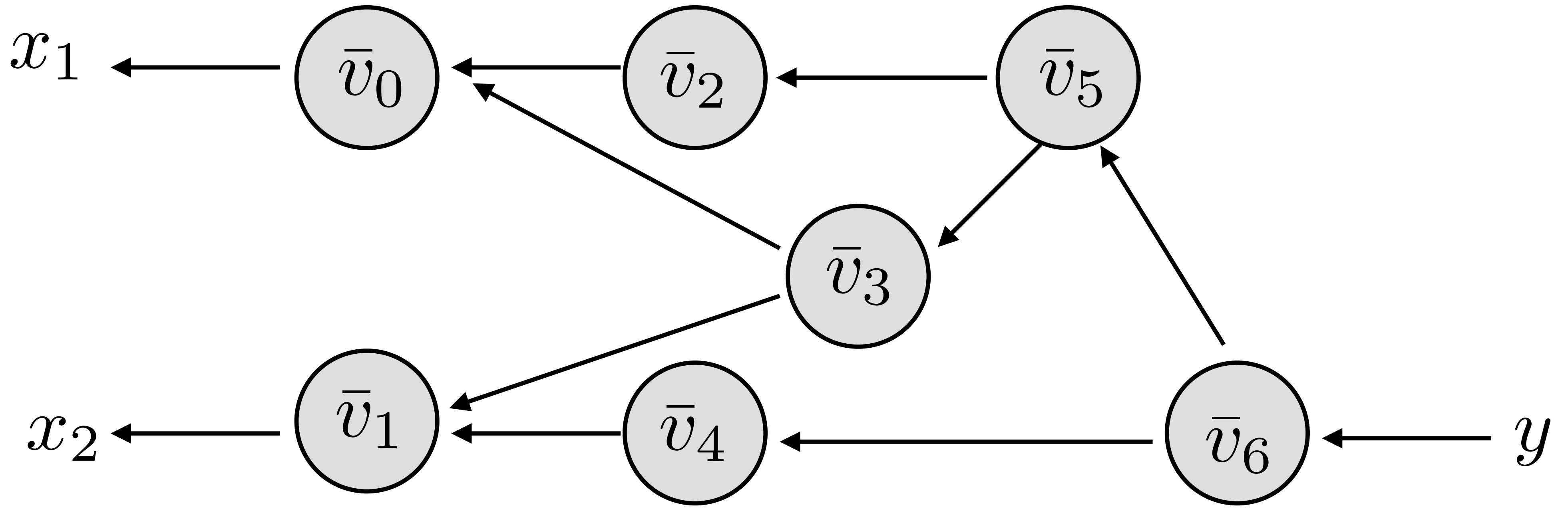
$\bar{v}_6 = \frac{\partial y}{\partial v_6}$	1

AutoDiff - **Reverse Mode**





Backwards Derivative Trace:

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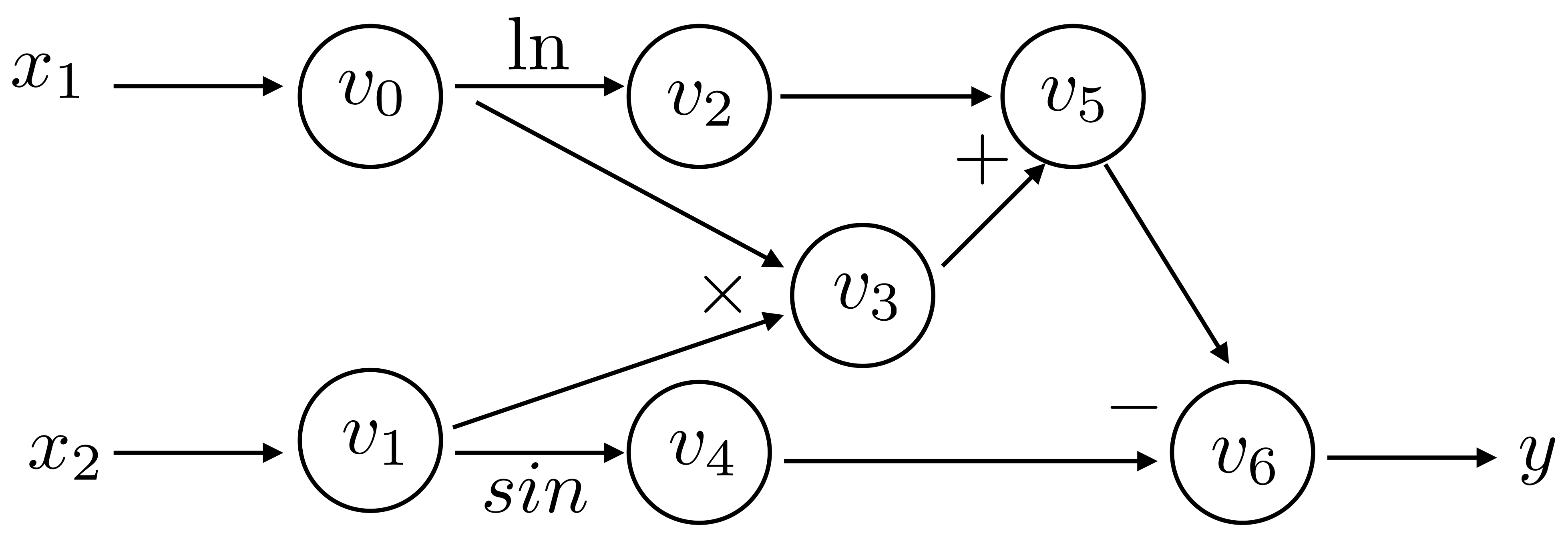
Automatic Differentiation (AutoDiff)

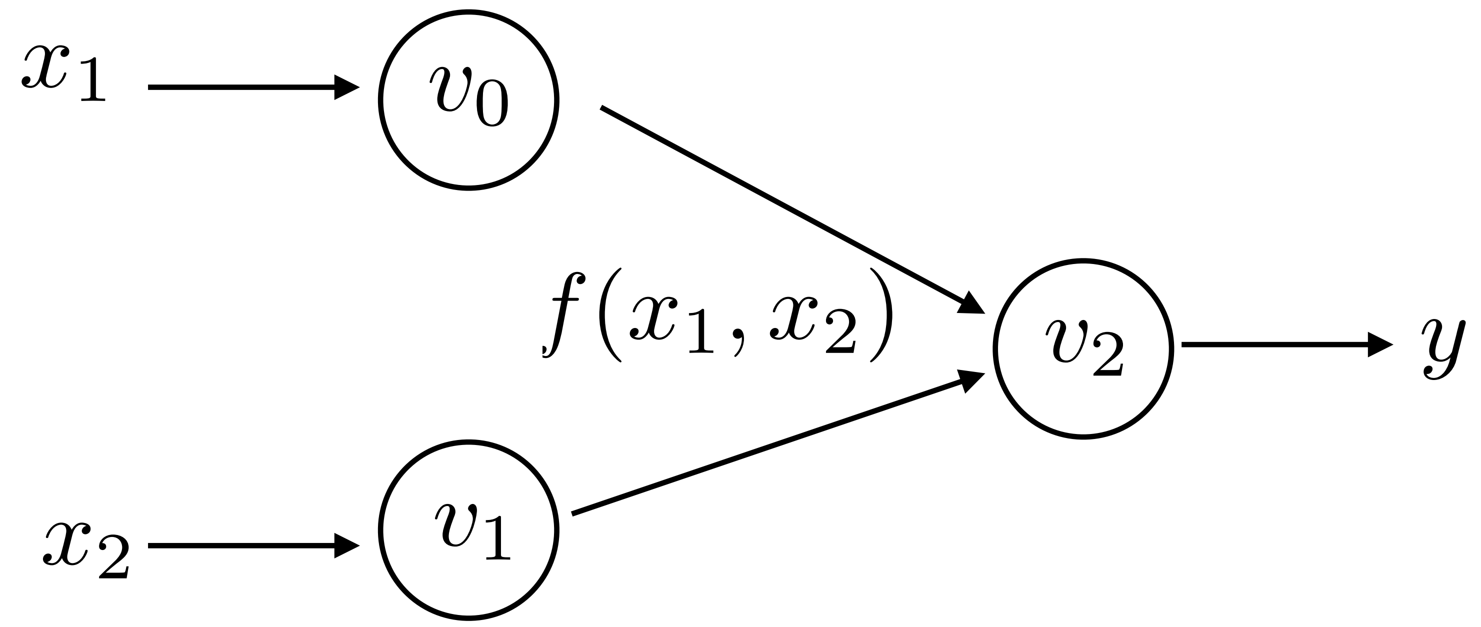
$$y = f(x_1, x_2) = \ln(x_1) + x_1 x_2 - sin(x_2)$$

AutoDiff can be done at various **granularities**

Elementary function granularity:

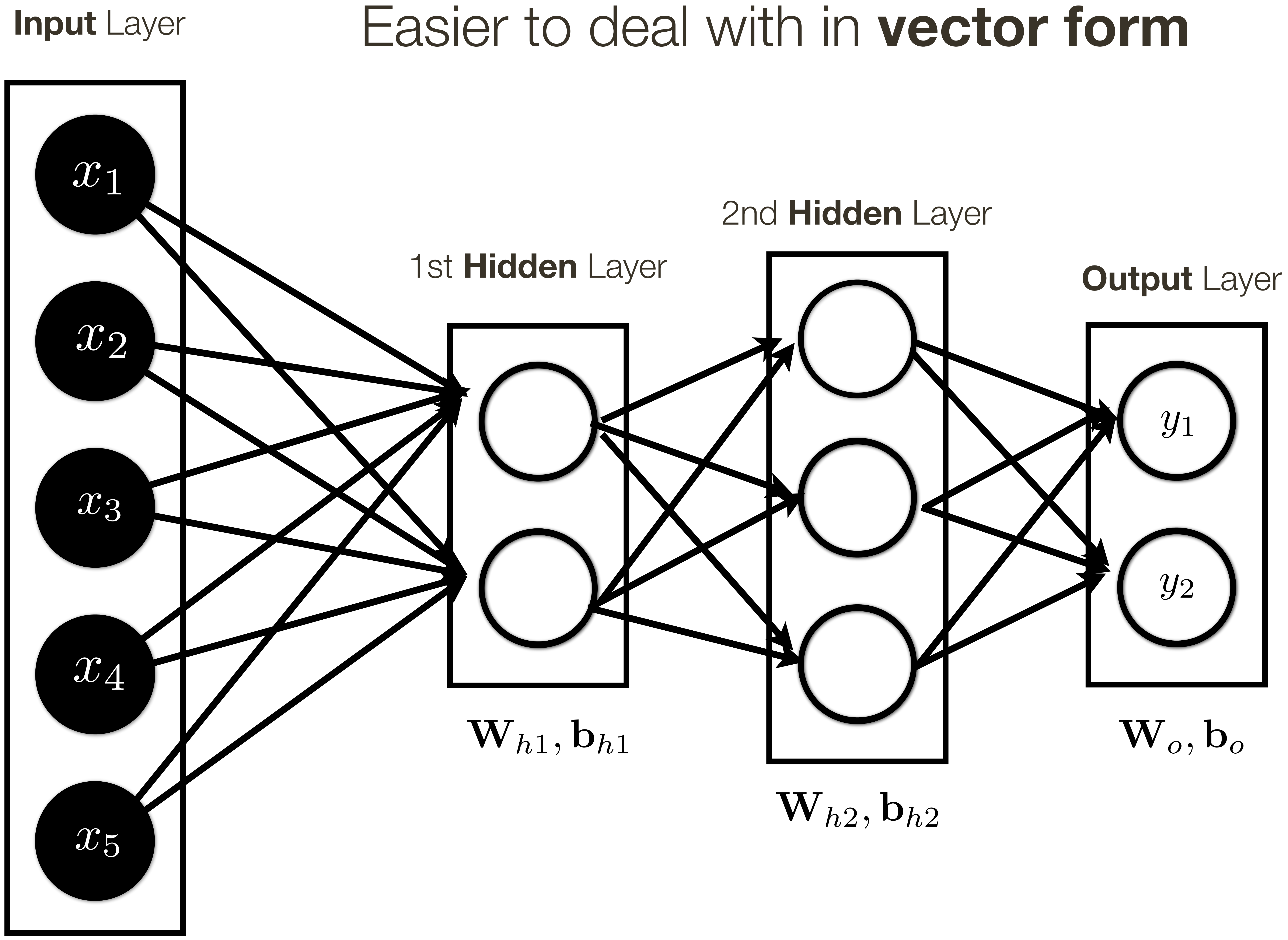


Complex function granularity:



