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

Lecture 2: Introduction to Deep Learning

Course **Logistics**

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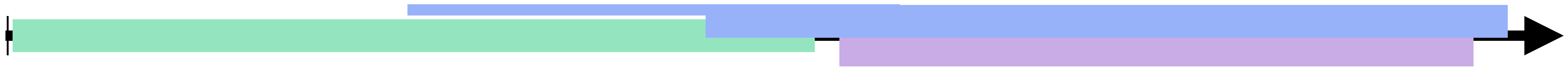
- Mine and TA office hours will be posted **today** (mine are **12:30-1:30 pm**)

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

Lecture 1: Introduction

Grading Criteria

- **Assignments** (programming) — 40% (total)
- **Research papers** — 20%
- **Project** — 40%



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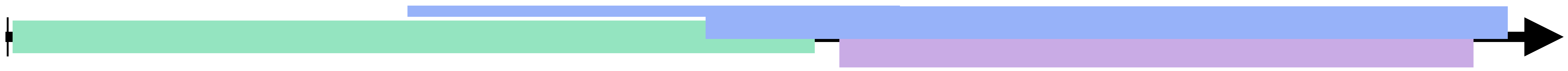
NO LATE SUBMISSIONS — If you don't complete the assignment, hand in what you have



Assignments (5 assignments and 40% of grade total)

- Assignment 0: **Introduction to PyTorch** (0%)
- Assignment 1: **Neural Network Introduction** (5%) — python™

Assignments all use **Python Jupiter Notebooks**, use `Canvas` to hand everything in. Assignments always due at **11:59pm PST** on due date.

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- Assignment 4: Neural Model for **Image Captioning / Retrieval** (10%) — PYTORCH

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- Assignment 4: Neural Model for **Image Captioning / Retrieval** (10%) — PYTORCH
- Assignment 5: Advanced Architectures **Graph NN** and **GANs** (10%) — PYTORCH

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Assignments (5 assignments and 40% of grade total)

I reserve the right to **change** release and due dates for the assignments to accommodate constraints of the course, do not take the dates on web-page as “set in stone”.

Research Papers (reviews and presentation, 20% of grade total)

Presentation - 10%

- You will need to **present 1 paper** individually or as a group (group size will be determined by # of people in class)
- Pick a paper from the syllabus individually (we will have process to pick #1, #2, #3 choices)
- Will need to prepare slides and **meet with me or TA** for feedback
- It is your responsibility to schedule these meetings
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Reading **Reviews** - 10%

- Individually, one for most lectures after the first half of semester
- Due 11:59pm a day before class where reading assigned, submitted via Canvas

Good **Presentation**

- You are effectively taking on responsibility for being an instructor for part of the class (**take it seriously**)

- What makes a **good presentation**?

  - High-level overview of the problem and motivation
  - Clear statement of the problem
  - Overview of the technical details of the method, including necessary background
  - Relationship of the approach and method to others discussed in class
  - Discussion of strengths and weaknesses of the approach
  - Discussion of strengths and weaknesses of the evaluation
  - Discussion of potential extensions (published or potential)

Reading **Reviews**

- Designed to make sure you read the material and have thought about it prior to class (to stimulate discussion)

  - Short summary of the paper (3-4 sentences)
  - Main contributions (2-3 bullet points)
  - Positive / negative points (2-3 bullet points each)
  - What did you not understand (was unclear) about the paper (2-3 bullet points)

Final **Project** (40% of grade total)

- Group project (groups of 3 are encouraged, but fewer maybe possible)
- Groups are self-formed, you will not be assigned to a group
- You need to come up with a project proposal and then work on the project as a group (each person in the group gets the same grade for the project)
- Project needs to be **research** oriented (not simply implementing an existing paper); you can use code of existing paper as a starting point though

Project proposal + class presentation: 15%
Project + final presentation (during finals week): 25%

Sample **Project Ideas**

- Translate an image into a cartoon or Picasso drawing better than existing approaches (e.g., experiment with loss functions, architectures)
- Generating video clips by retrieving images relevant to lyrics of songs
- Generating an image based on the sounds or linguistic description
- Compare different feature representation and role of visual attention in visual question answering
- Storyboarding movie scripts
- Grounding a language/sound in an image

… there are **endless possibilities** … think **creatively** and **have fun**!

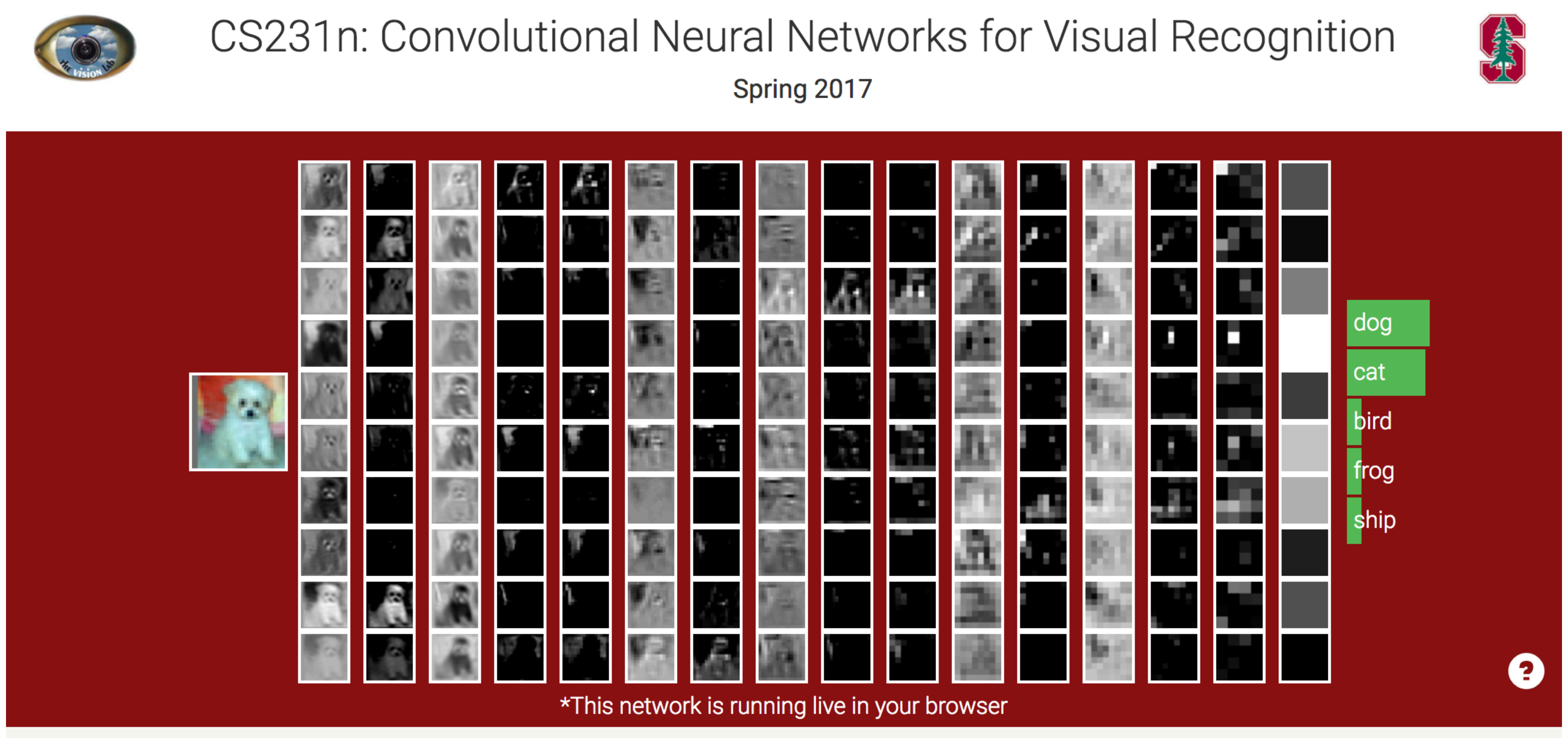
THE UNIVERSITY OF BRITISH COLUMBIA

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

Lecture 2: Introduction to Deep Learning

Introduction to **Deep Learning**

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



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

Covering: foundations and most important aspects of DNNs

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


Disney · PIXAR
TOY
STORY
4

Disney · PIXAR
2 0 1 8

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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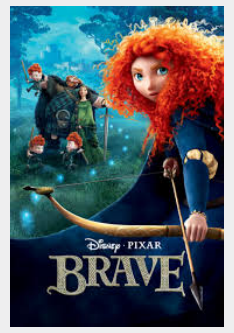

*slide adopted from V. Ordonex

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	$x_1^{(5)}$	$x_2^{(5)}$	$x_3^{(5)}$	$x_4^{(5)}$	$x_5^{(5)}$	$\hat{y}_j = \sum_i w_{ji} x_i + b_j$	

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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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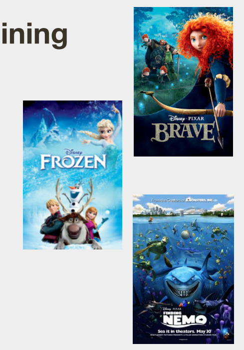

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$$\mathcal{L}(\mathbf{W}, \mathbf{b}) = \sum_{d=1}^{|D_{train}|} \underline{l(\hat{\mathbf{y}}^{(d)}, \mathbf{y}^{(d)})}$$

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

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

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

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Solution:

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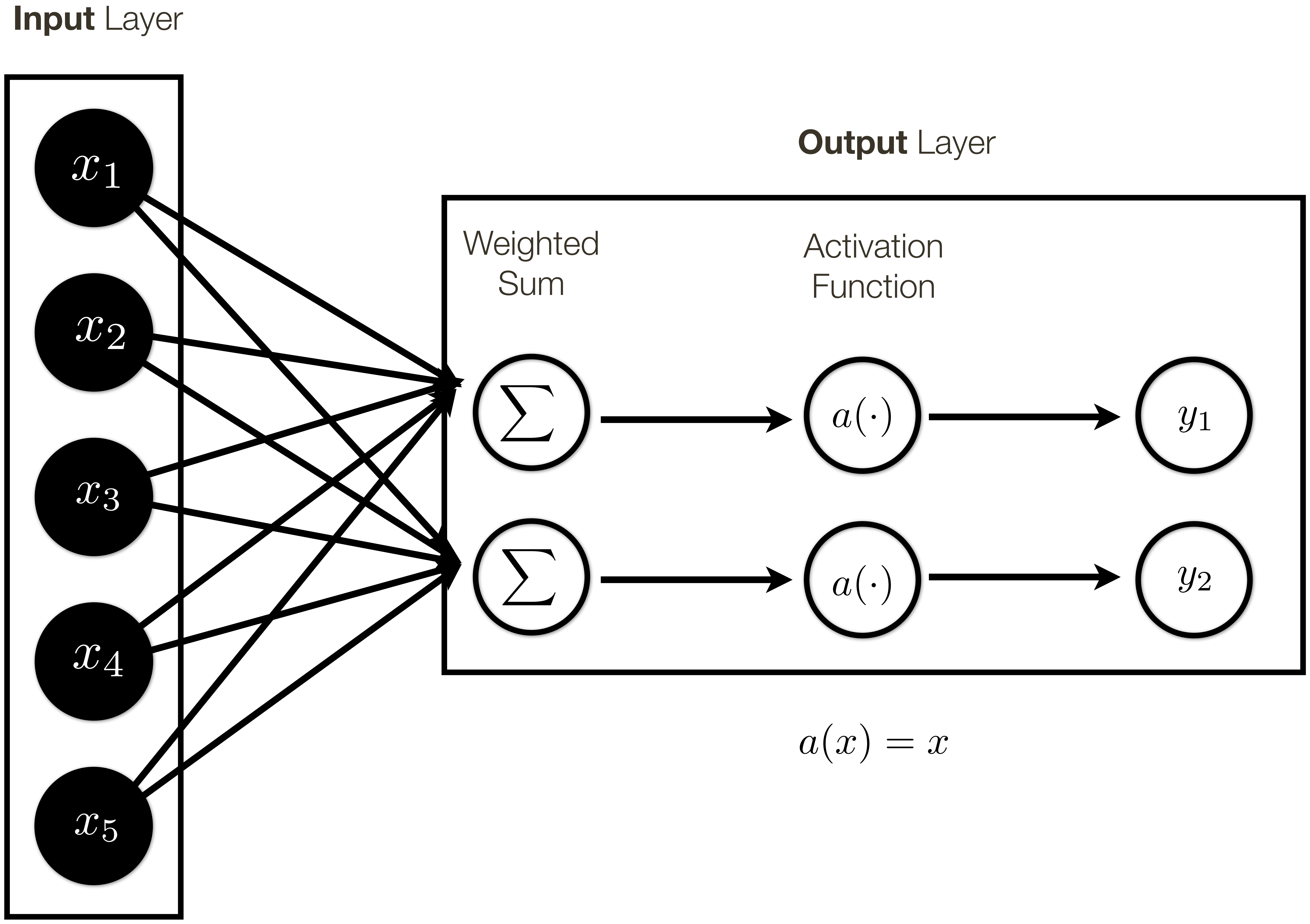
after some operations $\longrightarrow$ $\mathbf{W}^* = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{Y}$