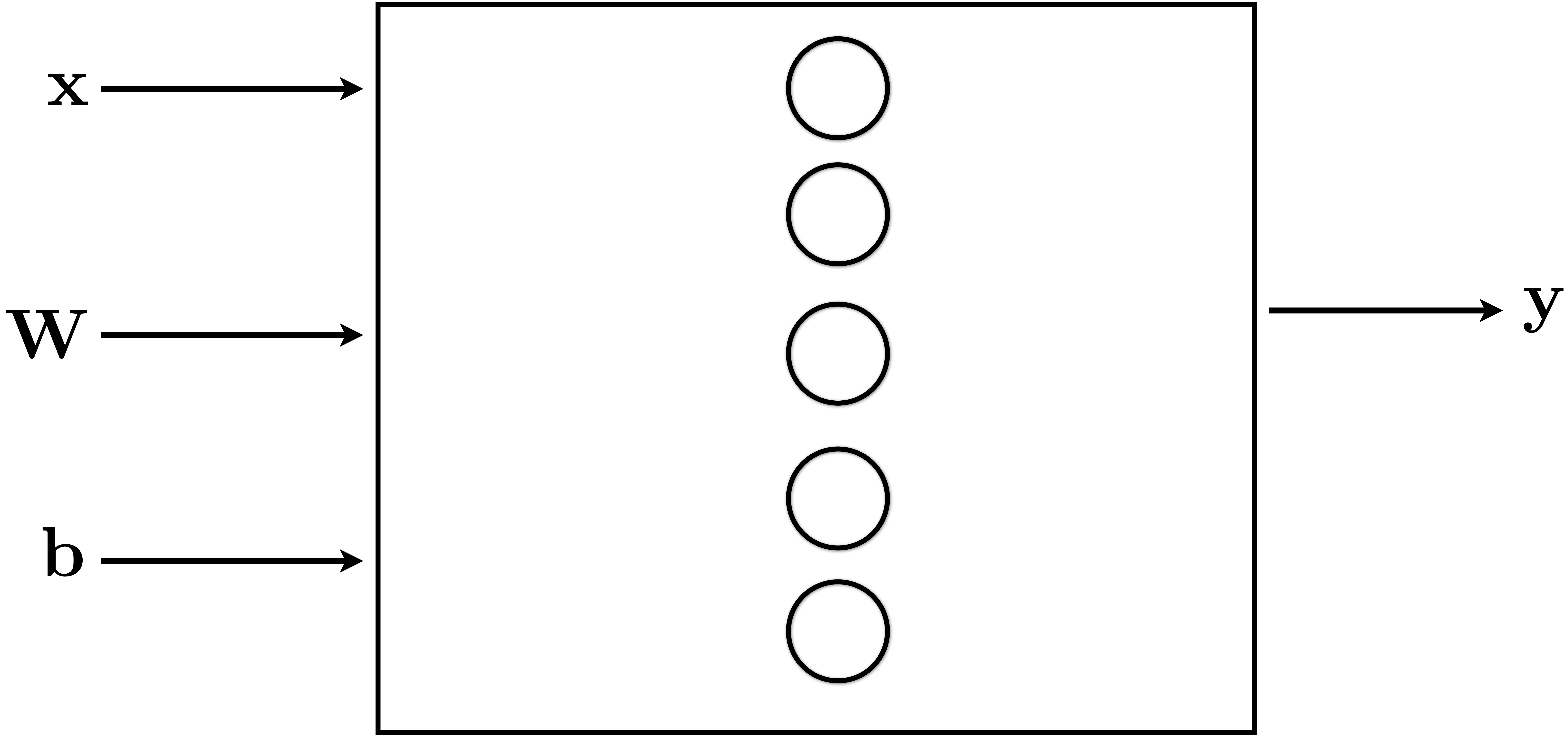
Backpropagation Practical Issues

Easier to deal with in **vector form**



Backpropagation Practical Issues

$$\mathbf{y} = f(\mathbf{W}, \mathbf{b}, \mathbf{x}) = \mathbf{sigmoid}(\mathbf{W} \cdot \mathbf{x} + \mathbf{b})$$

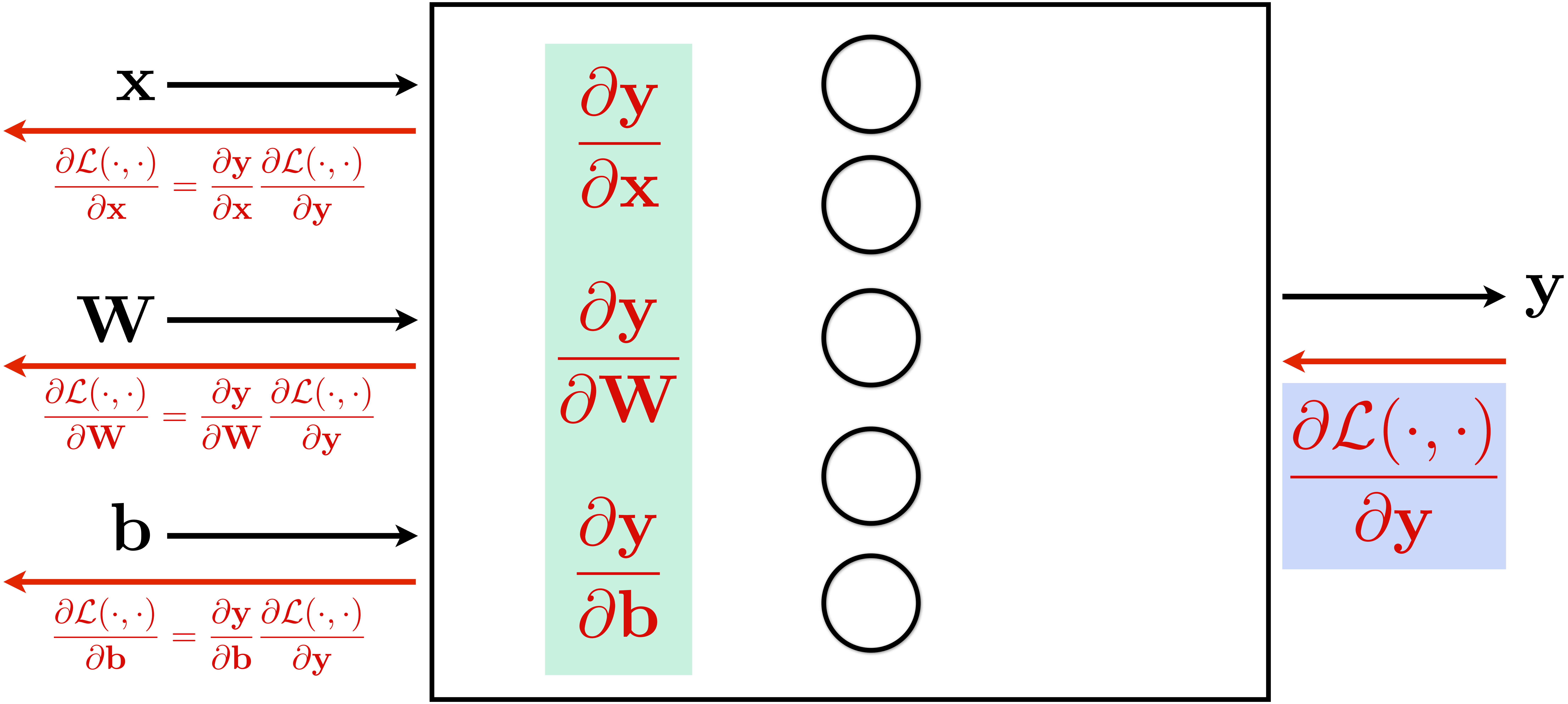


Backpropagation Practical Issues

"**local**" Jacobians
(matrix of partial derivatives, e.g. size |x| x |y|)

"**backprop**" Gradient

$$\mathbf{y} = f(\mathbf{W}, \mathbf{b}, \mathbf{x}) = \mathbf{sigmoid}(\mathbf{W} \cdot \mathbf{x} + \mathbf{b})$$



Jacobian of Sigmoid layer

$\mathbf{x}, \mathbf{y} \in \mathbb{R}^{2048}$

Element-wise sigmoid layer:

What is the dimension of **Jacobian**?

What does it look like?

If we are working with a mini batch of 100 inputs-output pairs, technically Jacobian is a matrix 204,800 x 204,800

Backpropagation: Common questions

Question: Does BackProp only work for certain layers?

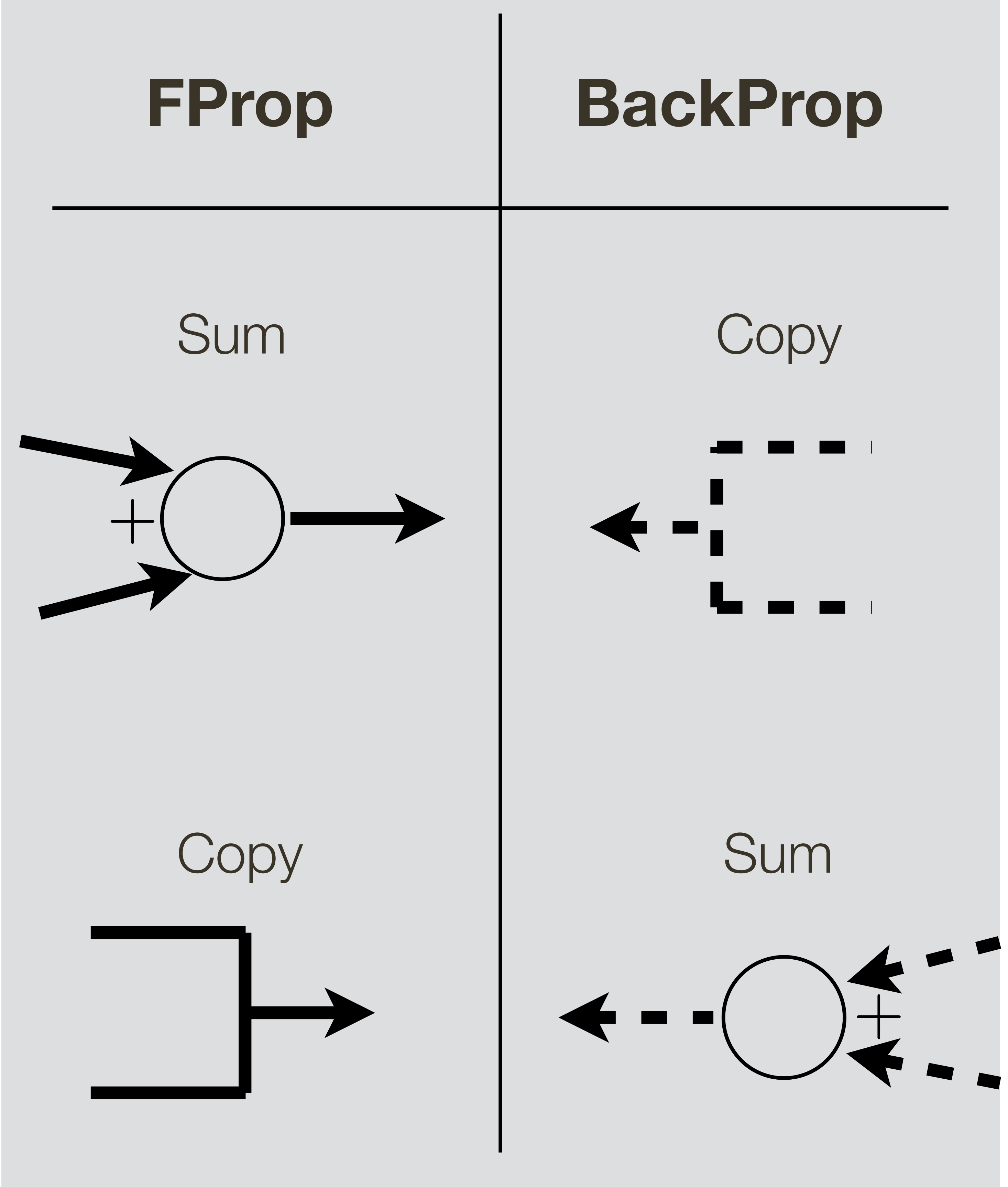
Answer: No, for any differentiable functions

Question: What is computational cost of BackProp?

Answer: On average about twice the forward pass

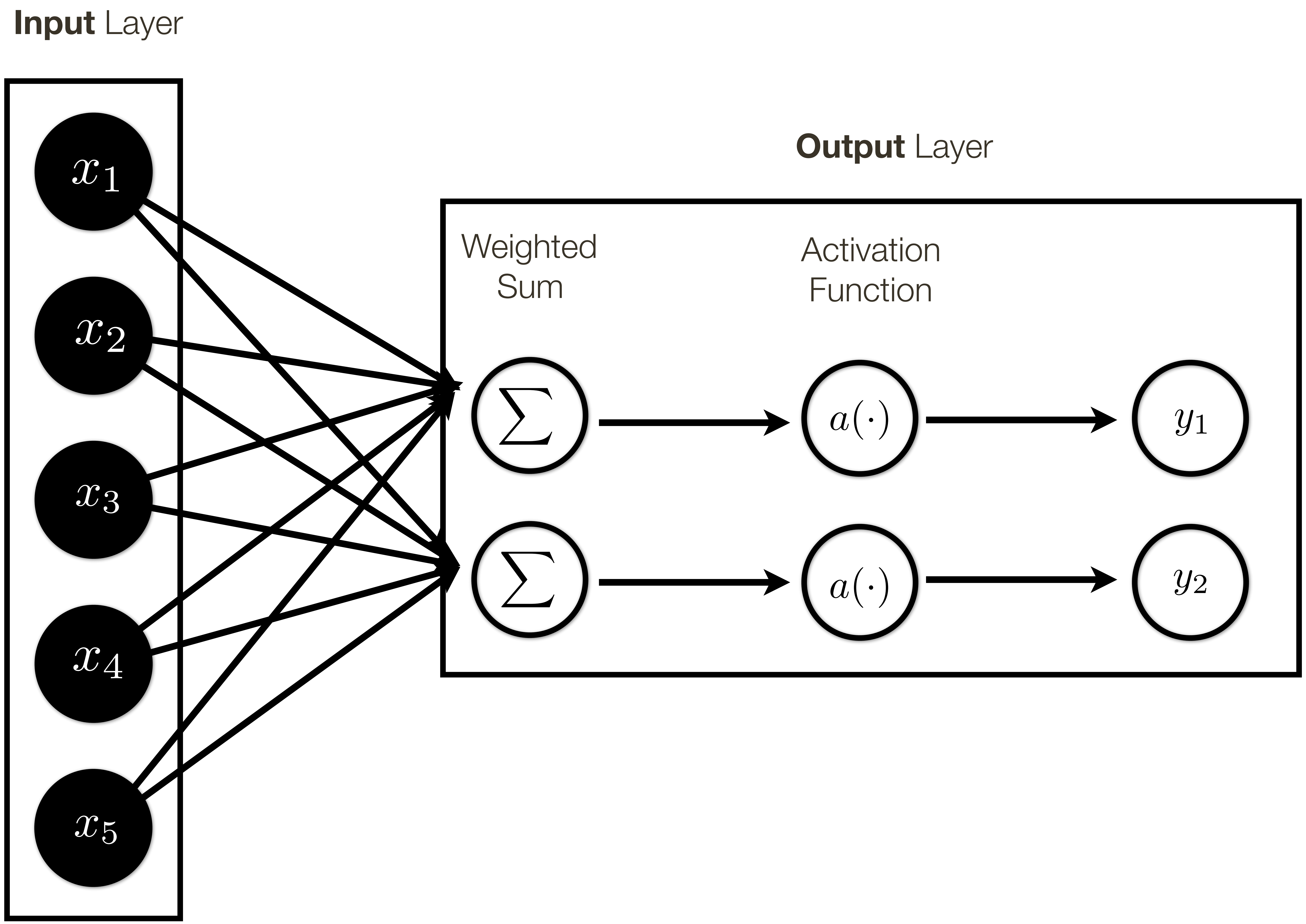
Question: Is BackProp a dual of forward propagation?