*slide adopted from V. Ordonex

One-layer **Neural Network**



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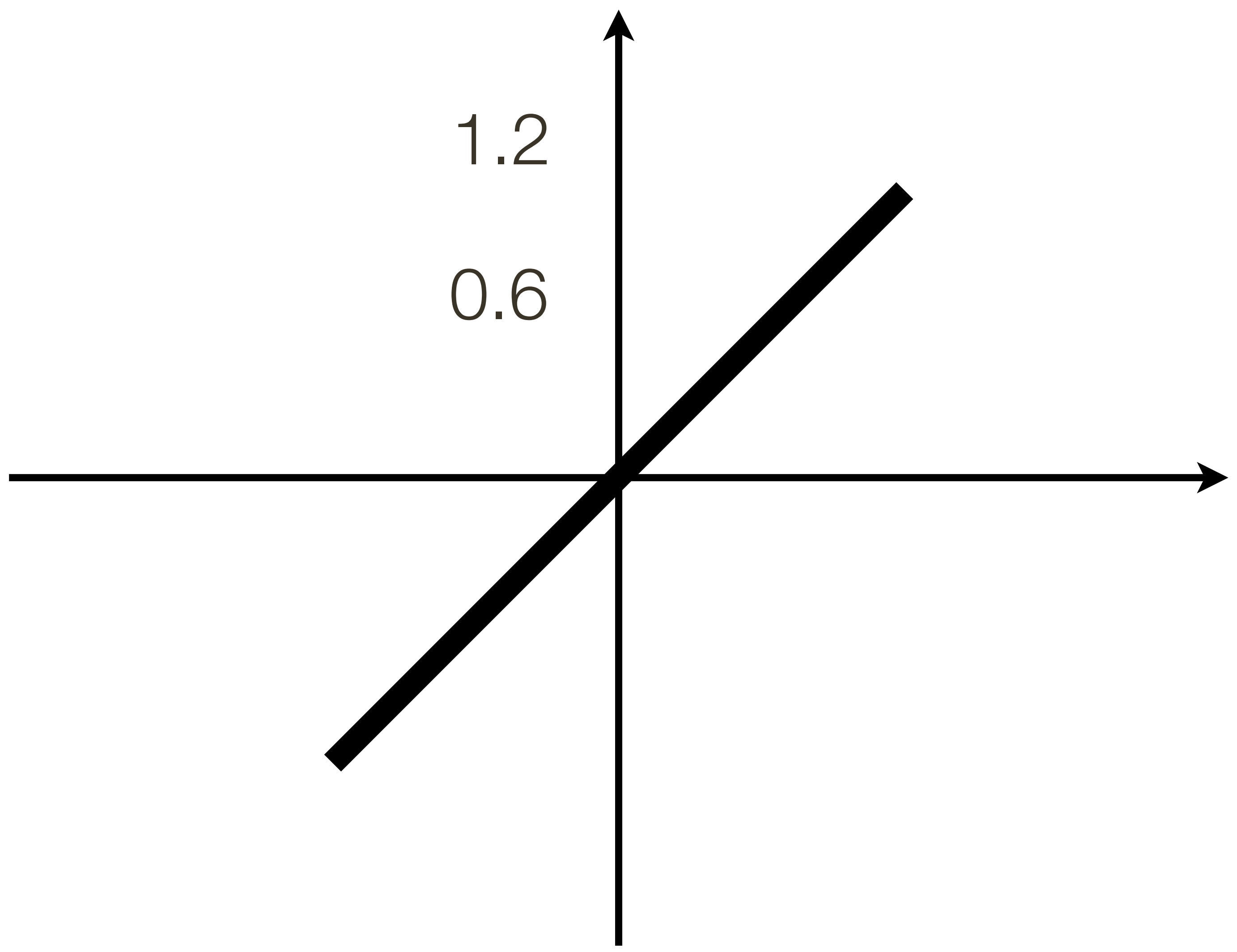
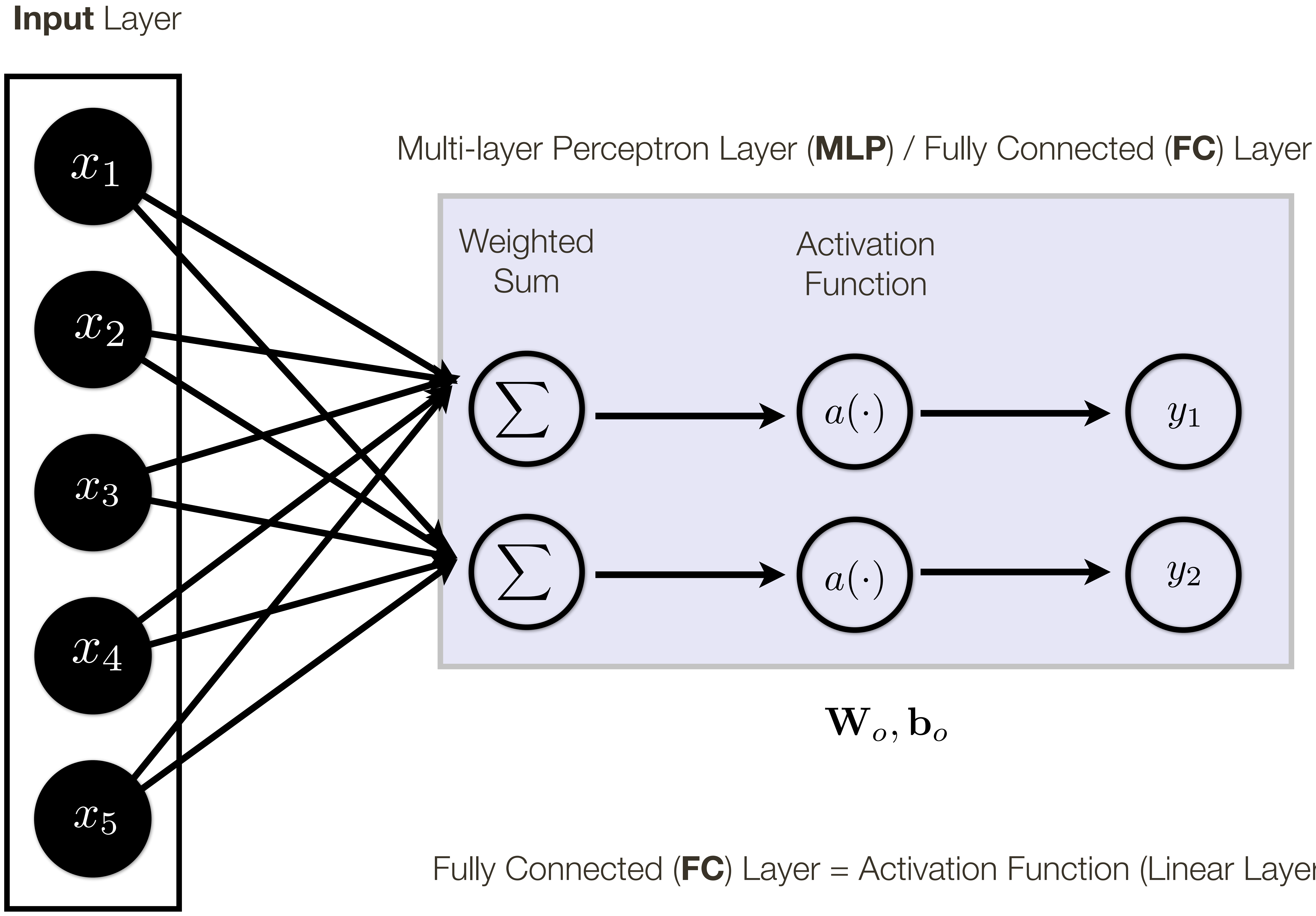


Linear Activation

One-layer **Neural Network**

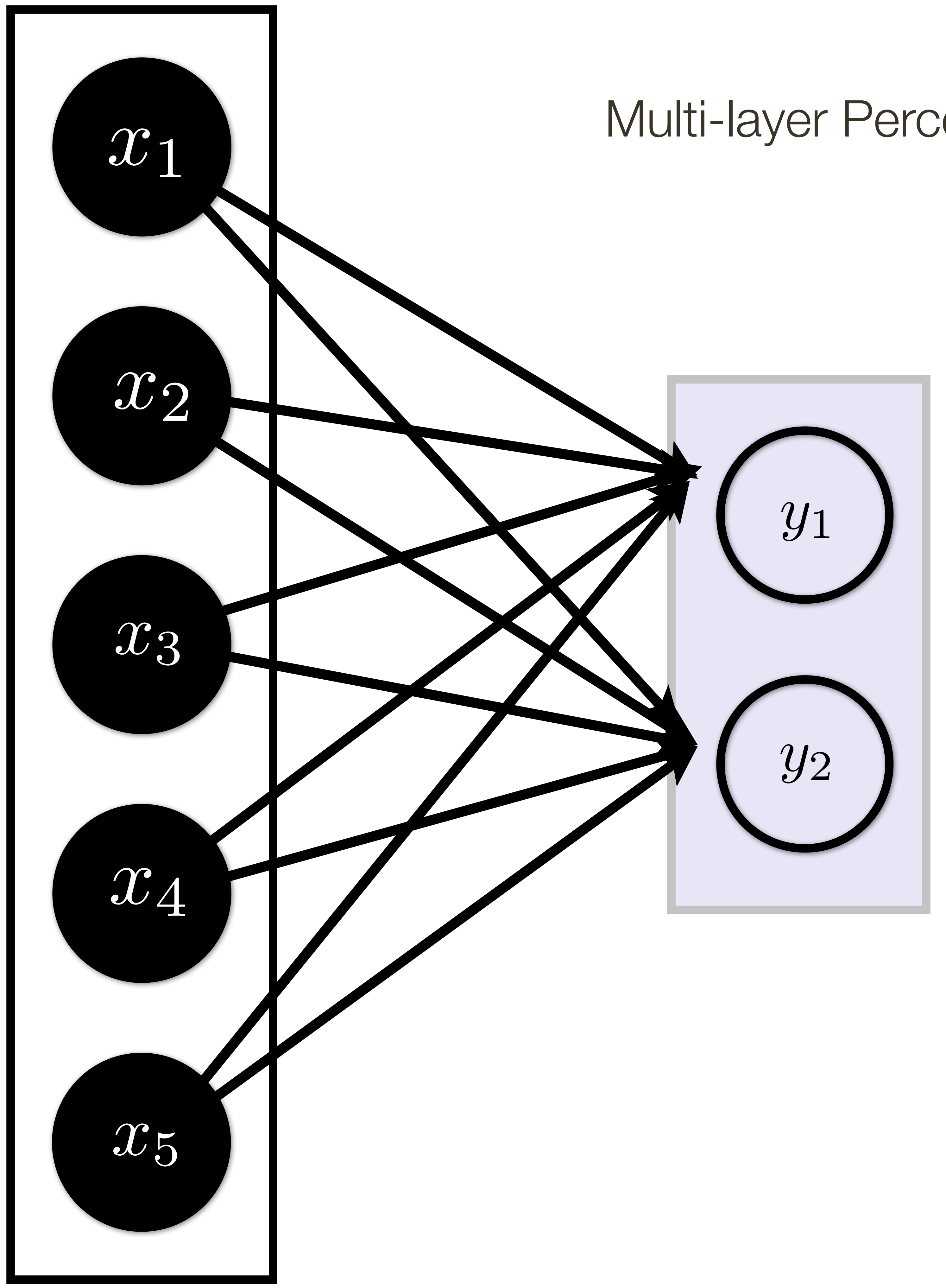


Fully Connected (**FC**) Layer = Activation Function (Linear Layer)

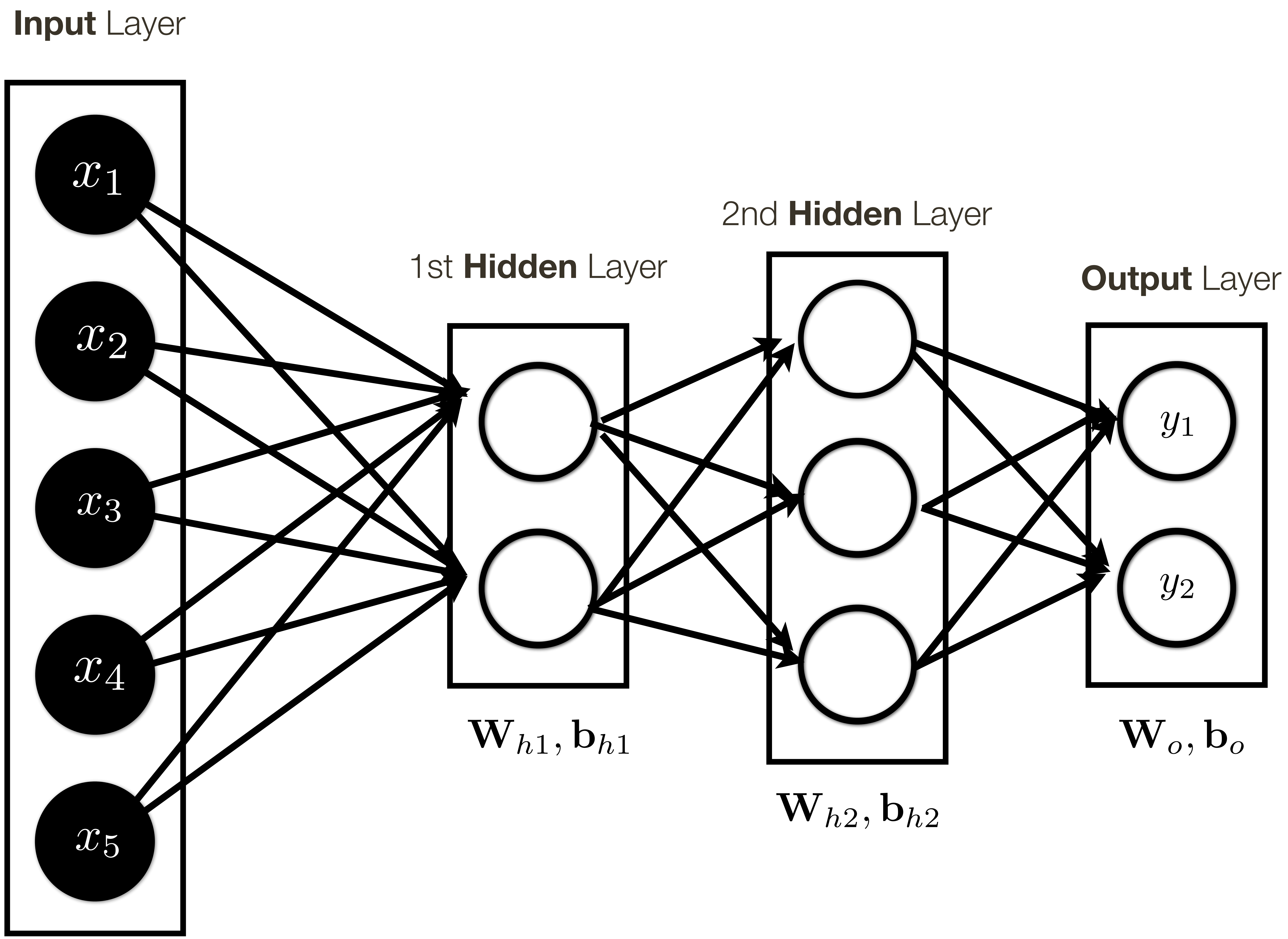
One-layer **Neural Network**

Input Layer

Multi-layer Perceptron Layer (**MLP**) / Fully Connected (**FC**) Layer



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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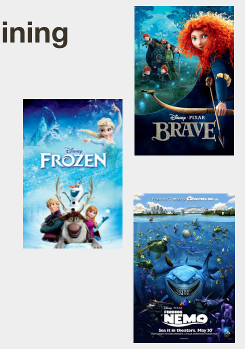
Training Set 	$x_1^{(1)}$	$x_2^{(1)}$	$x_3^{(1)}$	$x_4^{(1)}$	$x_5^{(1)}$	$y_1^{(1)}$	$y_2^{(1)}$
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	1	1	0	0	0		

e.g., hidden unit = production cost + promotion cost

e.g., p(film over budget) = sigmoid (hidden unit)

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Question: Why have many layers?