Answer: Yes

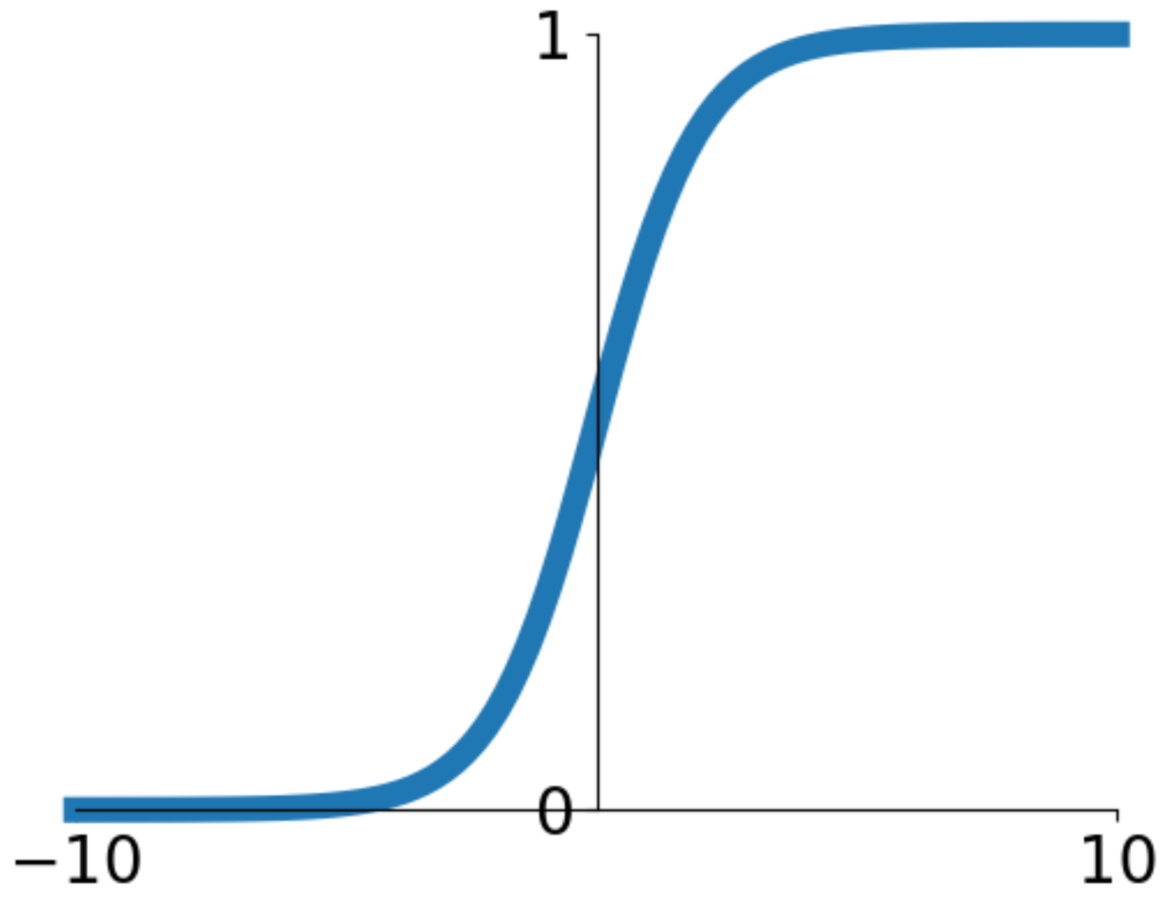


* Adopted from slides by Marc'Aurelio Ranzato

Activation Function: Sigmoid

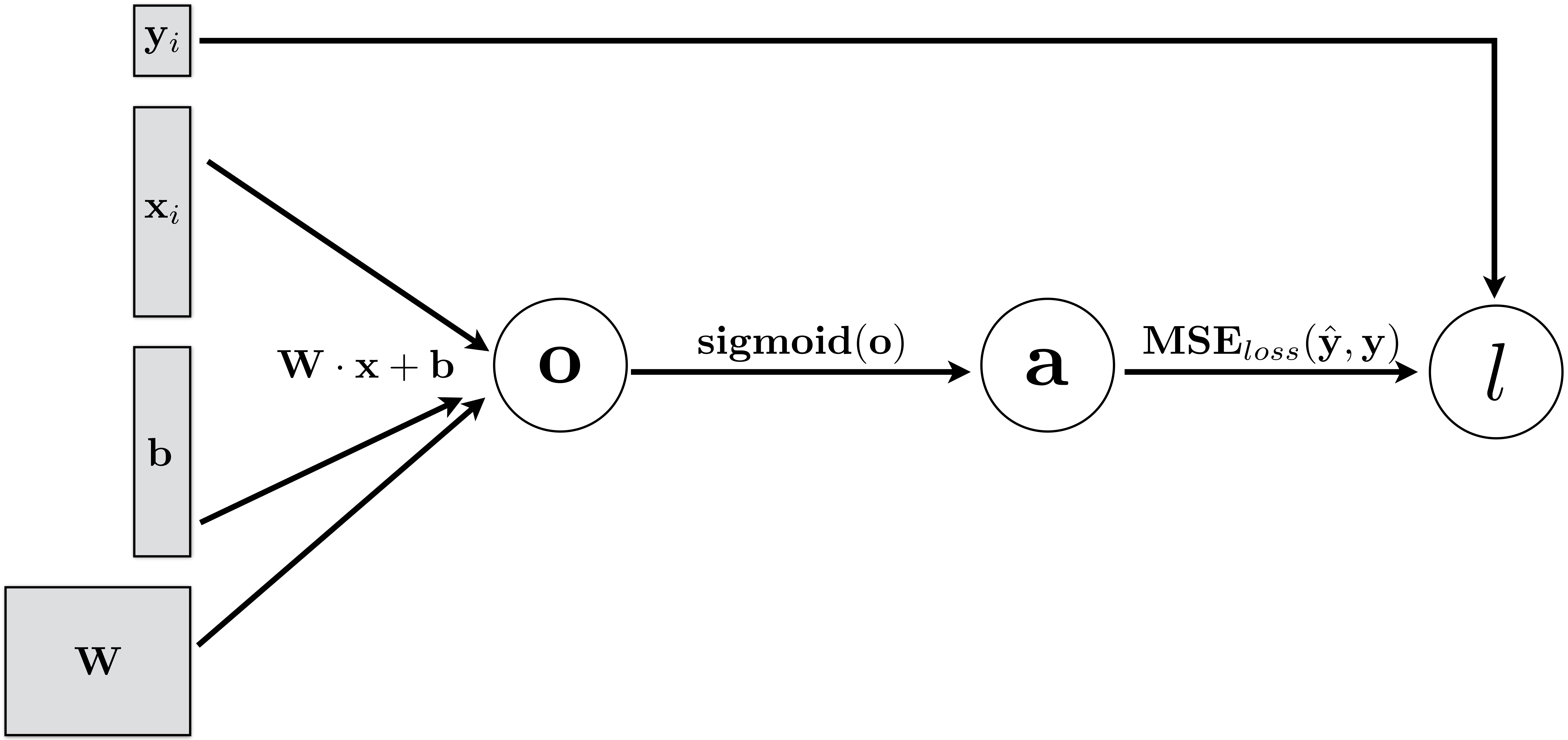


$$a(x) = \textbf{sigmoid}(x) = \frac{1}{1+e^{-x}}$$



Sigmoid Activation

Computational Graph: 1-layer network



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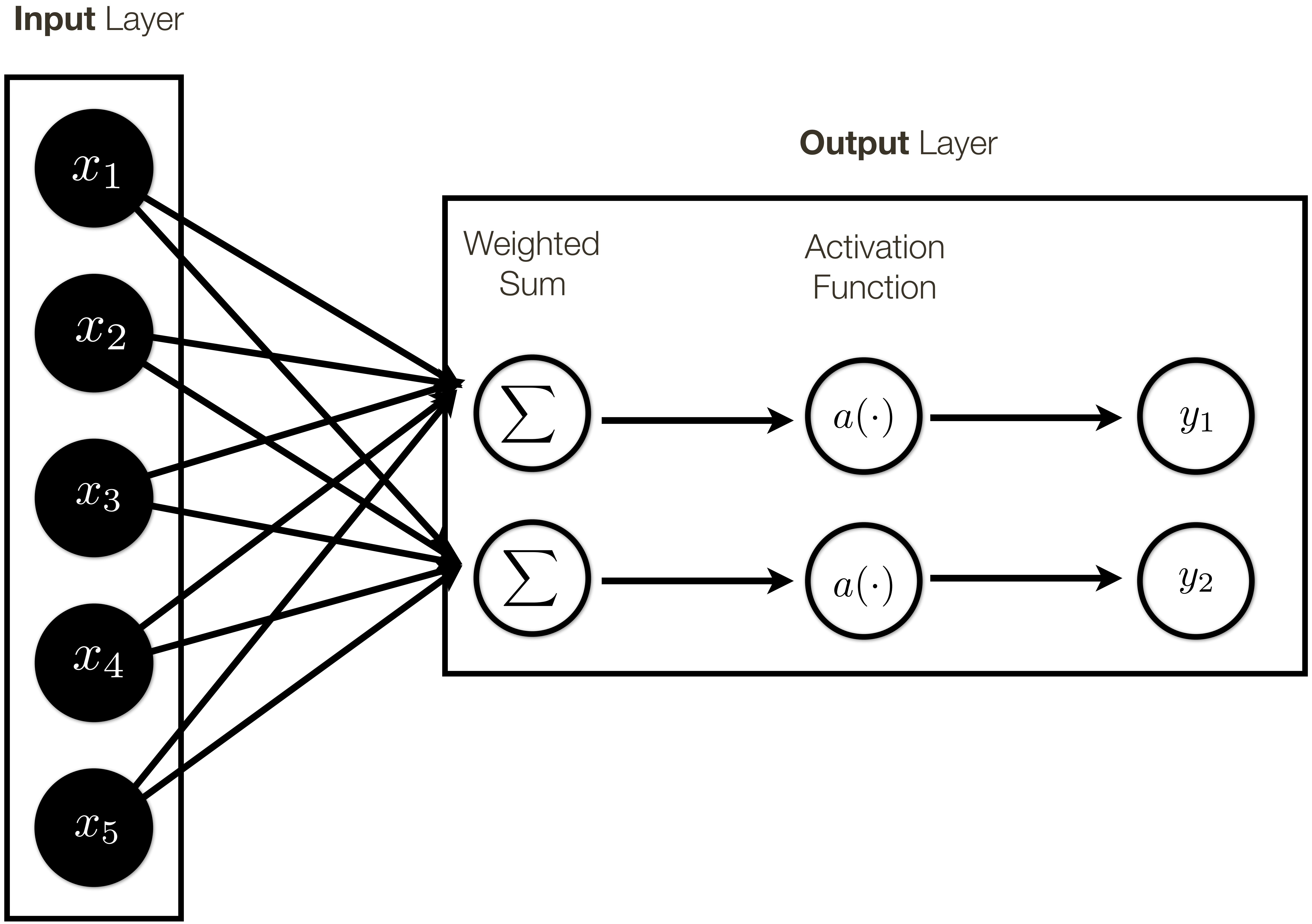

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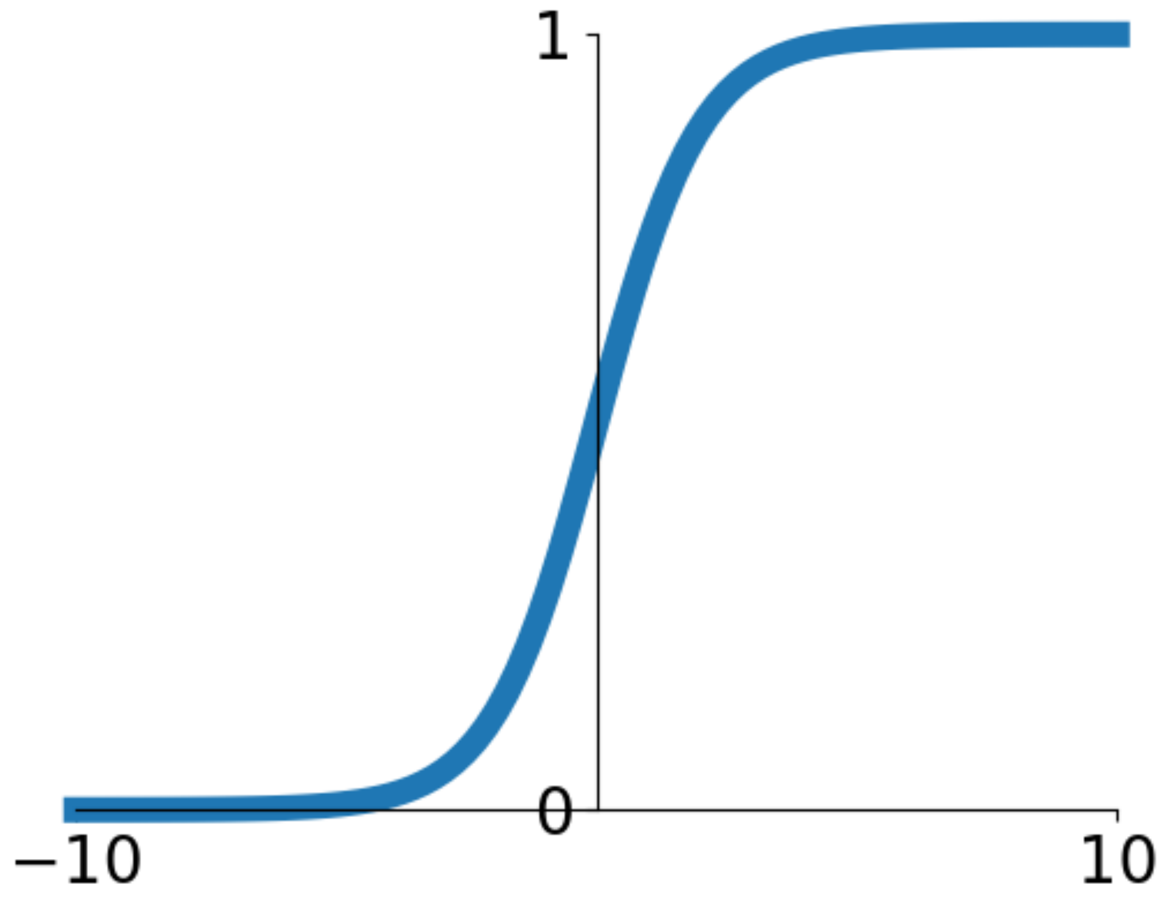


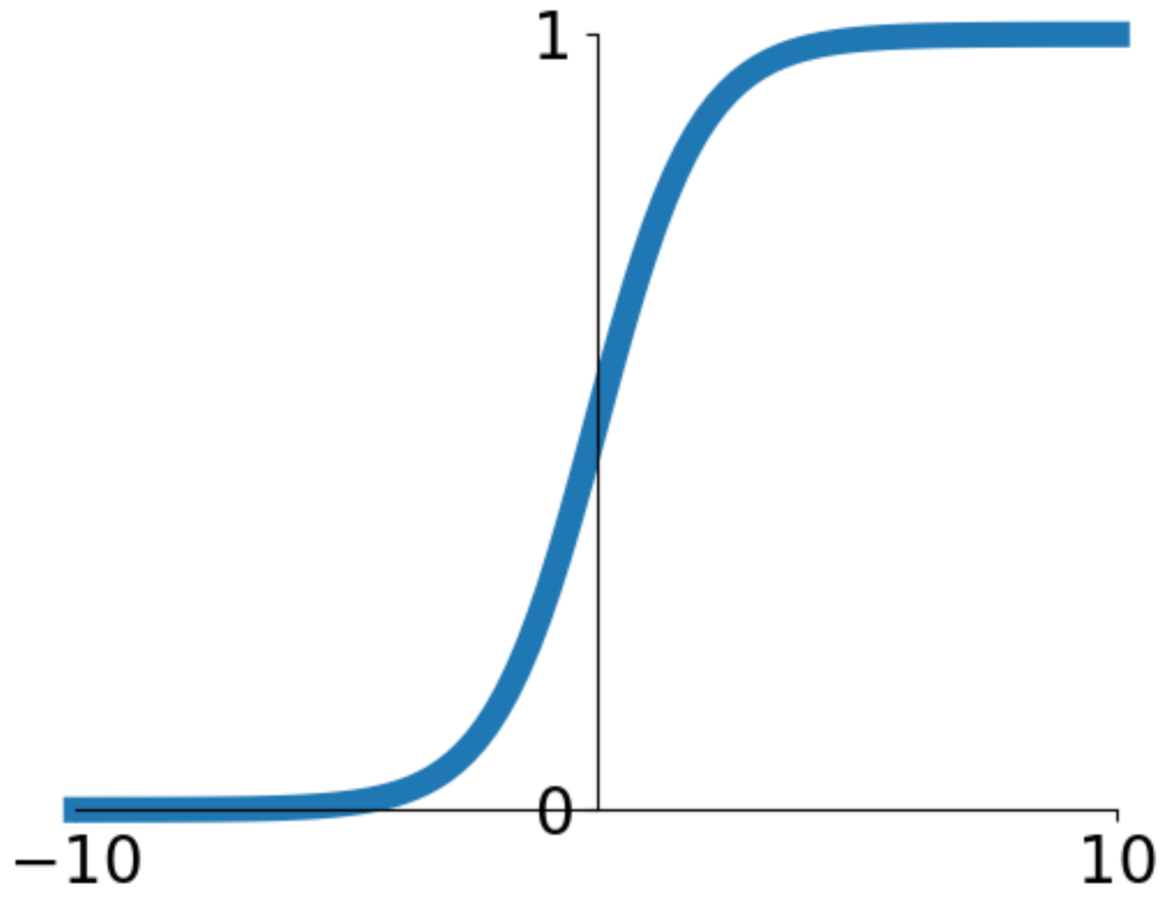
Sigmoid Activation

Activation Function: Sigmoid

$$a(x) = \mathbf{sigmoid}(x) = \frac{1}{1 + e^{-x}}$$

Pros:

- Squishes everything in the range [0,1]
- Can be interpreted as "probability"
- Has well defined gradient everywhere



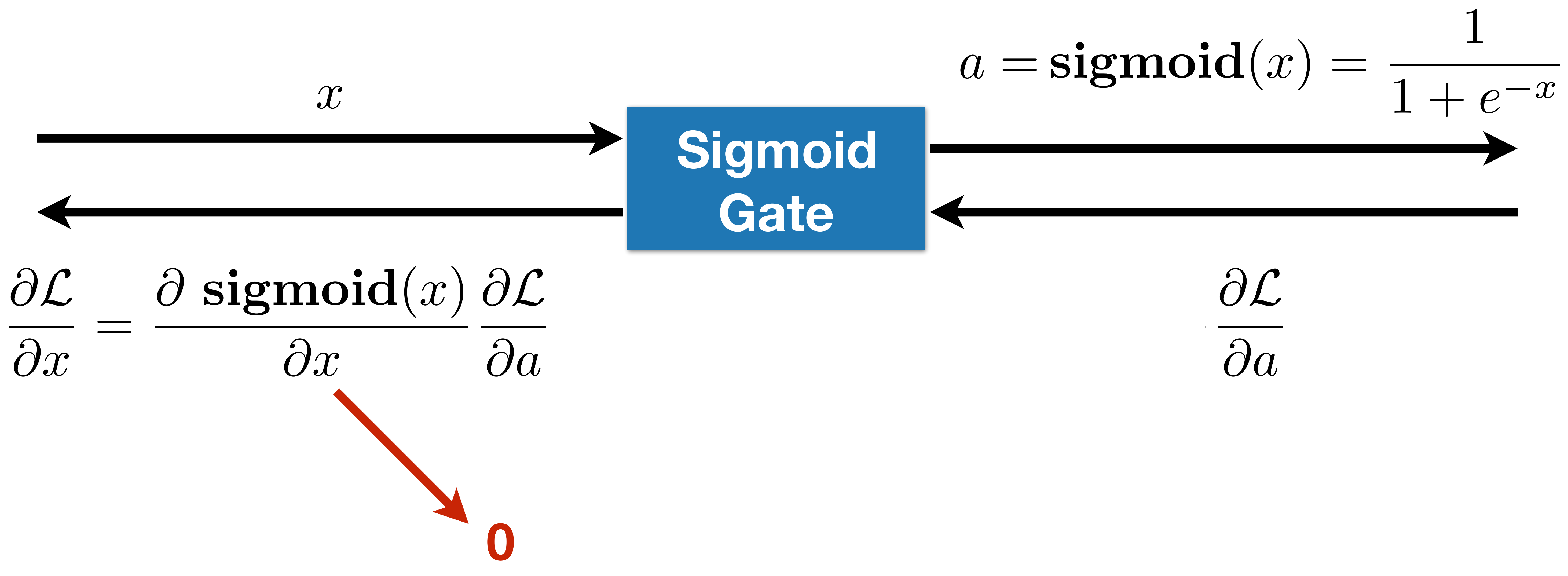
Sigmoid Activation

Cons:

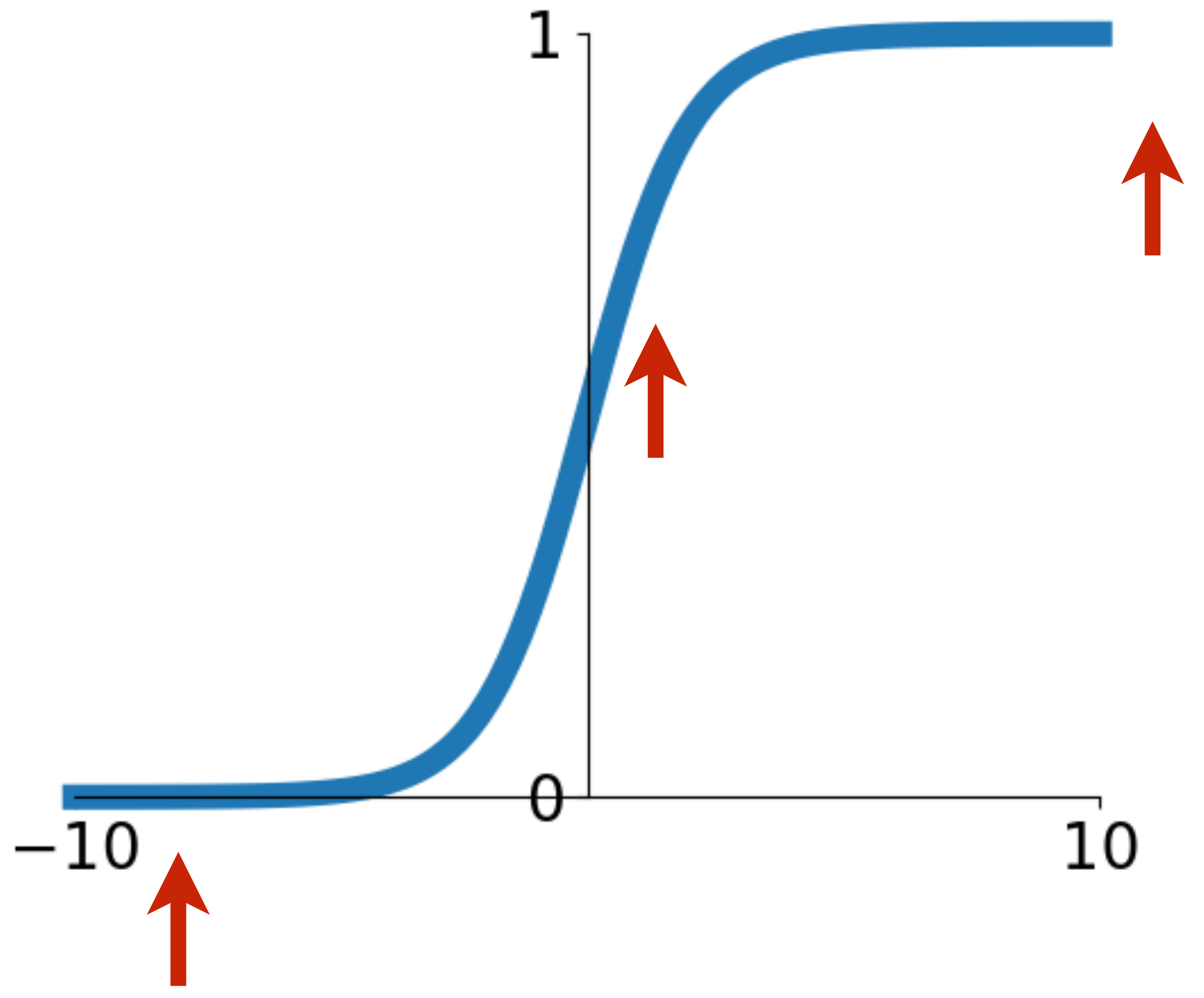
- Saturated neurons "kill" the gradients
- Non-zero centered
- Could be expensive to compute

* slide adopted from Li, Karpathy, Johnson's **CS231n at Stanford**

Activation Function: Sigmoid



$$a(x) = \mathbf{sigmoid}(x) = \frac{1}{1+e^{-x}}$$



Sigmoid Activation

Cons:

- Saturated neurons **“kill” the gradients**
- Non-zero centered
- Could be expensive to compute