Answer: 1) More layers = more complex functional mapping

2) More efficient due to distributed representation

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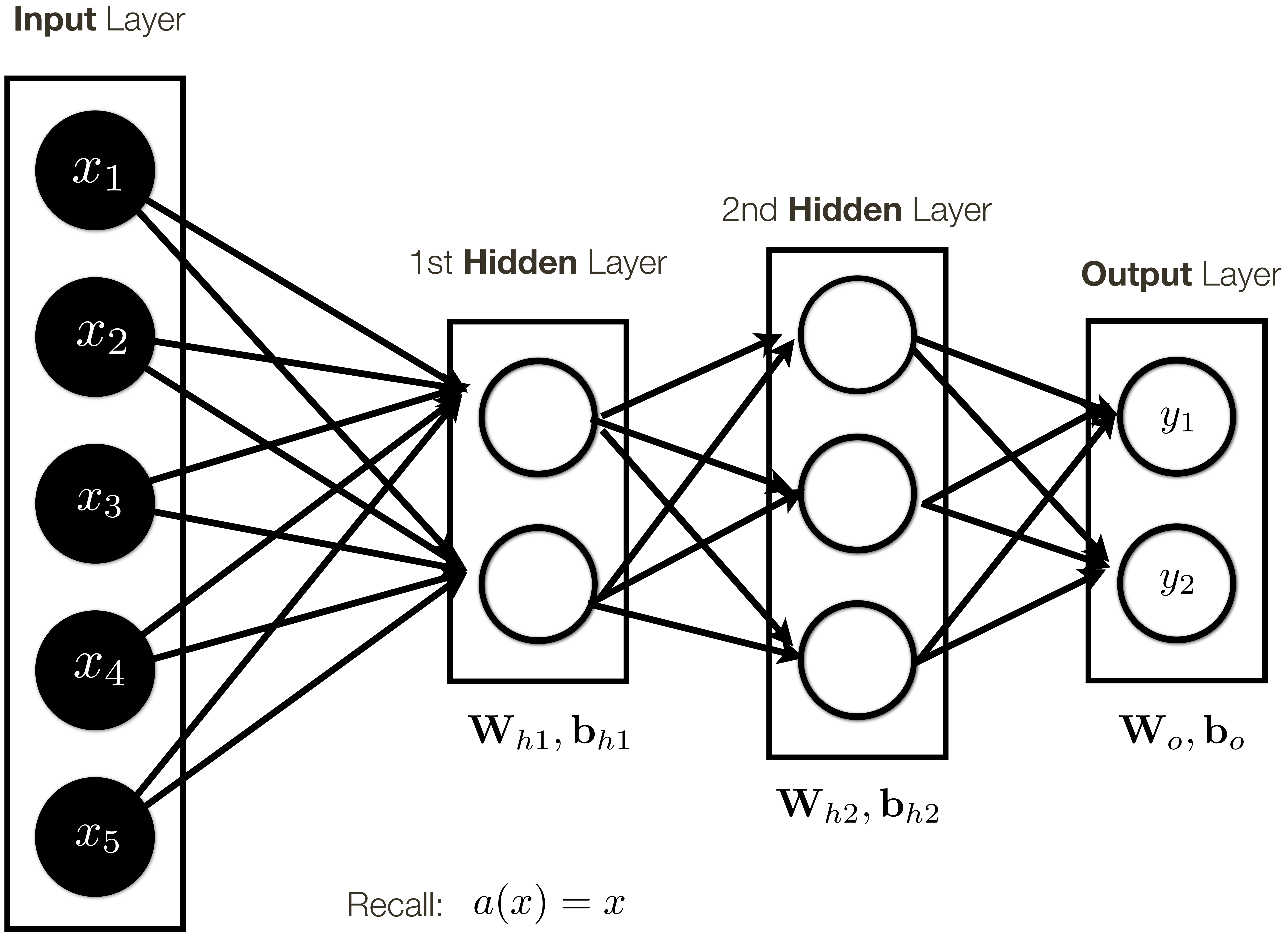
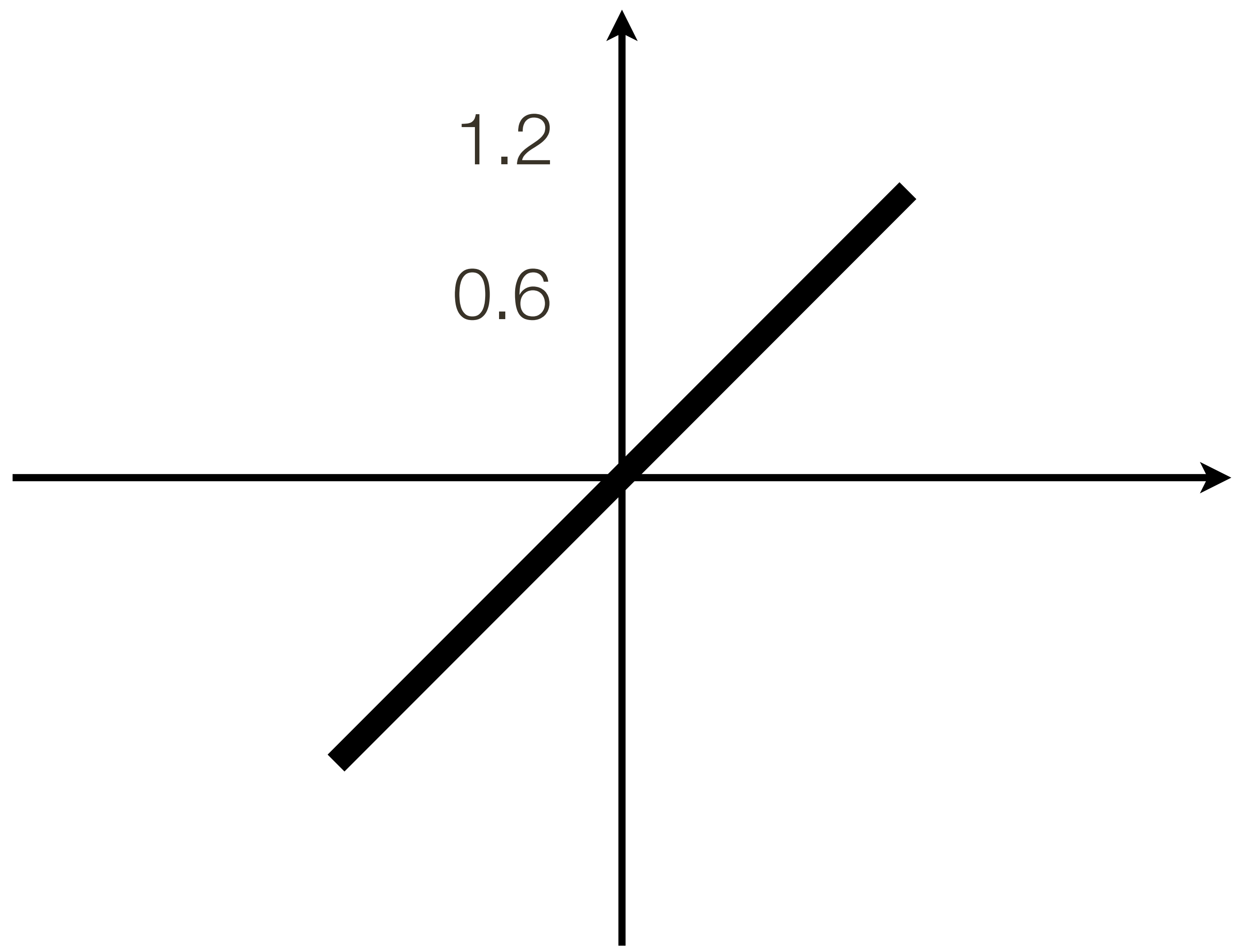
Multi-layer **Neural Network**



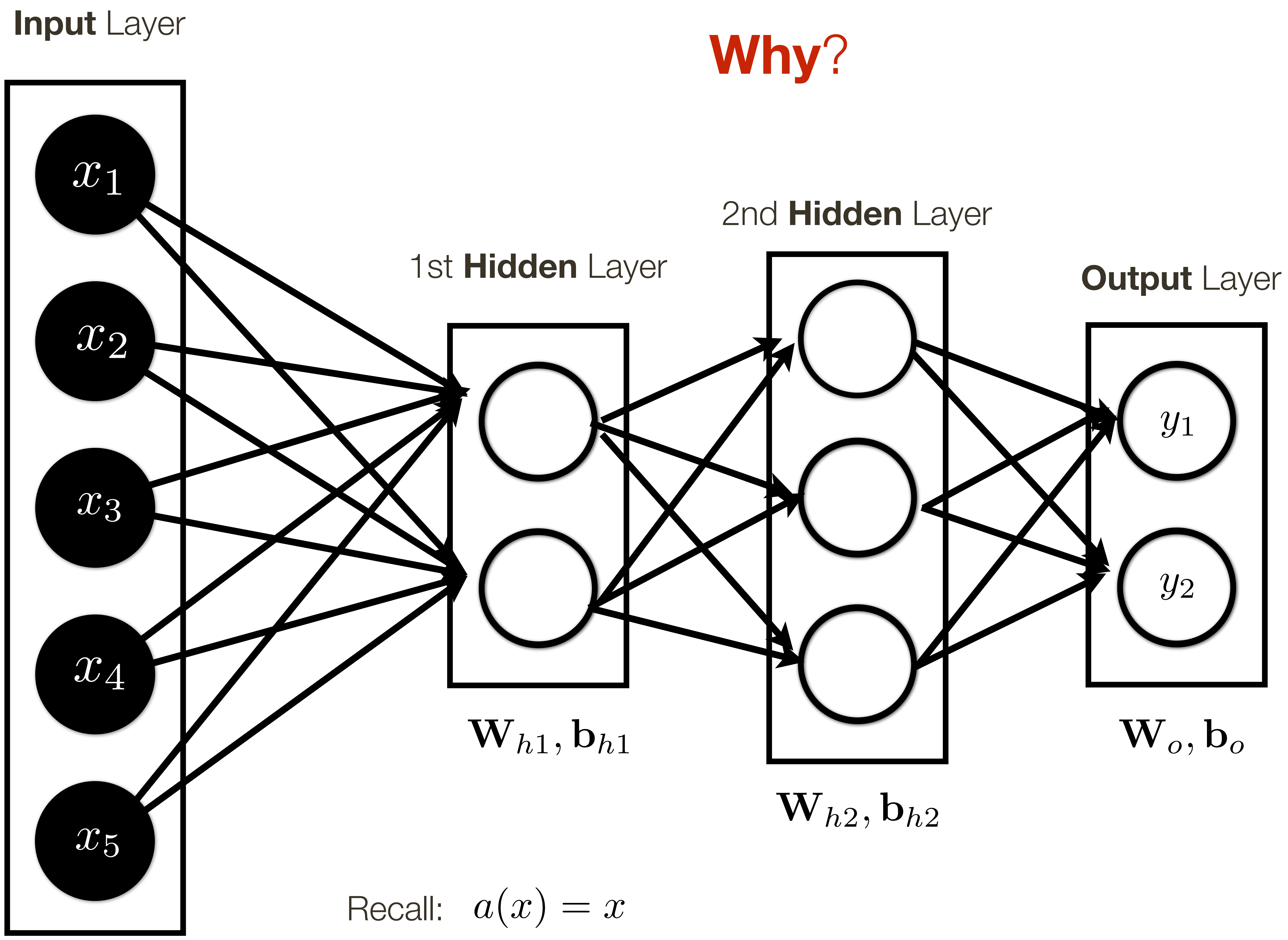
Recall: $a(x) = x$

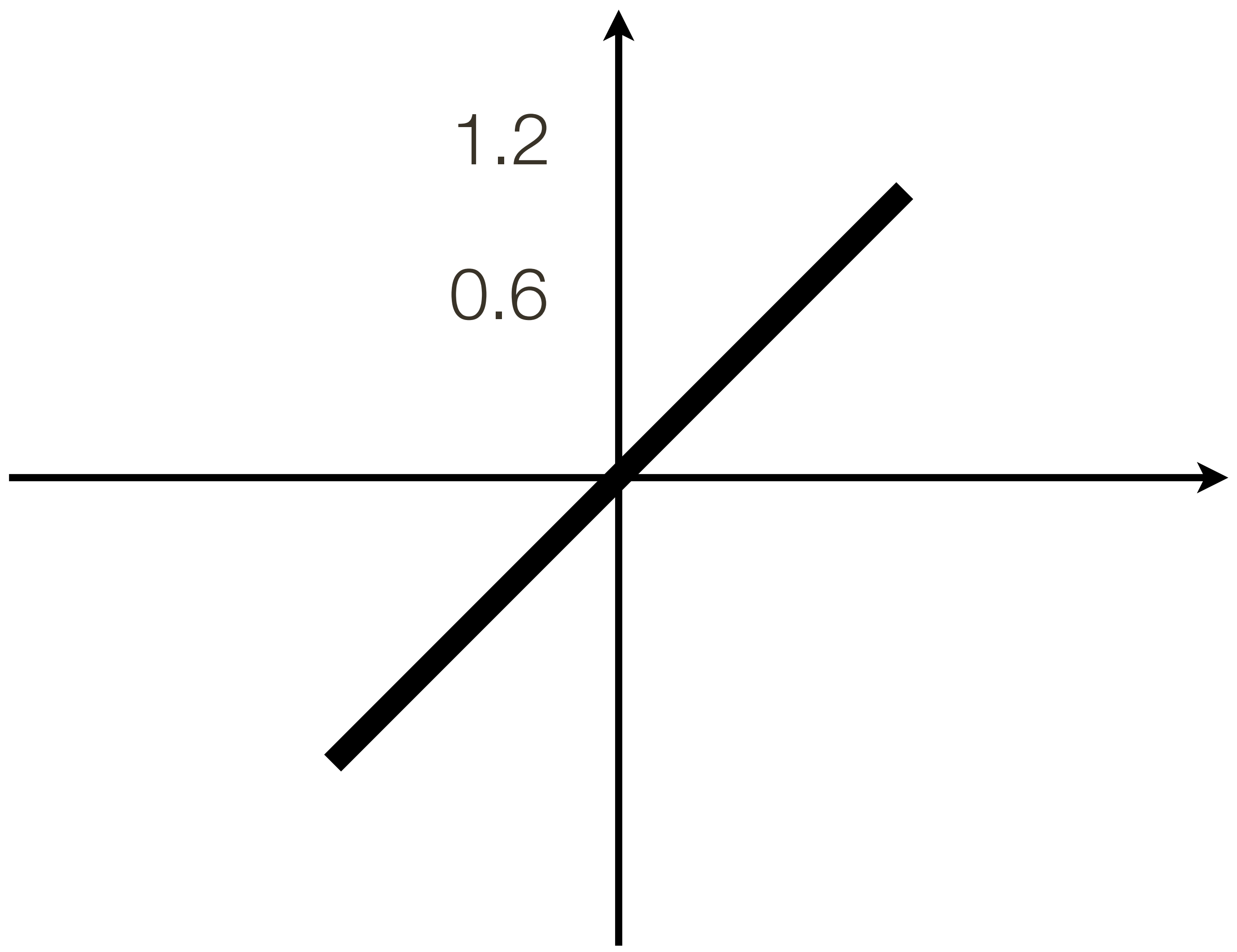


Linear Activation

Multi-layer **Neural Network**

Why?





Linear Activation

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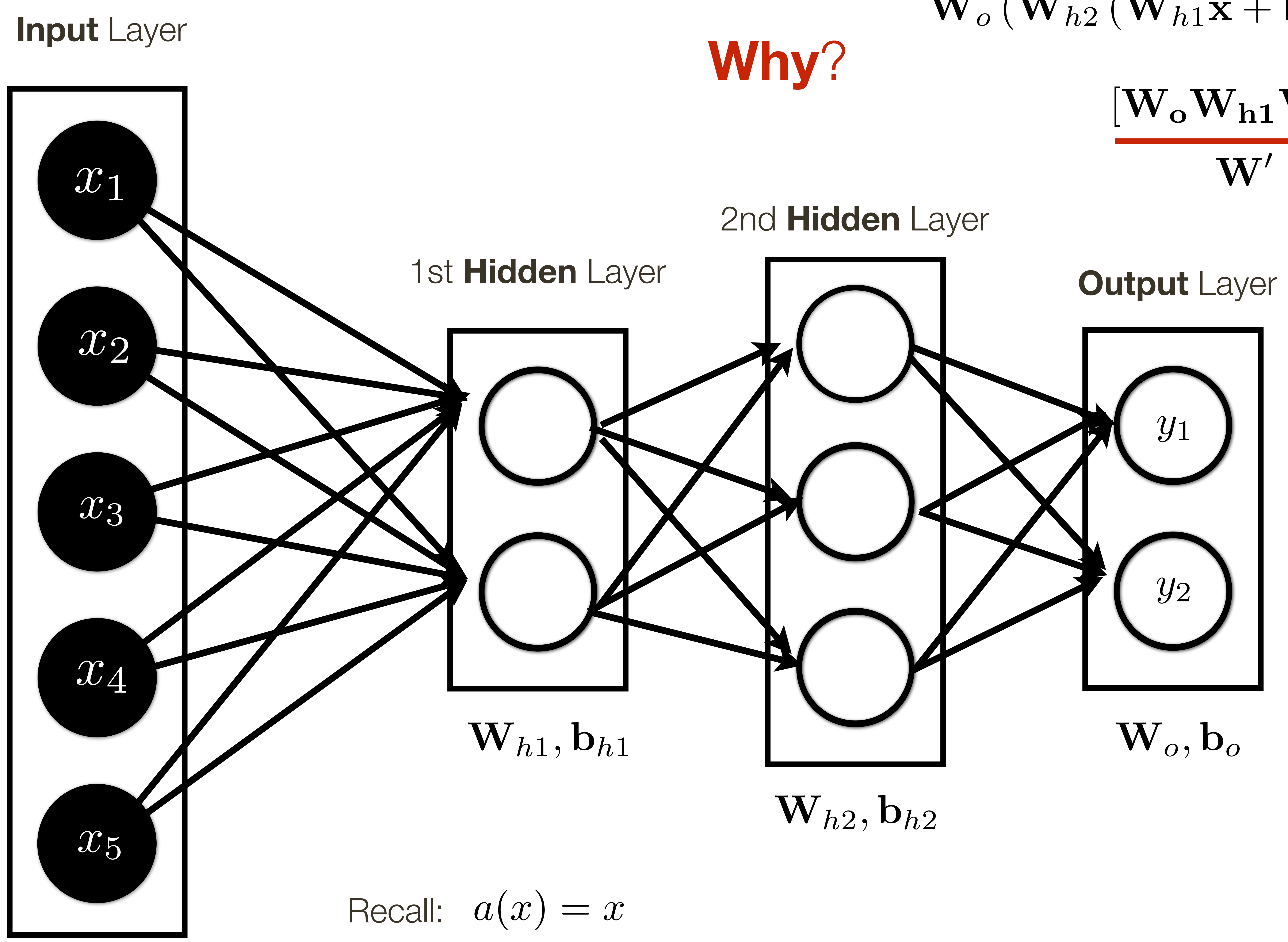
Multi-layer **Neural Network**

Why?