Activation Function: Tanh

$$a(x) = \mathbf{tanh}(x) = 2 \cdot \mathbf{sigmoid}(2x) - 1$$

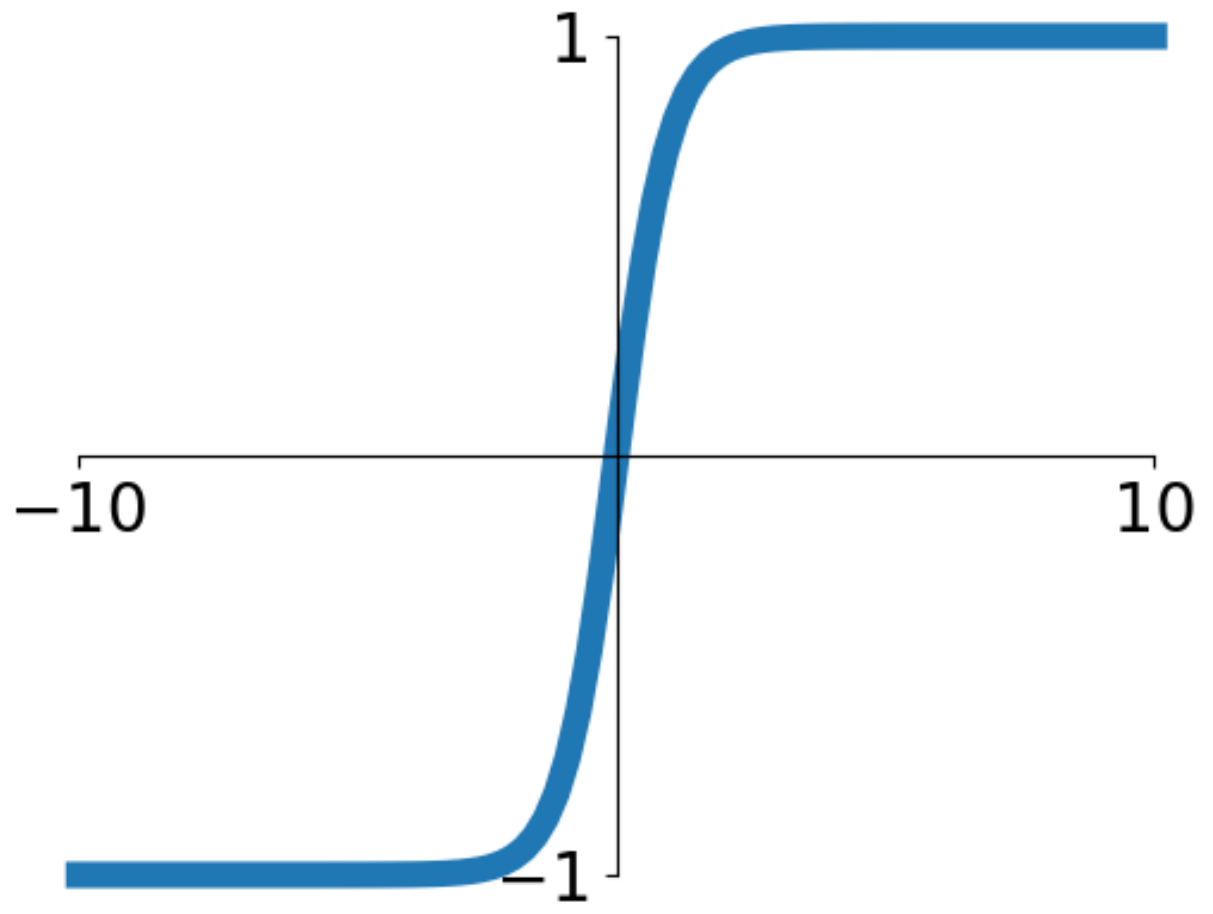
$$a(x) = \mathbf{tanh}(x) = \frac{2}{1 + e^{-2x}} - 1$$

Pros:

- Squishes everything in the range [-1,1]
- Centered around zero
- Has well defined gradient everywhere

Cons:

- Saturated neurons "kill" the gradients



Tanh Activation

* slide adopted from Li, Karpathy, Johnson's **CS231n at Stanford**

Activation Function: Rectified Linear Unit (ReLU)

$$a(x) = max(0, x)$$

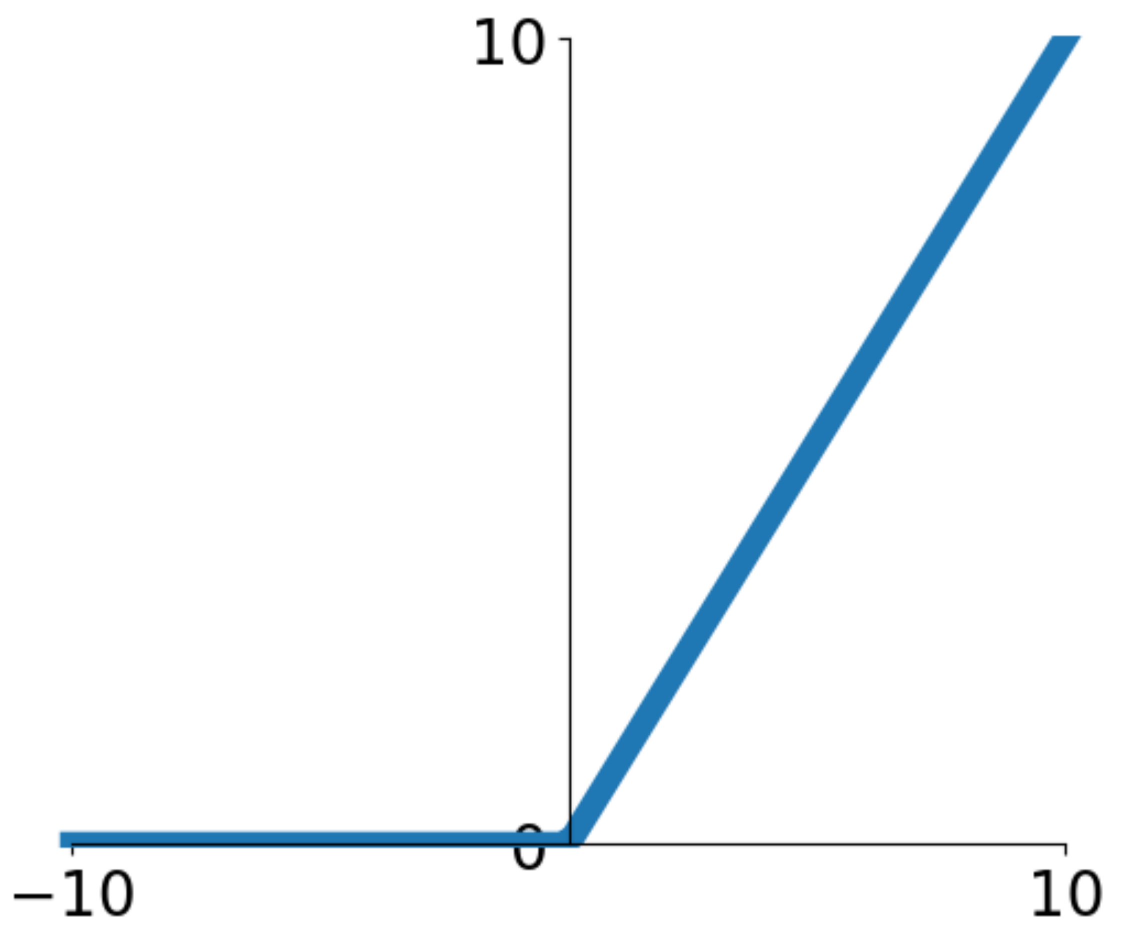
$$a'(x) = \begin{cases} 1 & \text{if } x \geq 0 \\ 0 & \text{if } x < 0 \end{cases}$$

Pros:

- Does not saturate (for x > 0)
- Computationally very efficient
- Converges faster in practice (e.g. 6 times faster)

Cons:

- Not zero centered



ReLU Activation

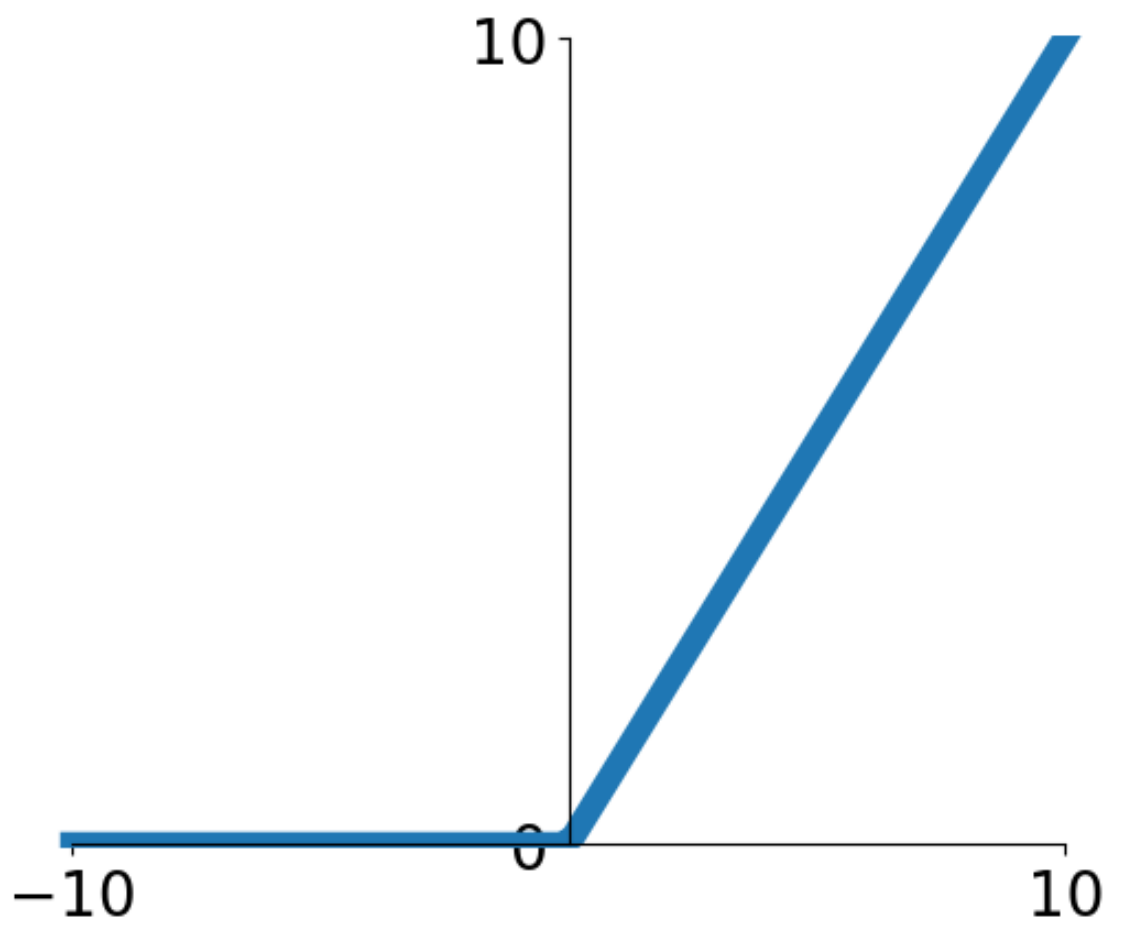
Activation Function: Rectified Linear Unit (ReLU)

$$a(x) = max(0, x)$$

$$a'(x) = \begin{cases} 1 & \text{if } x \geq 0 \\ 0 & \text{if } x < 0 \end{cases}$$

Question: What do ReLU layers accomplish?