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

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



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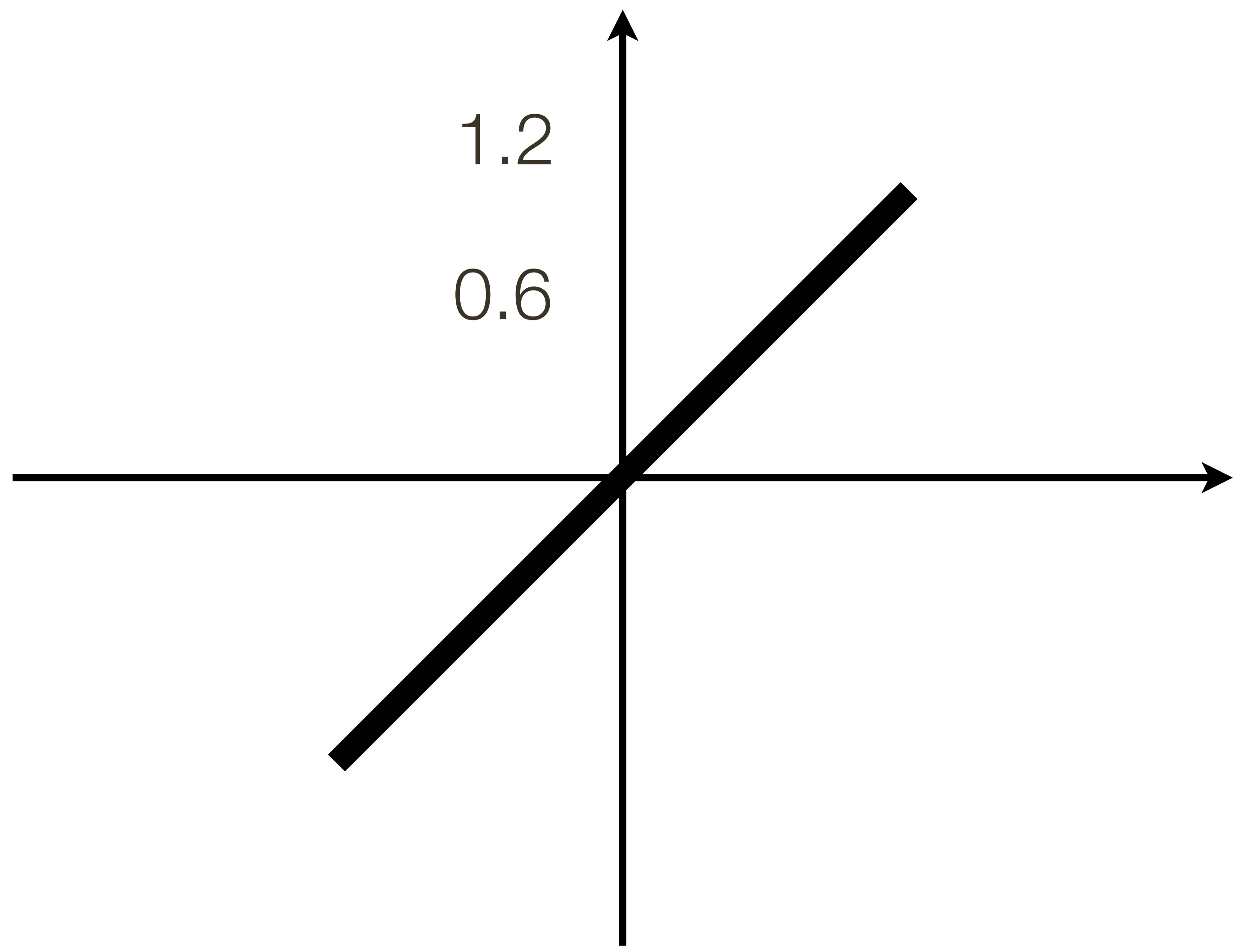

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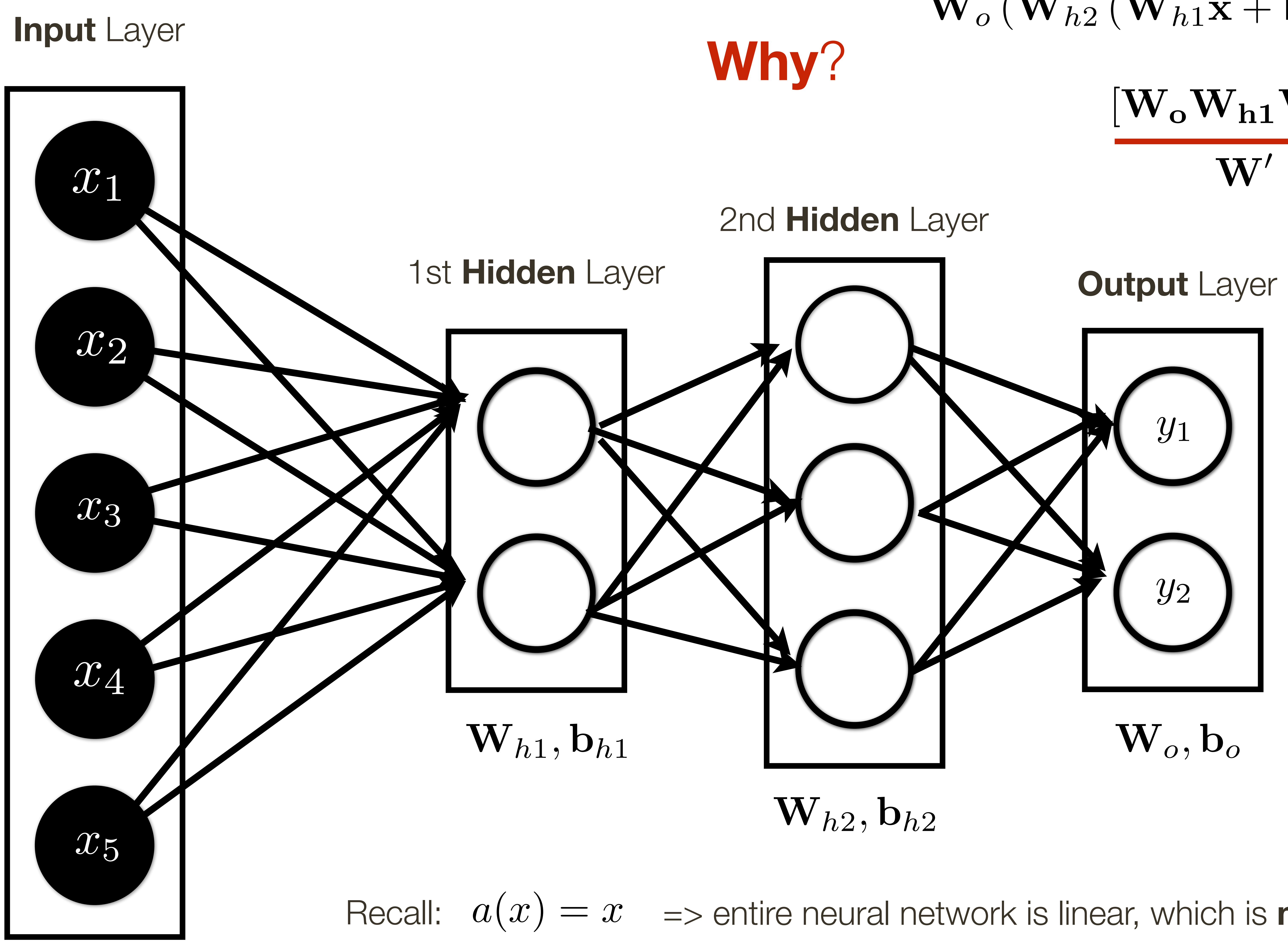
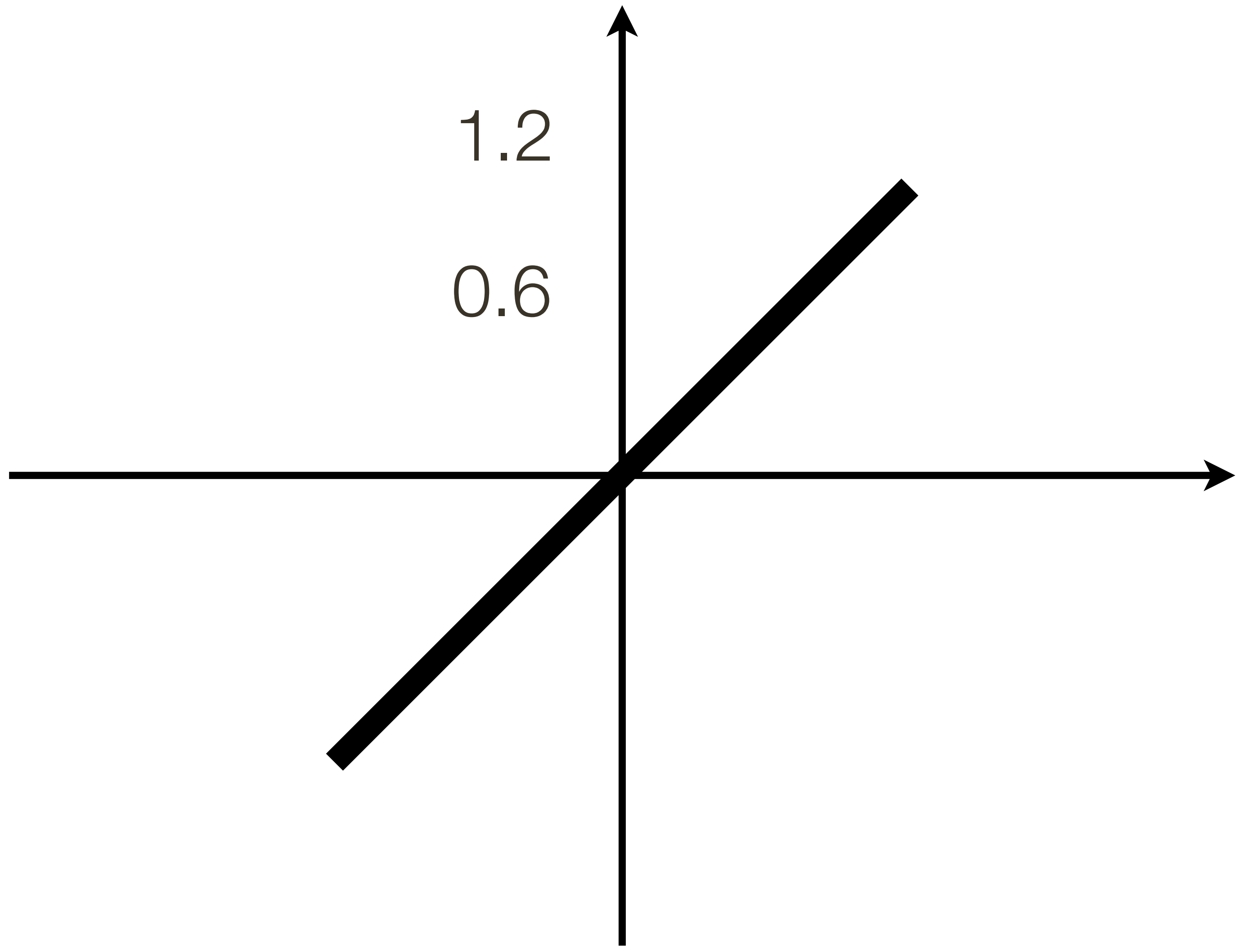
$$\mathbf{W}_o\left(\mathbf{W}_{h2}\left(\mathbf{W}_{h1}\mathbf{x}+\mathbf{b}_{h1}\right)+\mathbf{b}_{h2}\right)+\mathbf{b}_o =$$

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

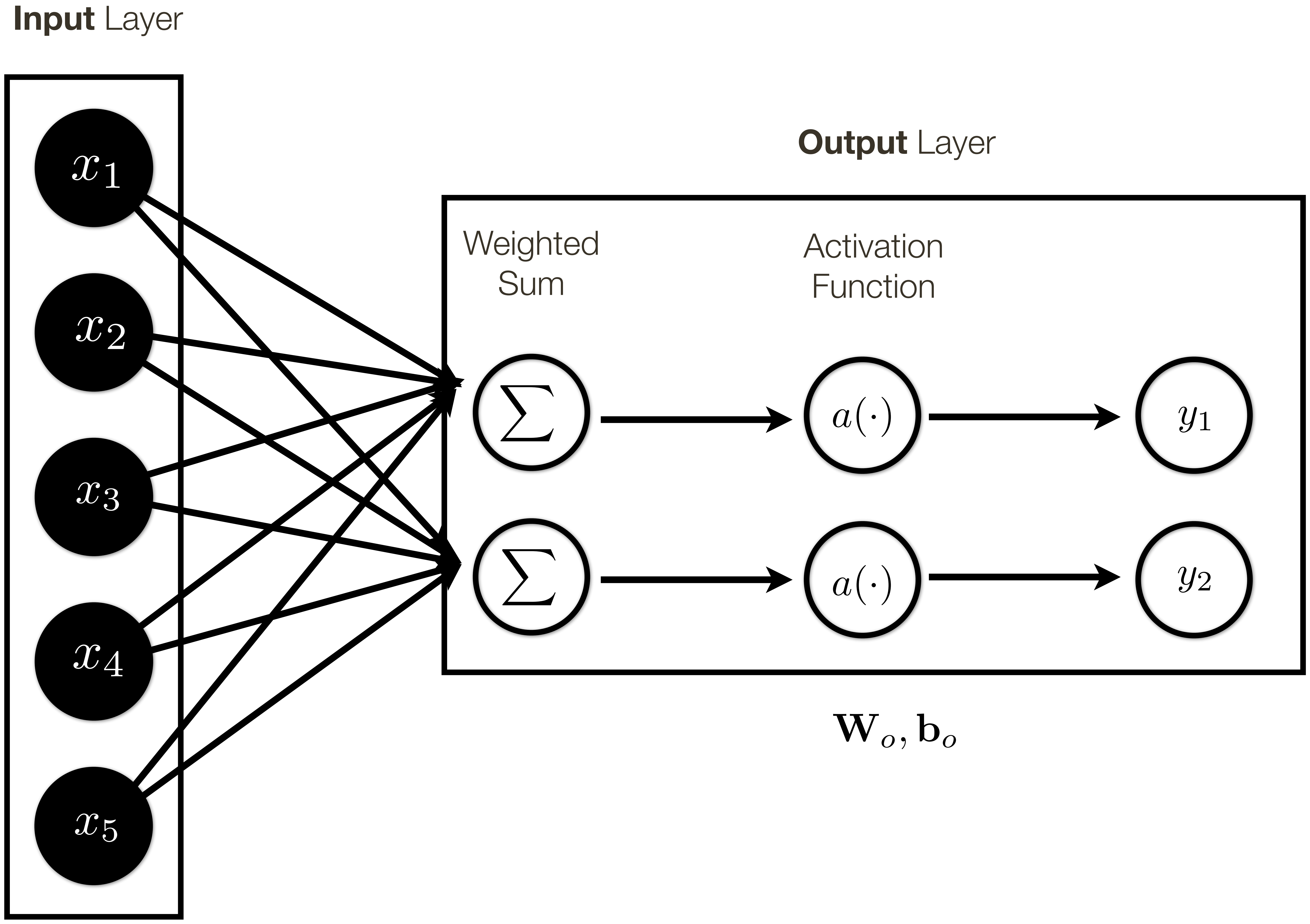




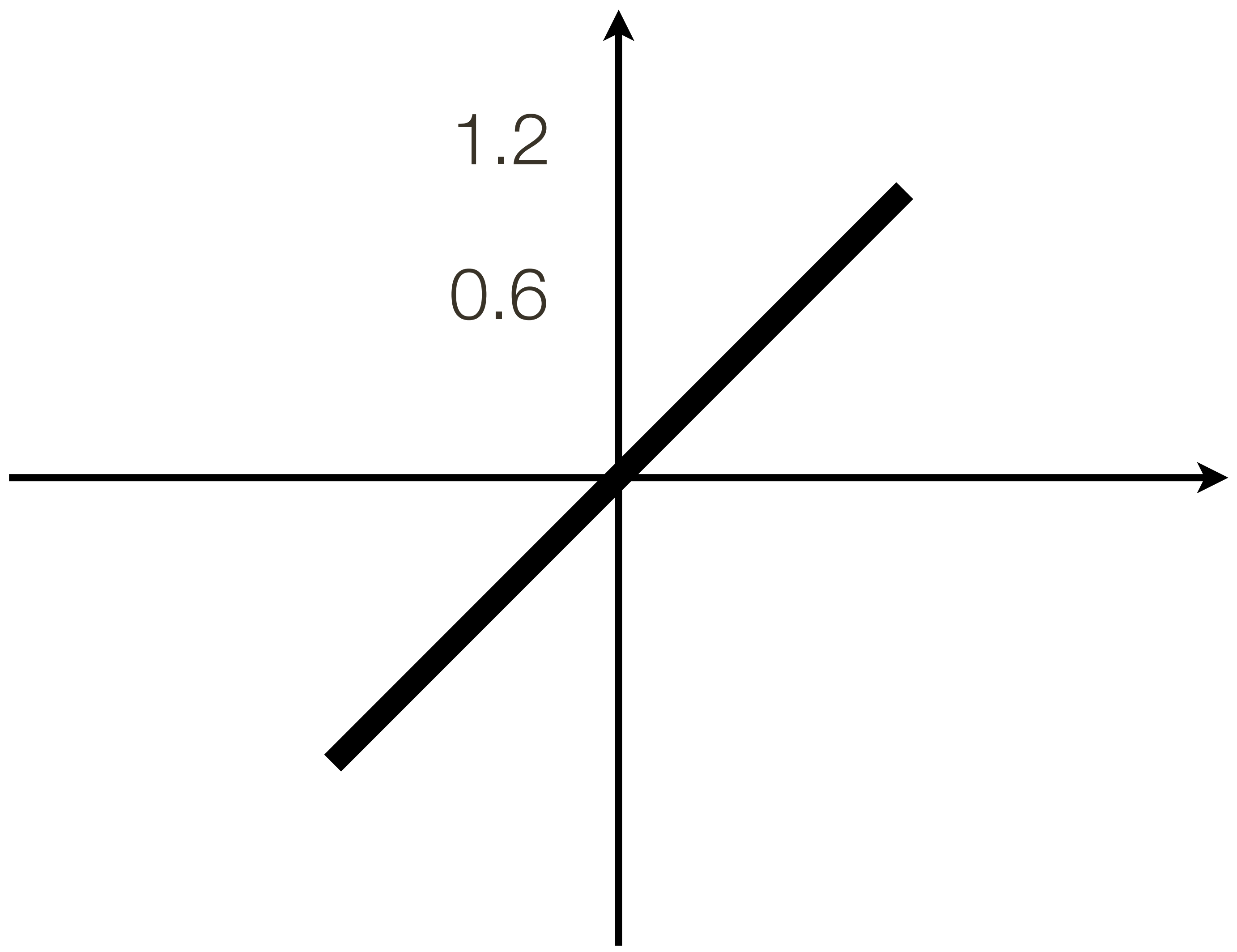
Linear Activation

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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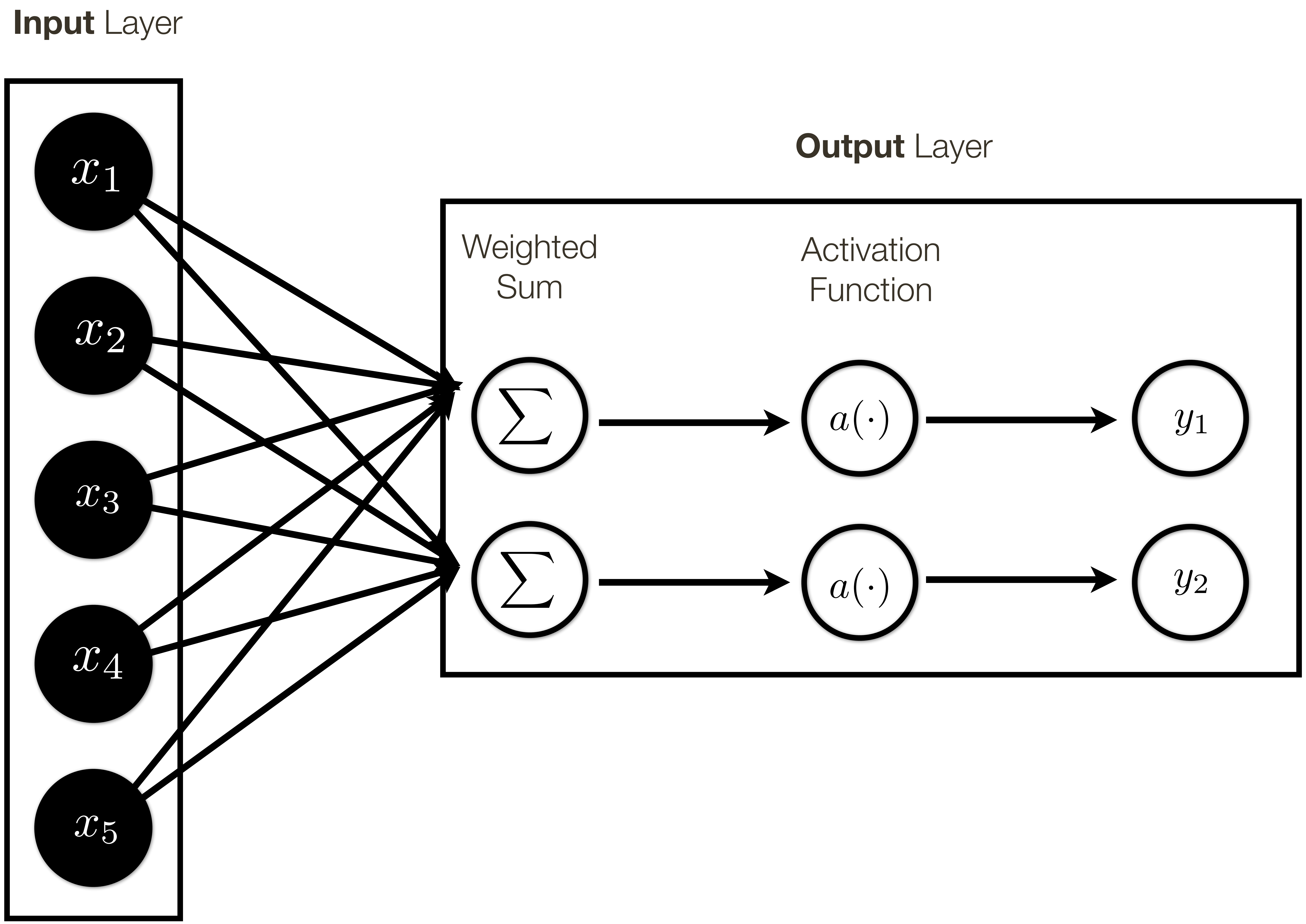
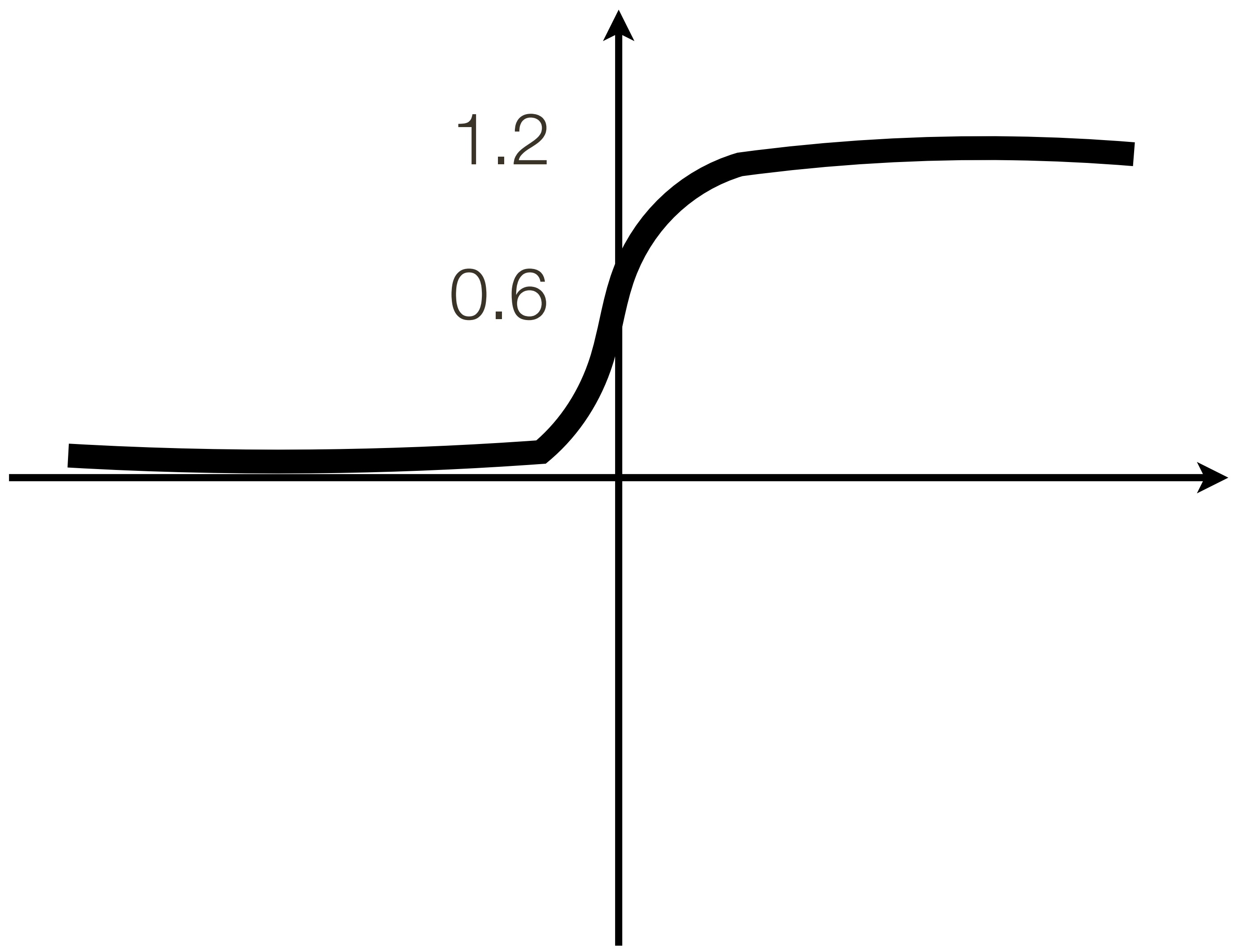


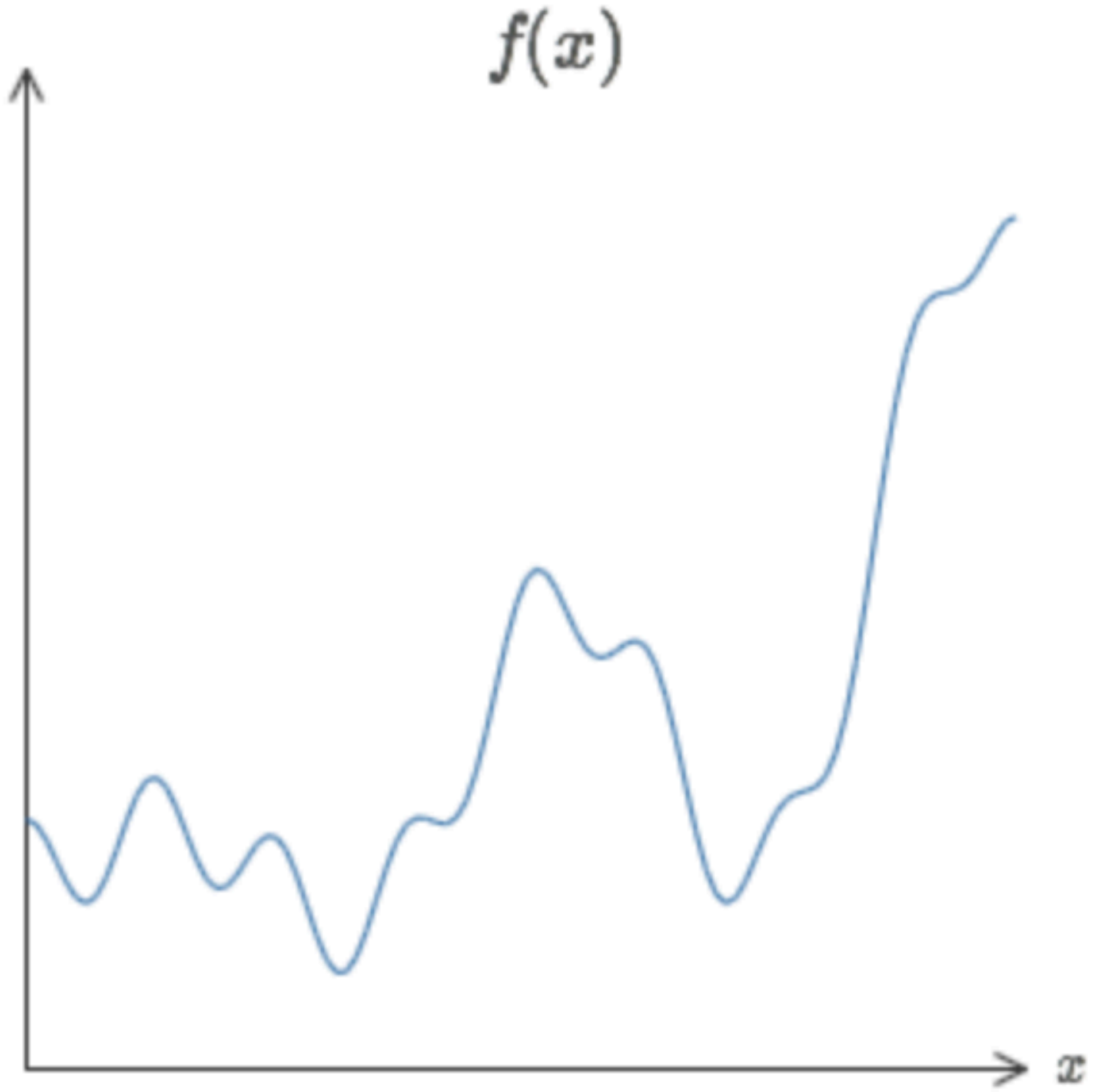
$$a(x) = \textbf{sigmoid}(x) = \frac{1}{1+e^{-x}}$$