Answer: Locally linear tiling, function is locally linear



ReLU Activation

Recall:

Conditions needed to prove NN is a universal approximator: Activation function needs to be well defined

$$\lim_{x \to \infty} a(x) = A$$

$$\lim_{x \to -\infty} a(x) = B$$

$$A \neq B$$

*slide adopted from http://neuralnetworksanddeeplearning.com/chap4.html

Recall:

Conditions needed to prove NN is a universal approximator: Activation function needs to be well defined

$$\lim_{x \to \infty} a(x) = A$$

$$\lim_{x \to -\infty} a(x) = B$$

$$A \neq B$$

Fun **Exercise:** Try to prove that network with ReLU is still a universal approximator (not too difficult if you think about it visually)

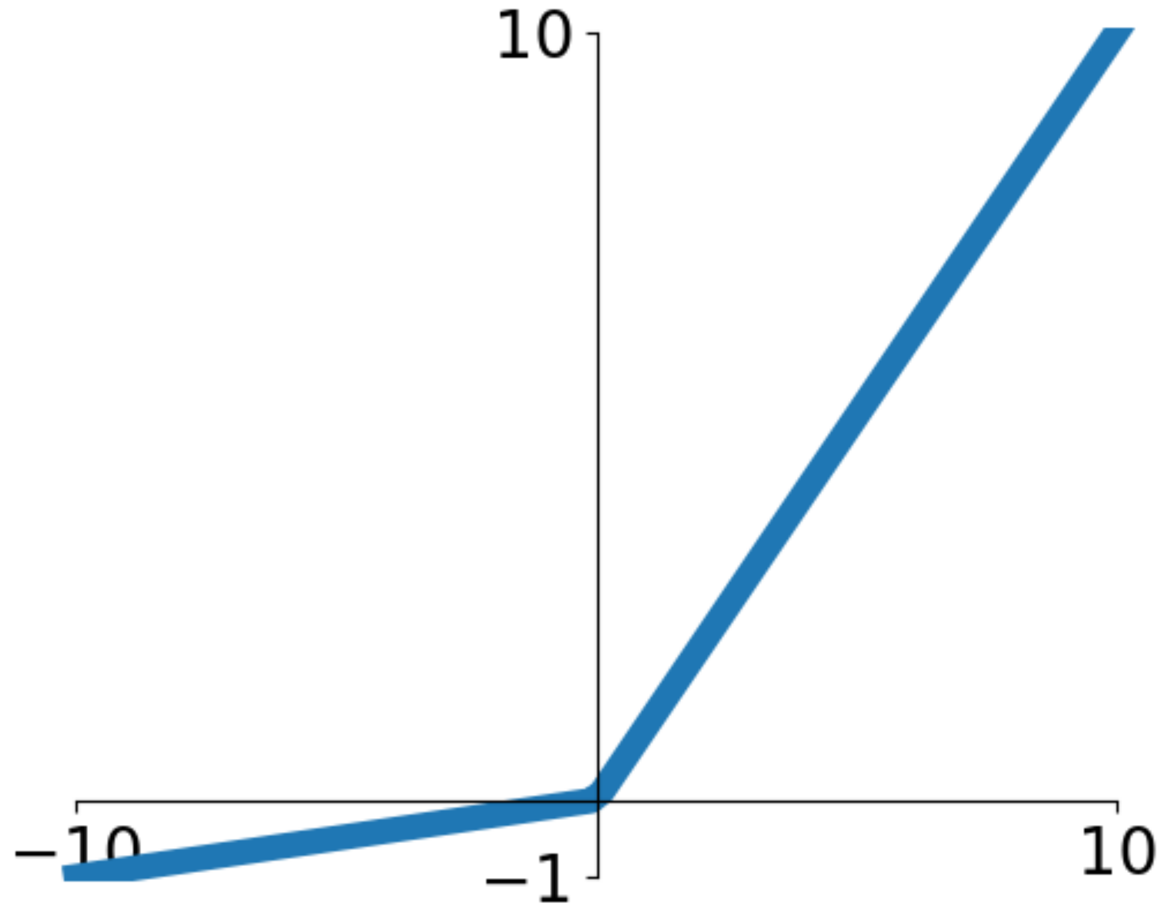
*slide adopted from http://neuralnetworksanddeeplearning.com/chap4.html

Activation Function: Leaky / Parametrized ReLU

Leaky: alpha is fixed to a small value (e.g., 0.01)

$$a(x) = \begin{cases} x & \text{if } x \geq 0 \\ \alpha x & \text{if } x < 0 \end{cases}$$

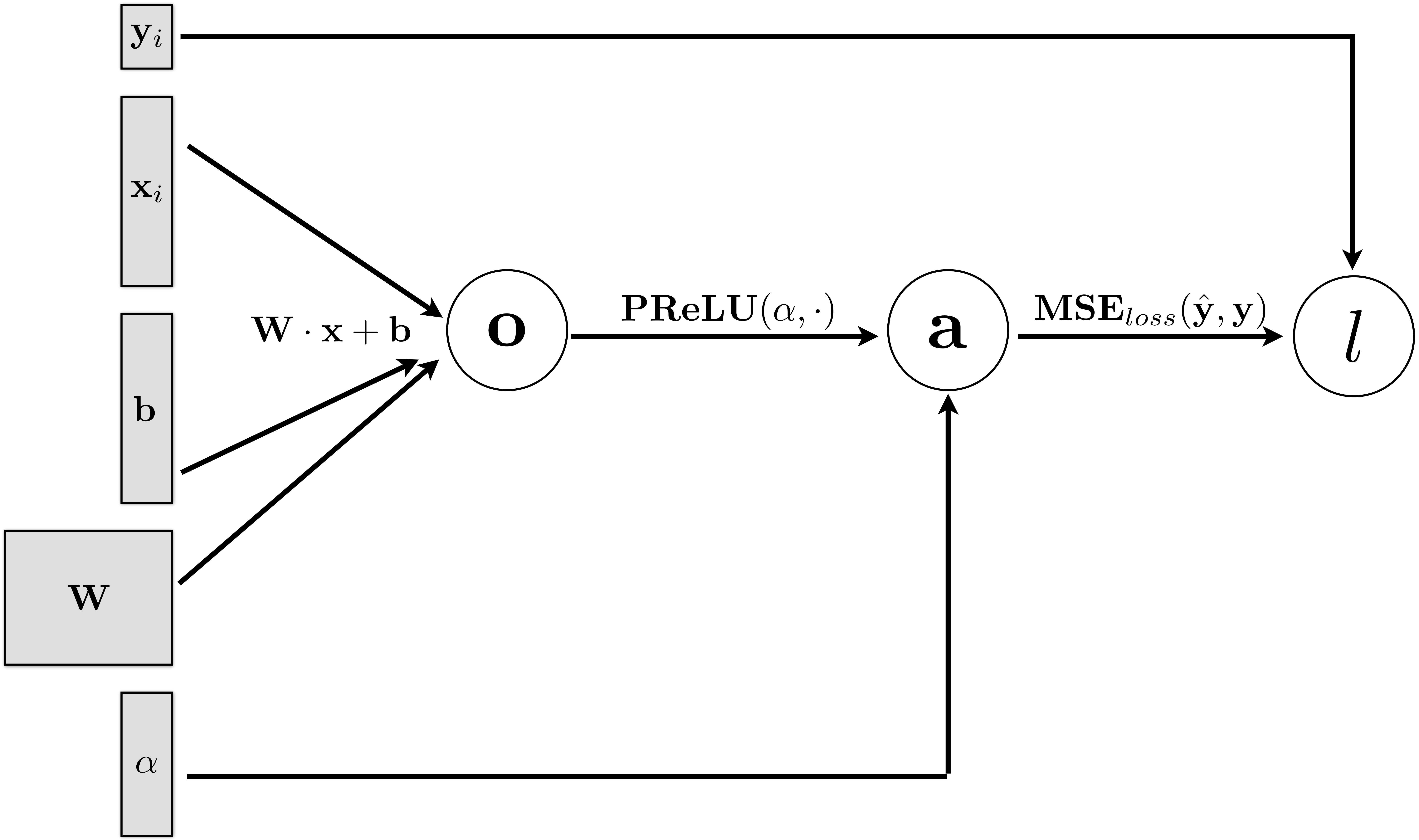
Parametrized: alpha is optimized as part of the network (BackProp through)



Leaky / Parametrized ReLU Activation

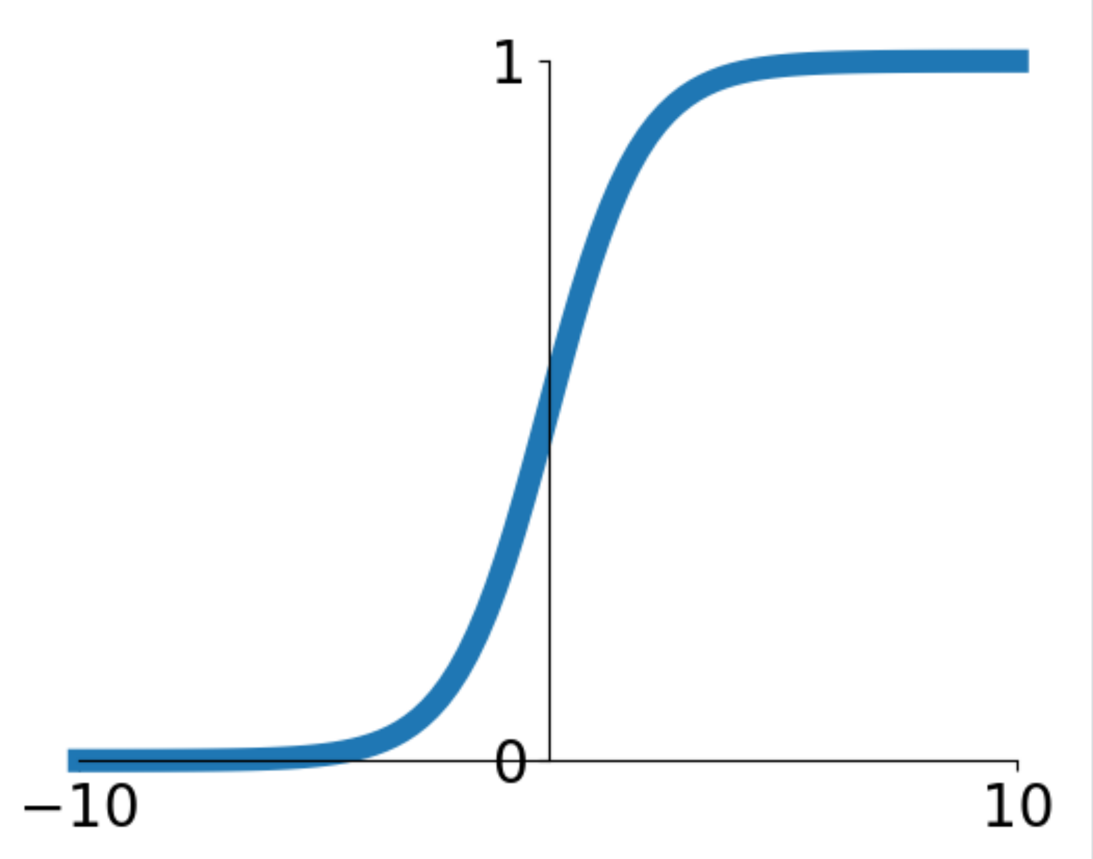
Pros:
- Does not saturate
- Computationally very efficient
- Converges faster in practice (e.g. 6x)