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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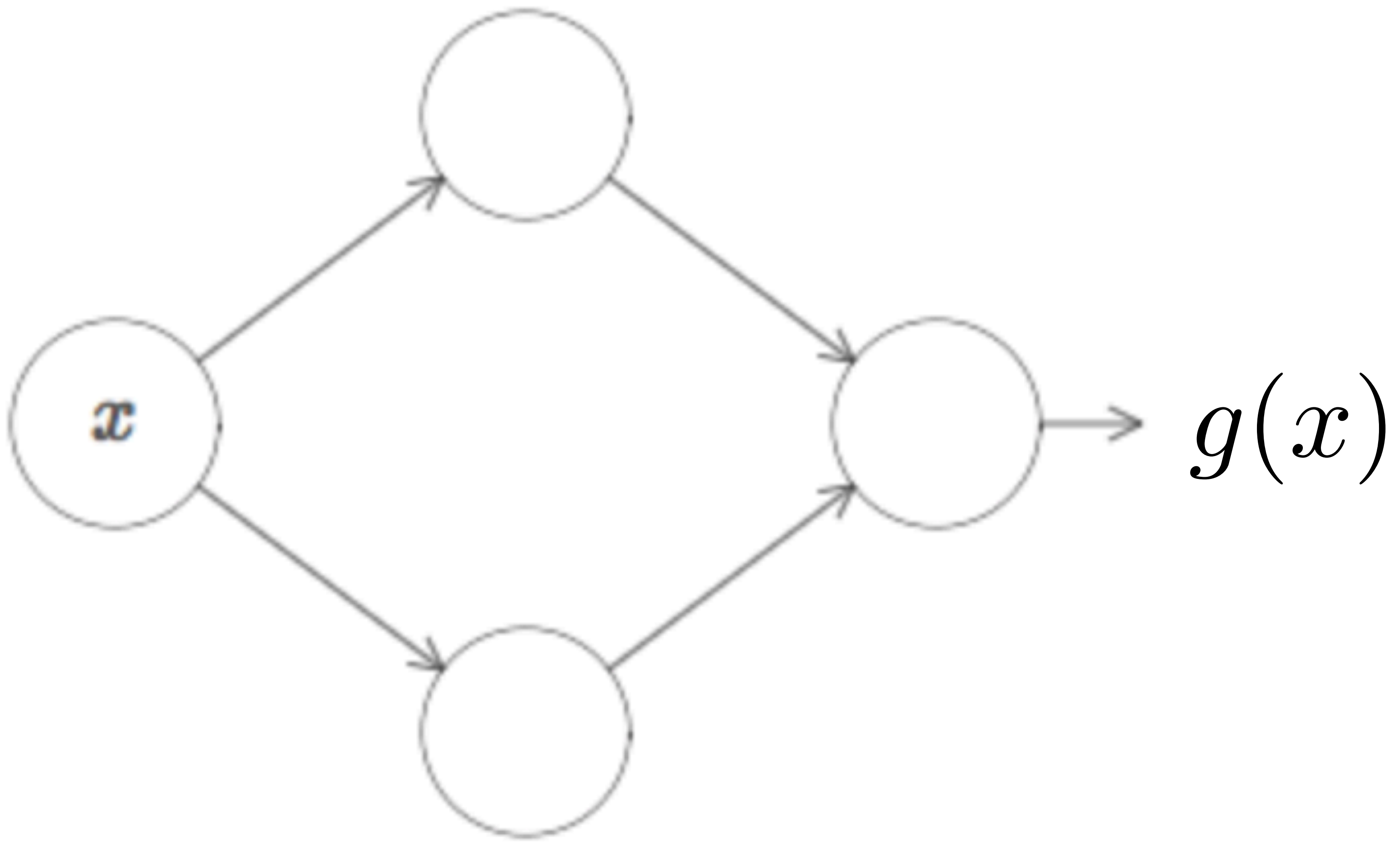
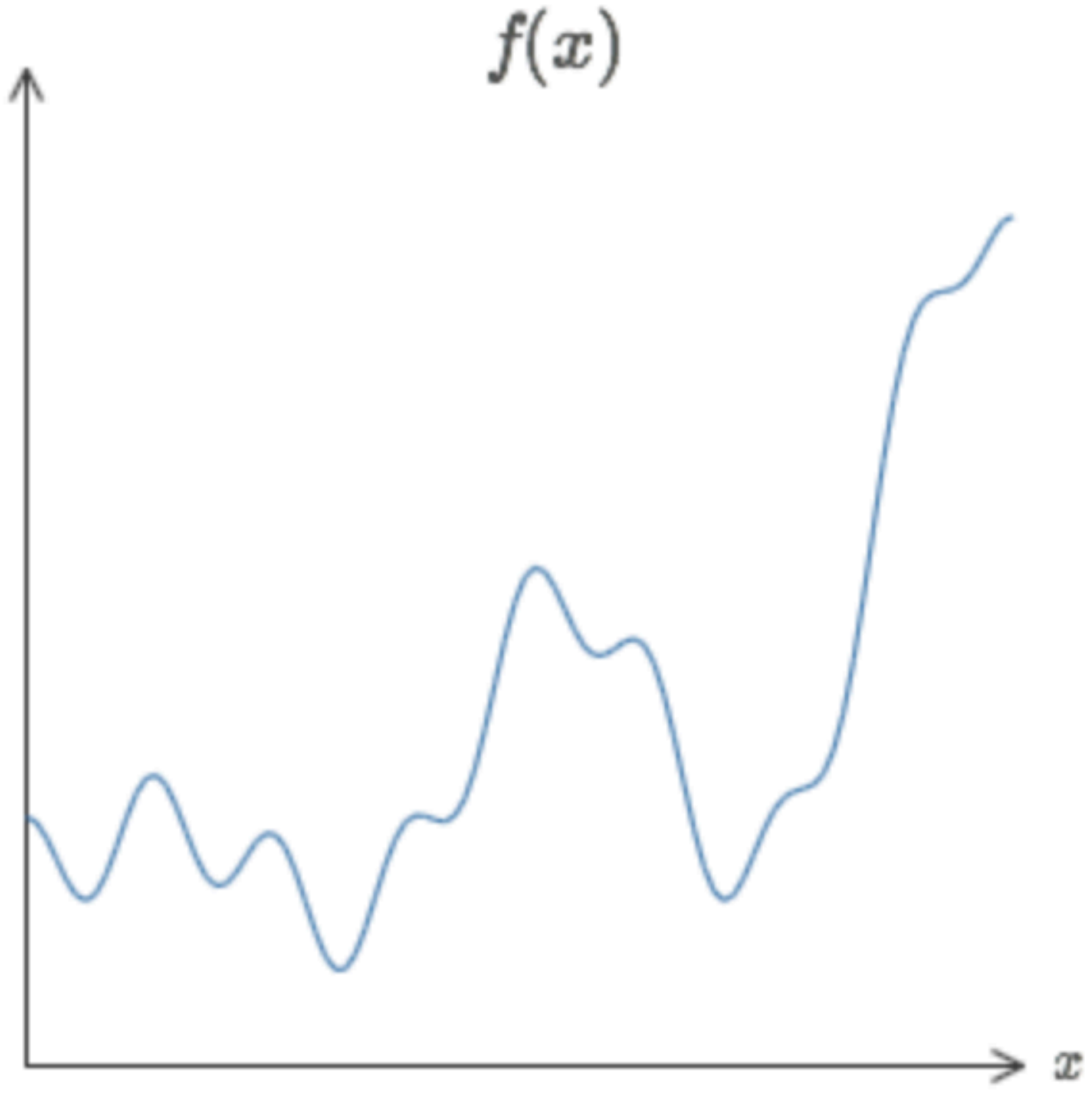


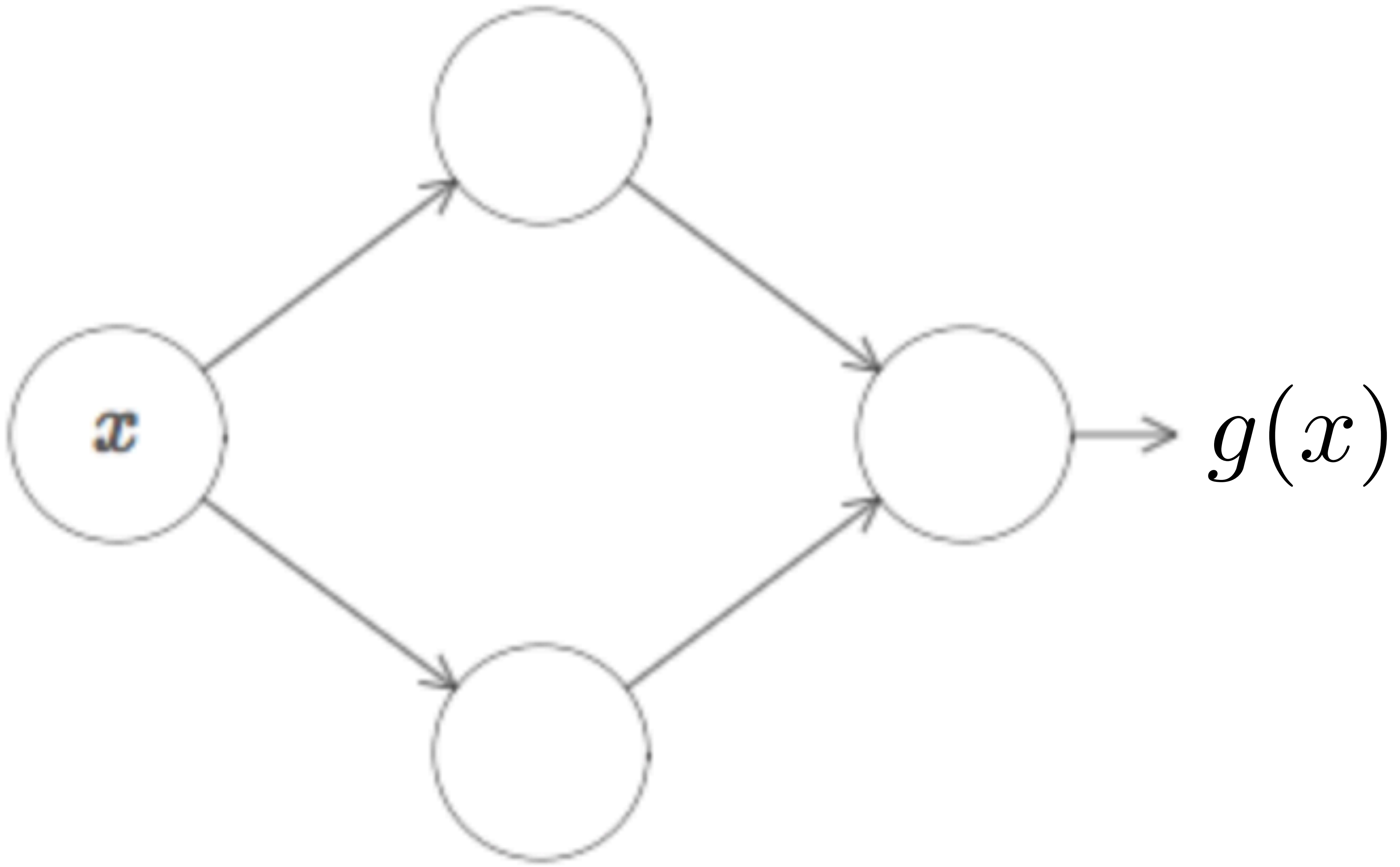


The guarantee is that by using enough hidden neurons we can always find a neural network whose output $g(x)$ satisfies $|g(x) - f(x)| < \epsilon$ for an arbitrarily small ϵ

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

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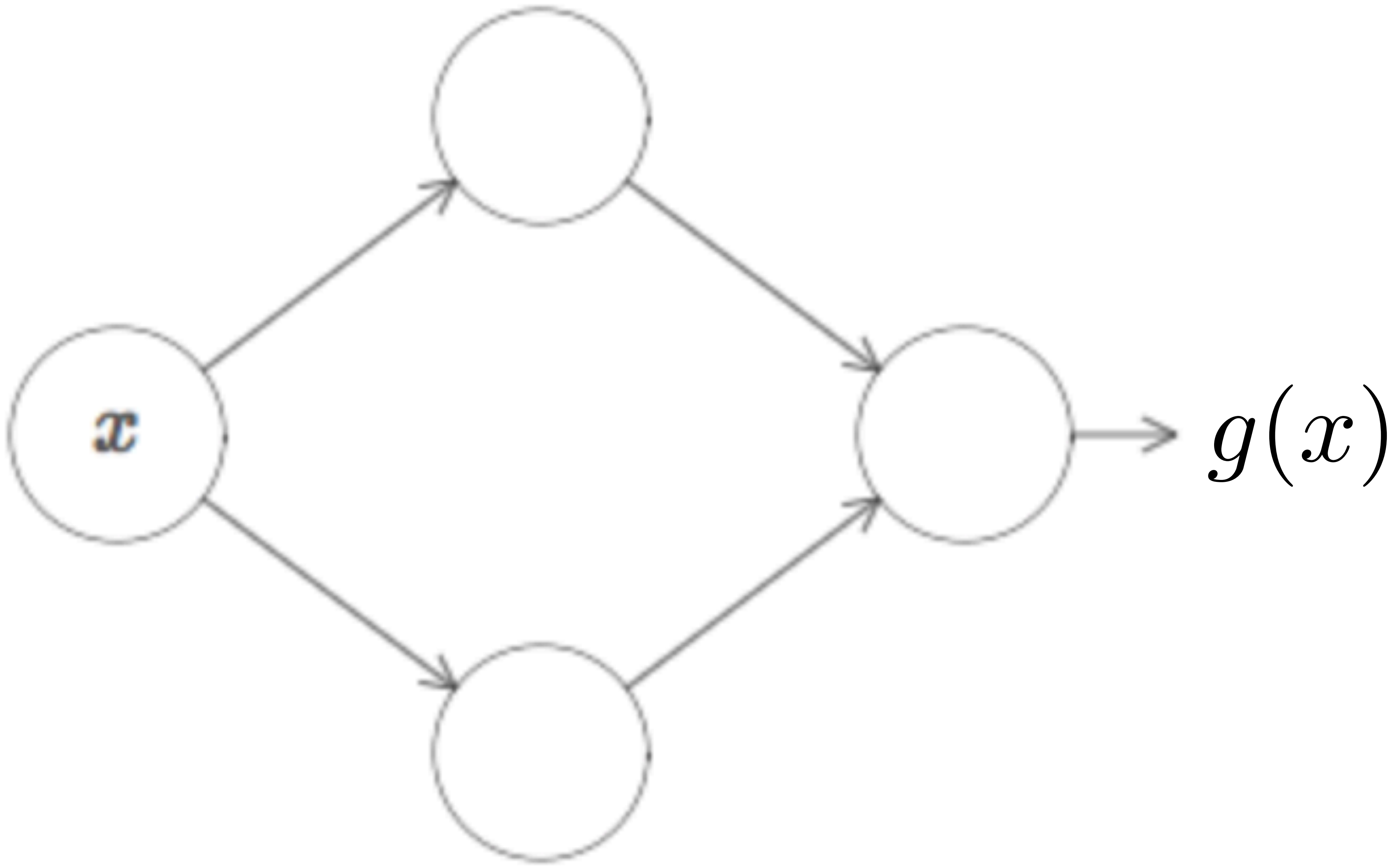
Let's look at output of this (hidden) neuron as a function of parameters (weight, bias)



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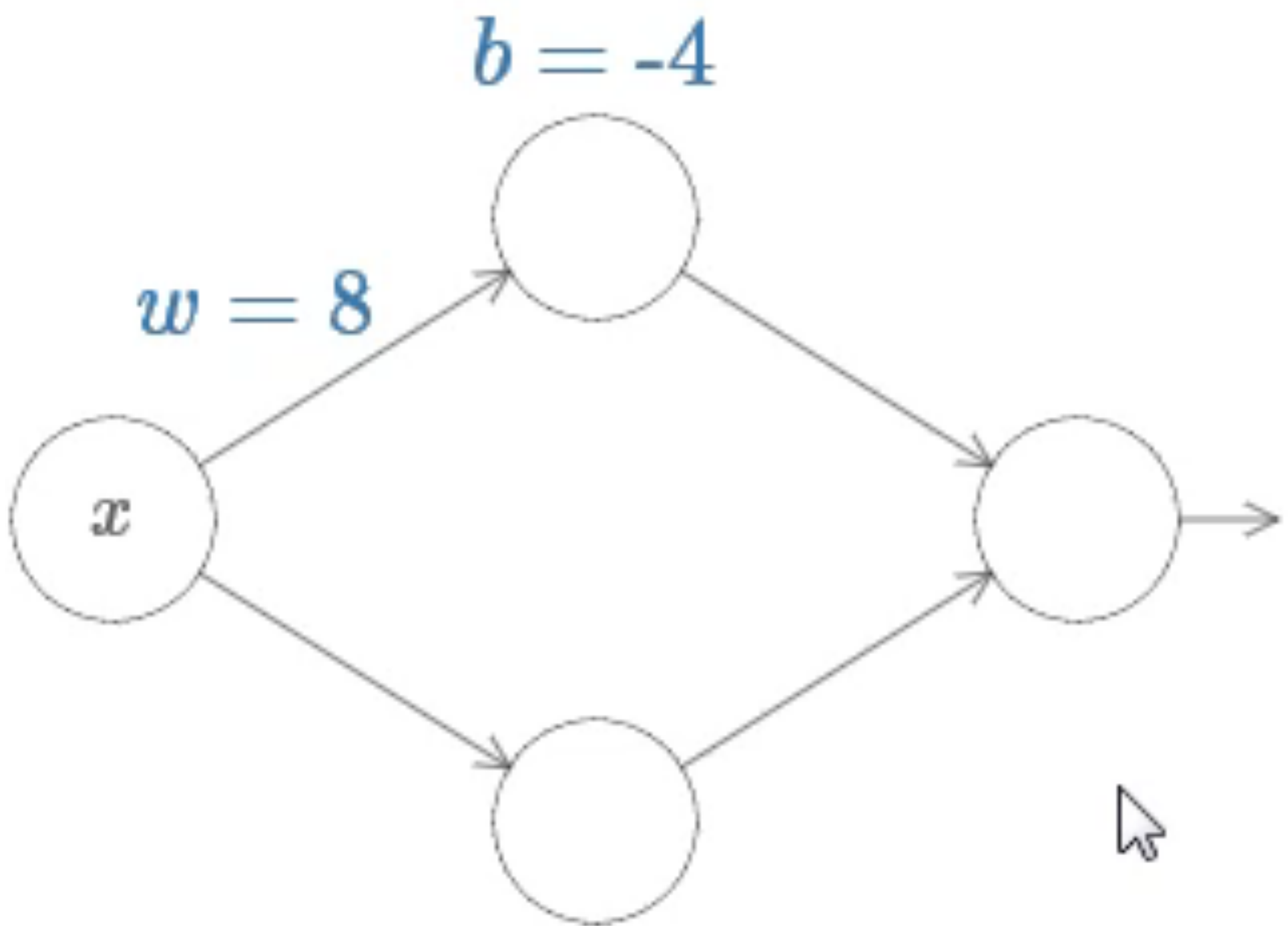

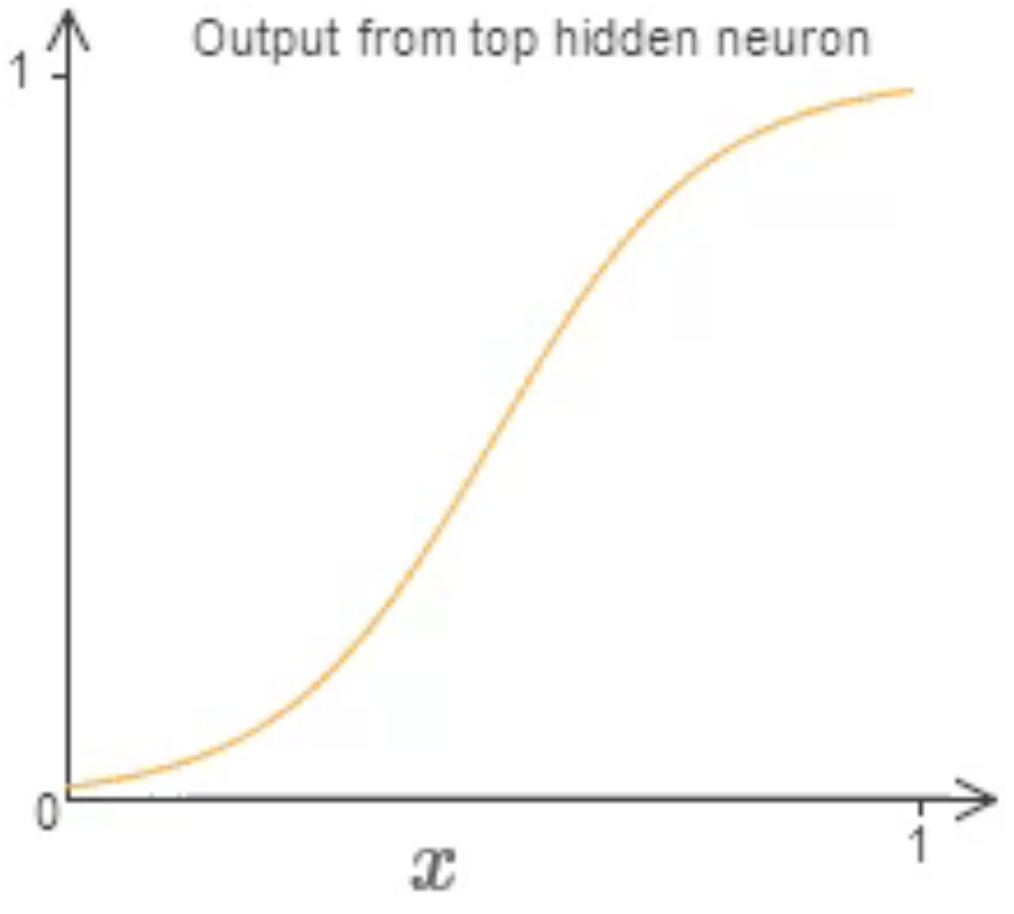

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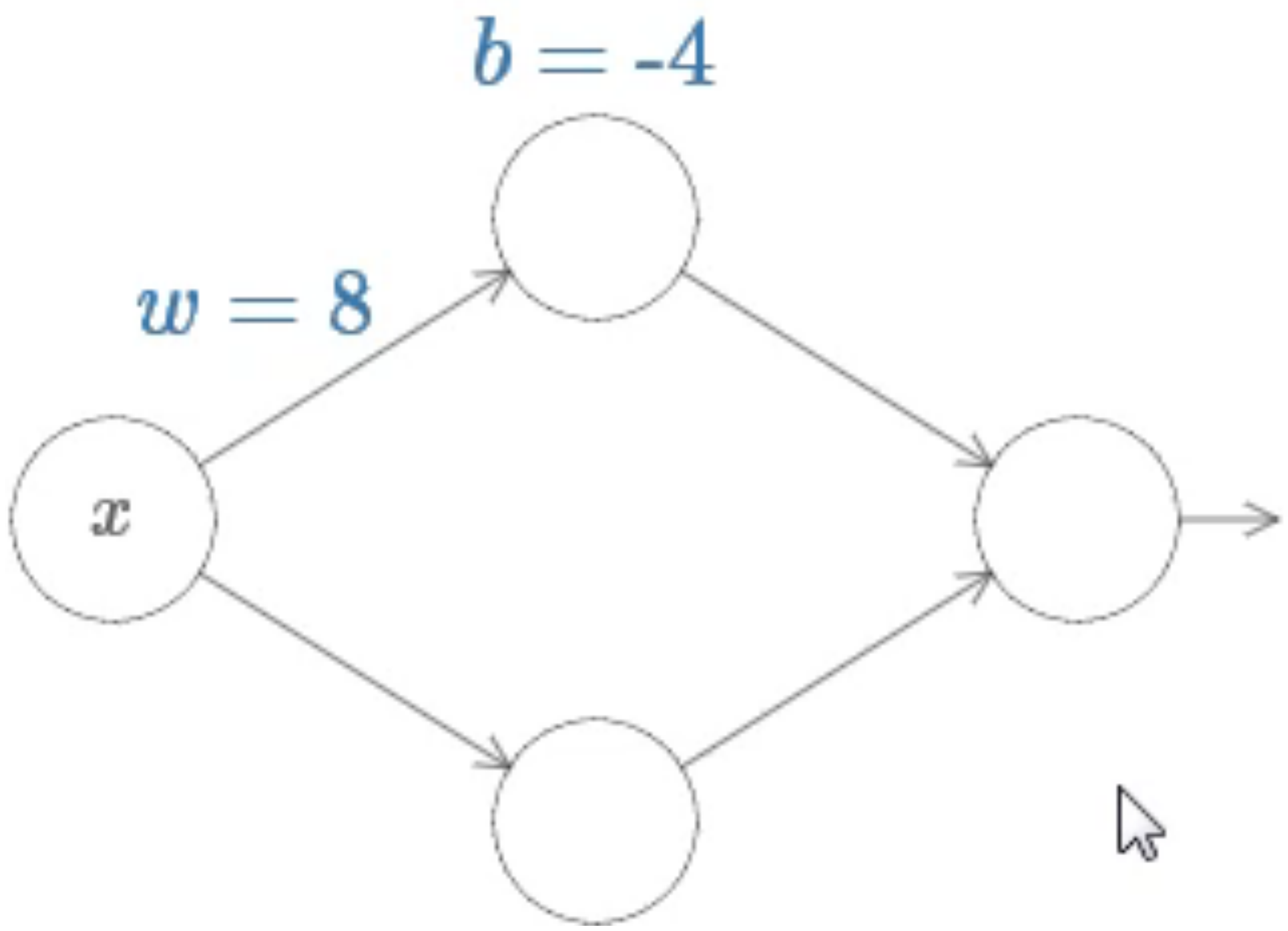

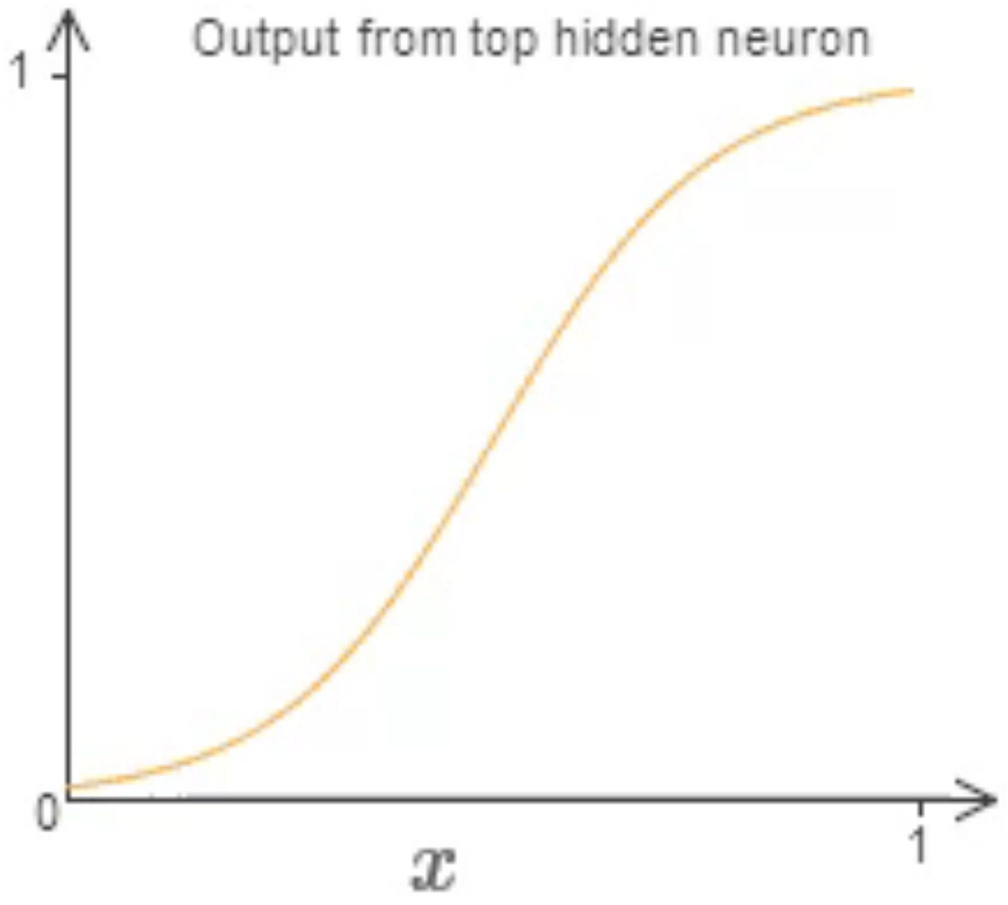

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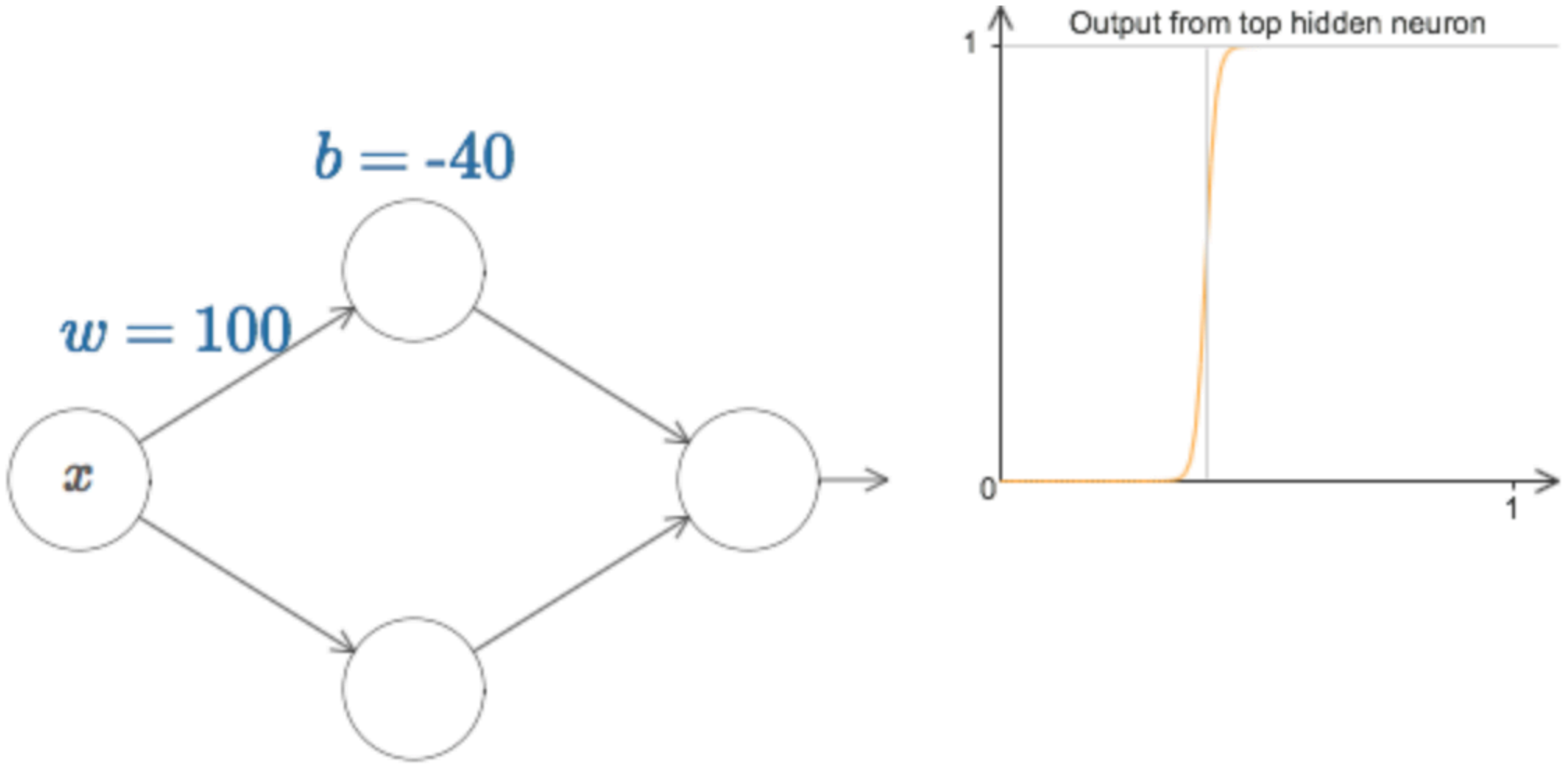
Light Theory: Neural Network as Universal Approximator