Computational Graph: 1-layer with PReLU



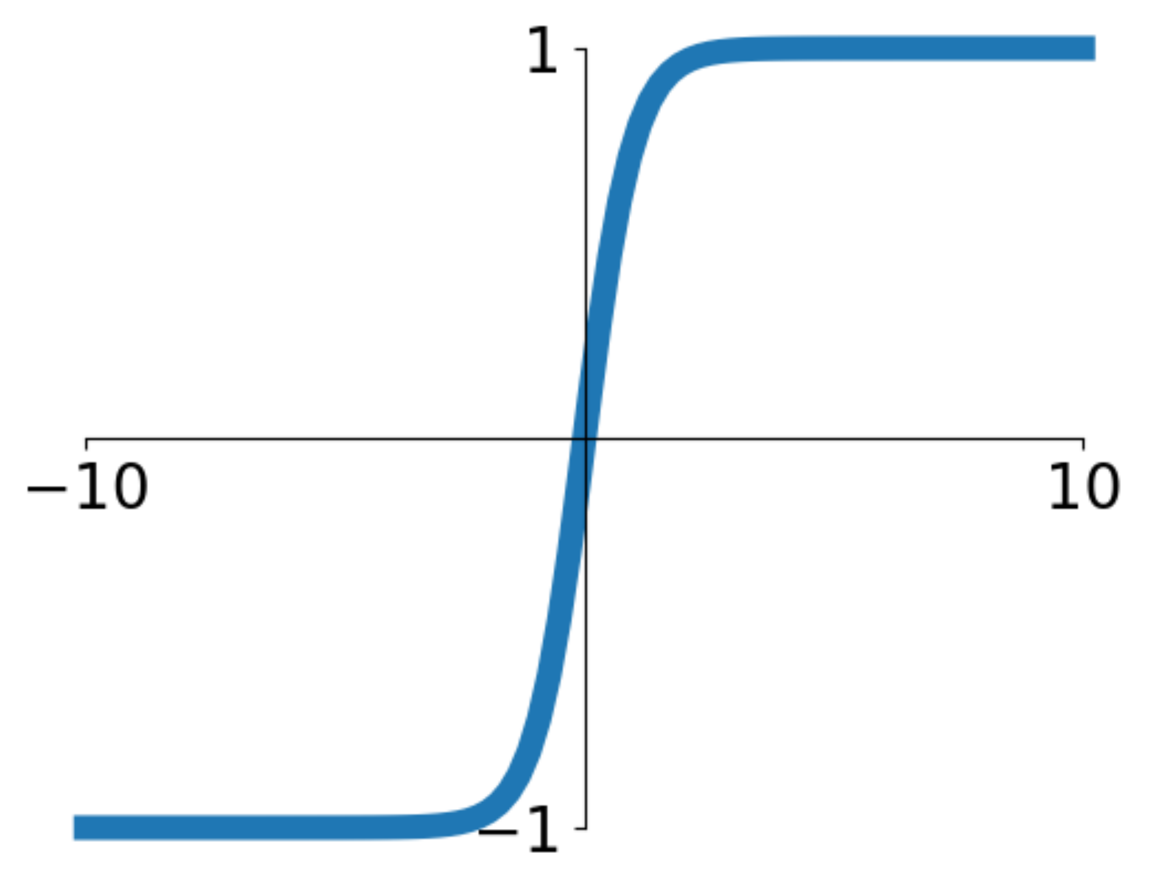
Activation Functions: Review

$$a(x) = \textbf{sigmoid}(x) = \frac{1}{1+e^{-x}}$$



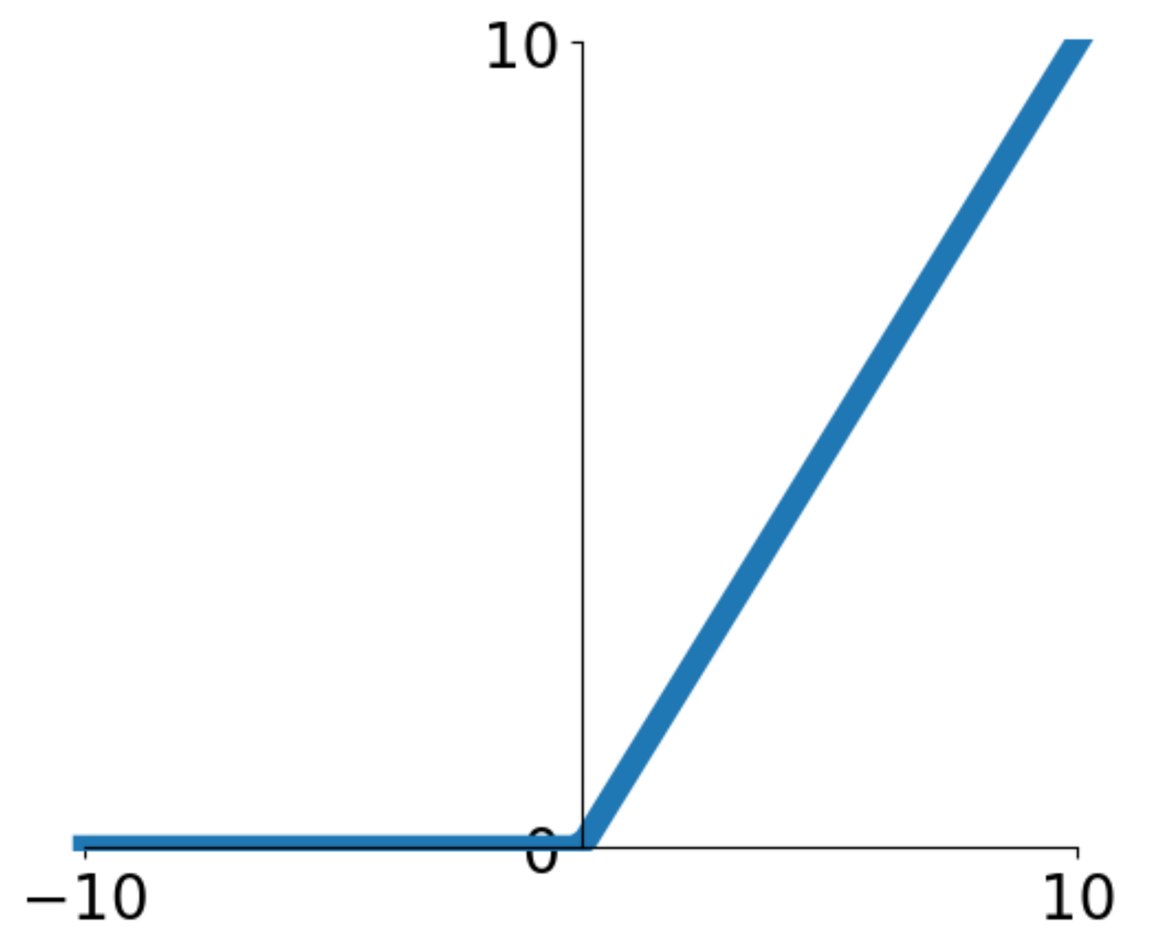
Sigmoid

$$a(x) = \textbf{tanh}(x) = \frac{2}{1+e^{-2x}} - 1$$



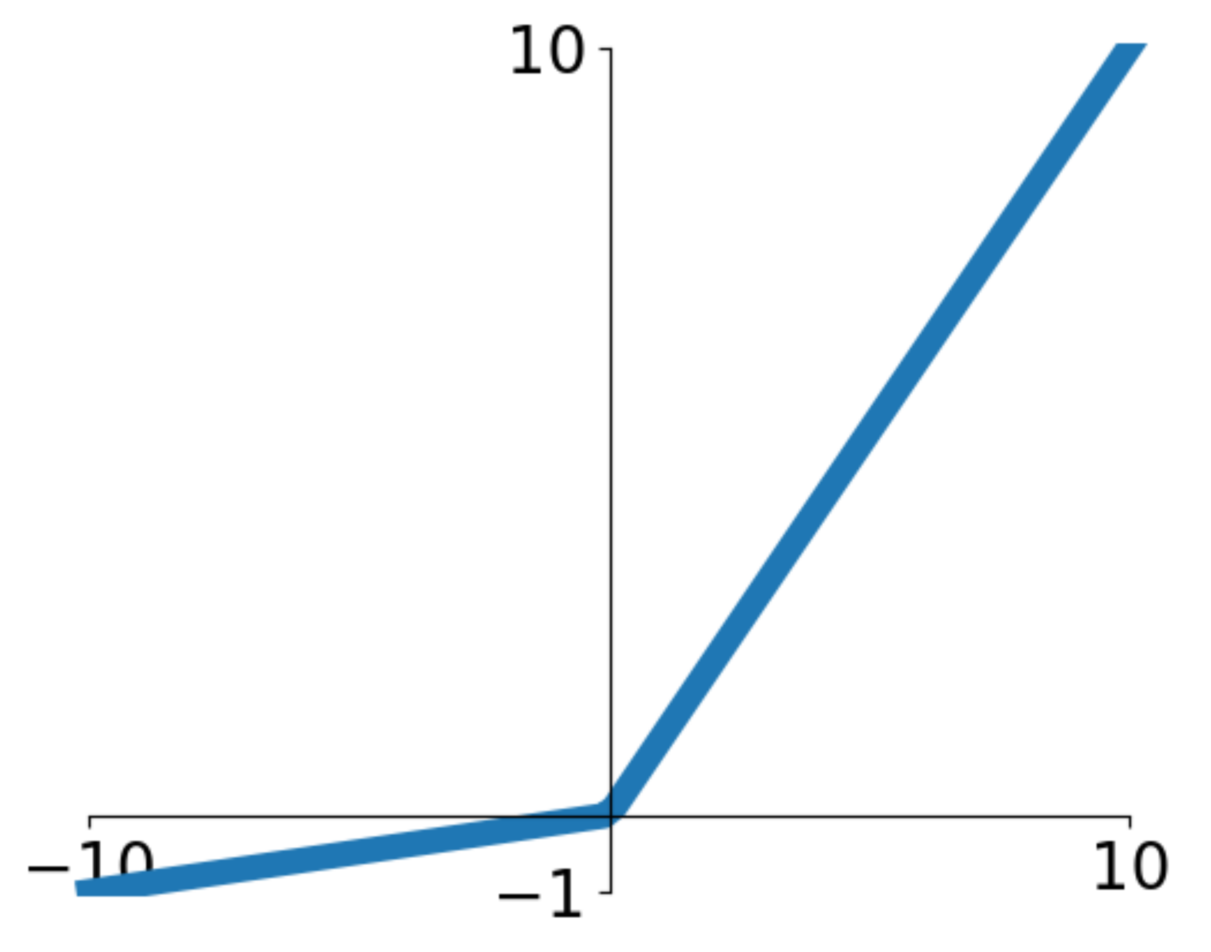
Tanh

$$a(x) = max(0, x)$$



ReLU

$$a(x) = \begin{cases} x & \text{if } x \geq 0 \\ \alpha x & \text{if } x < 0 \end{cases}$$



Leaky / Parametrized **ReLU**