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



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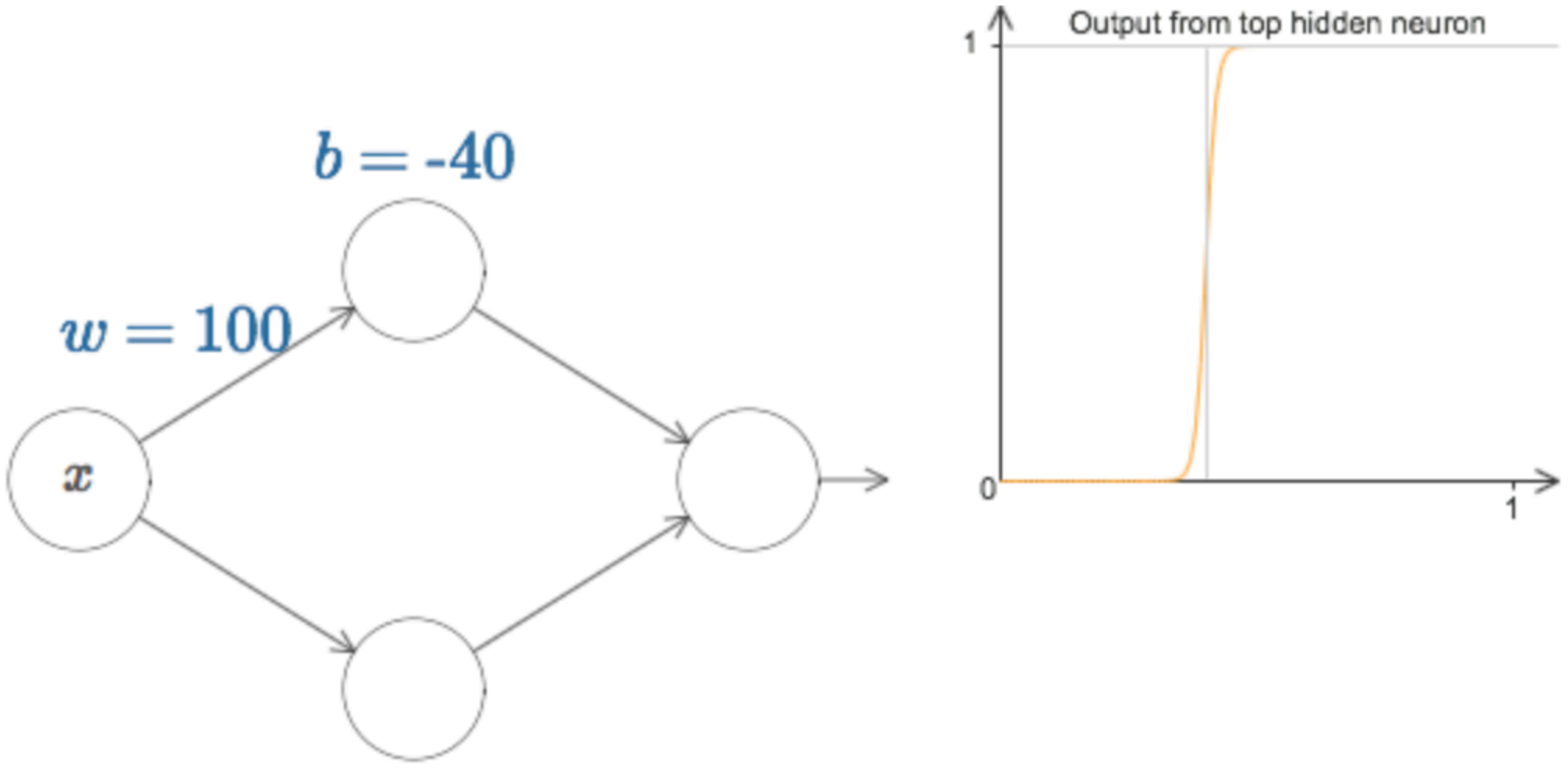
It is easier to work with sums of step functions, so we can assume that every neuron outputs a step function.



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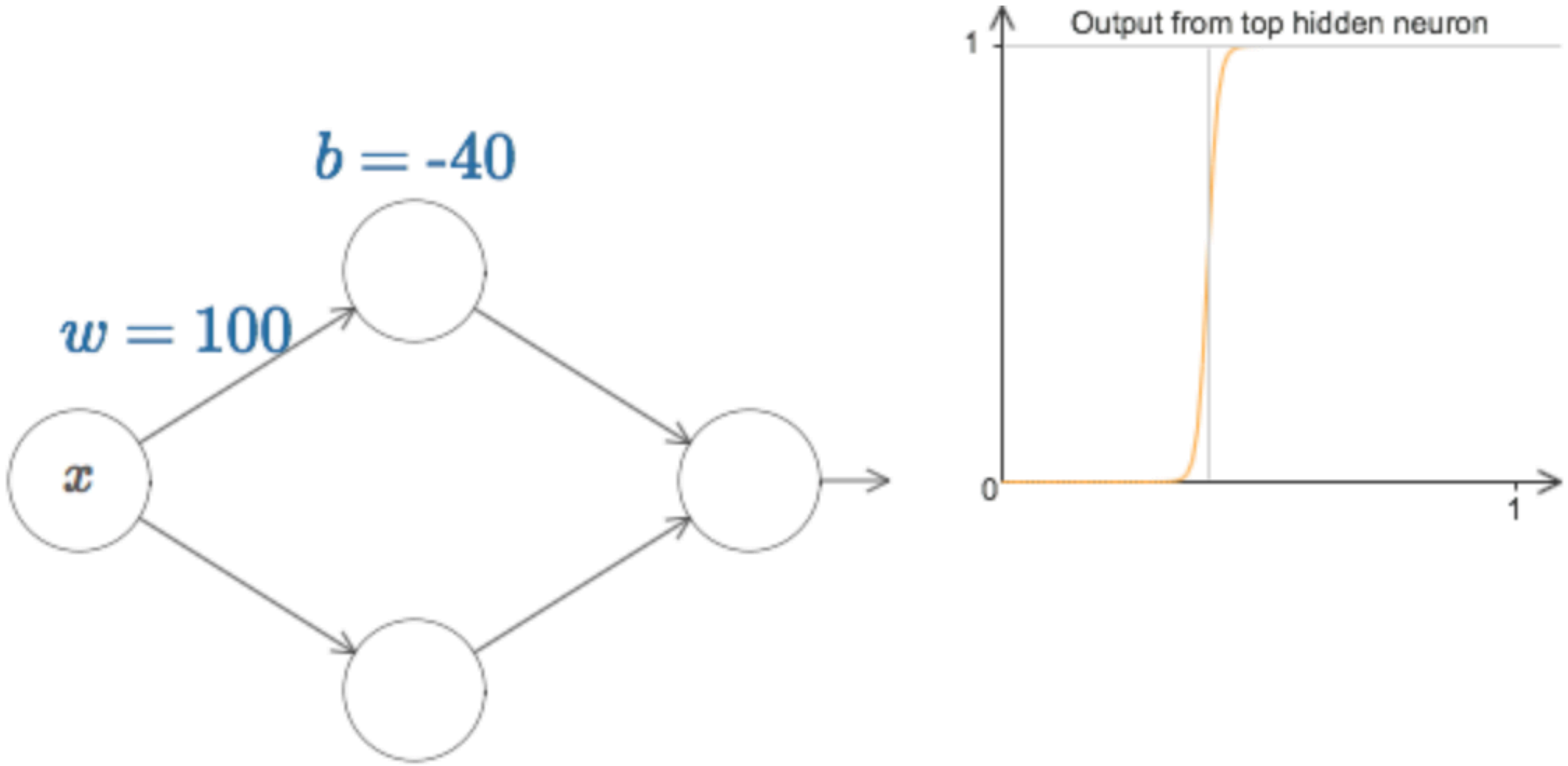

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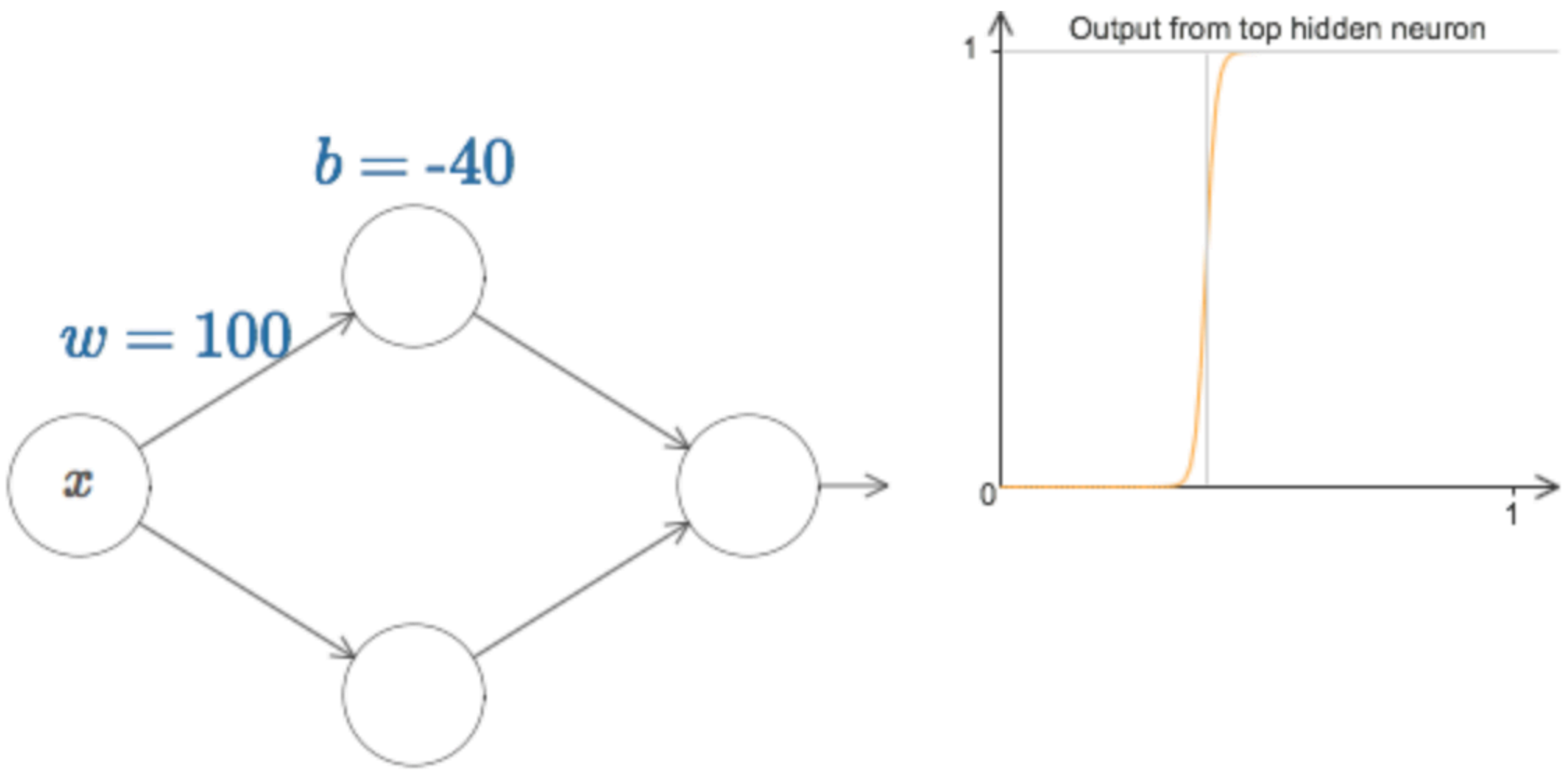

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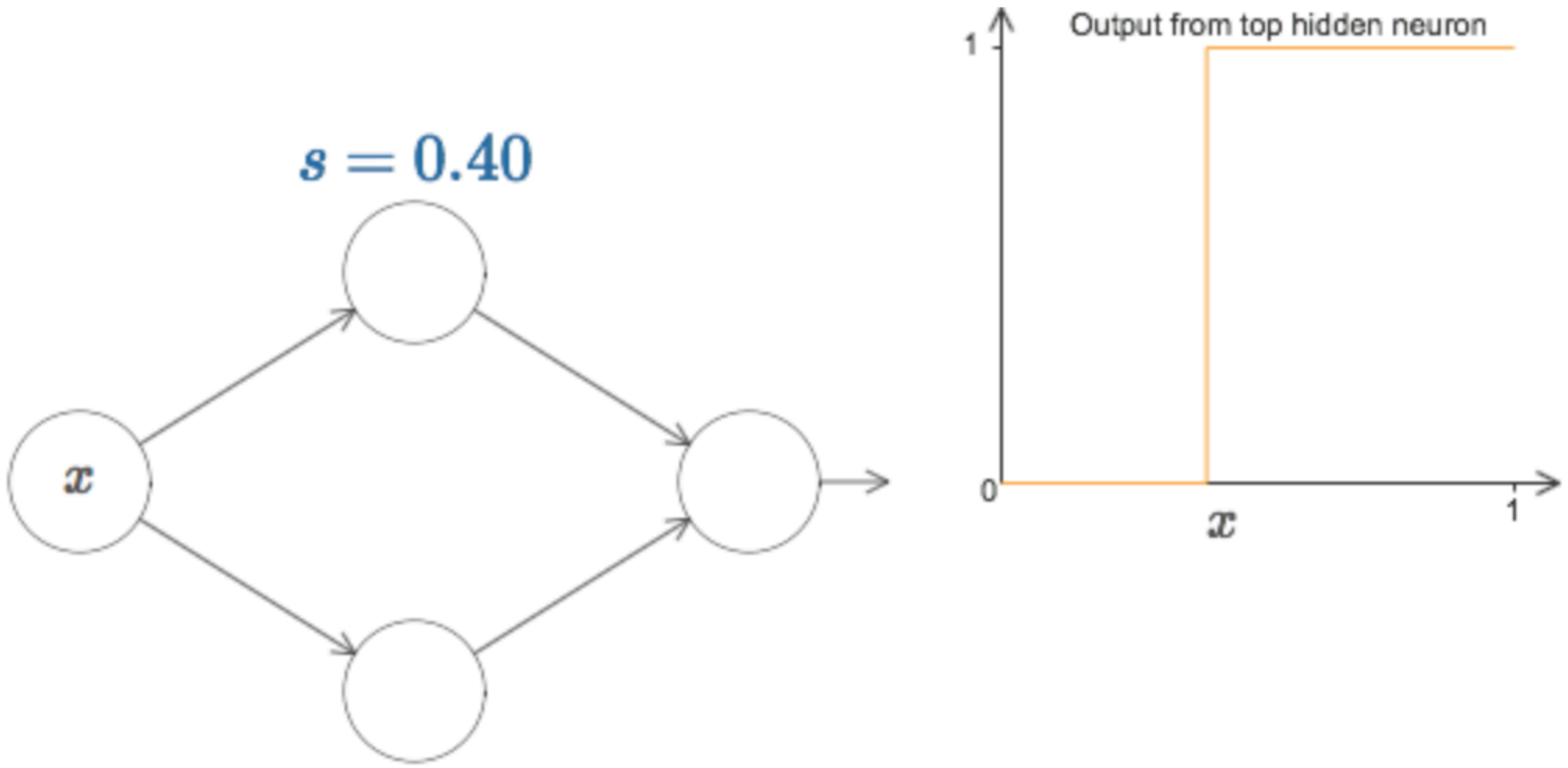

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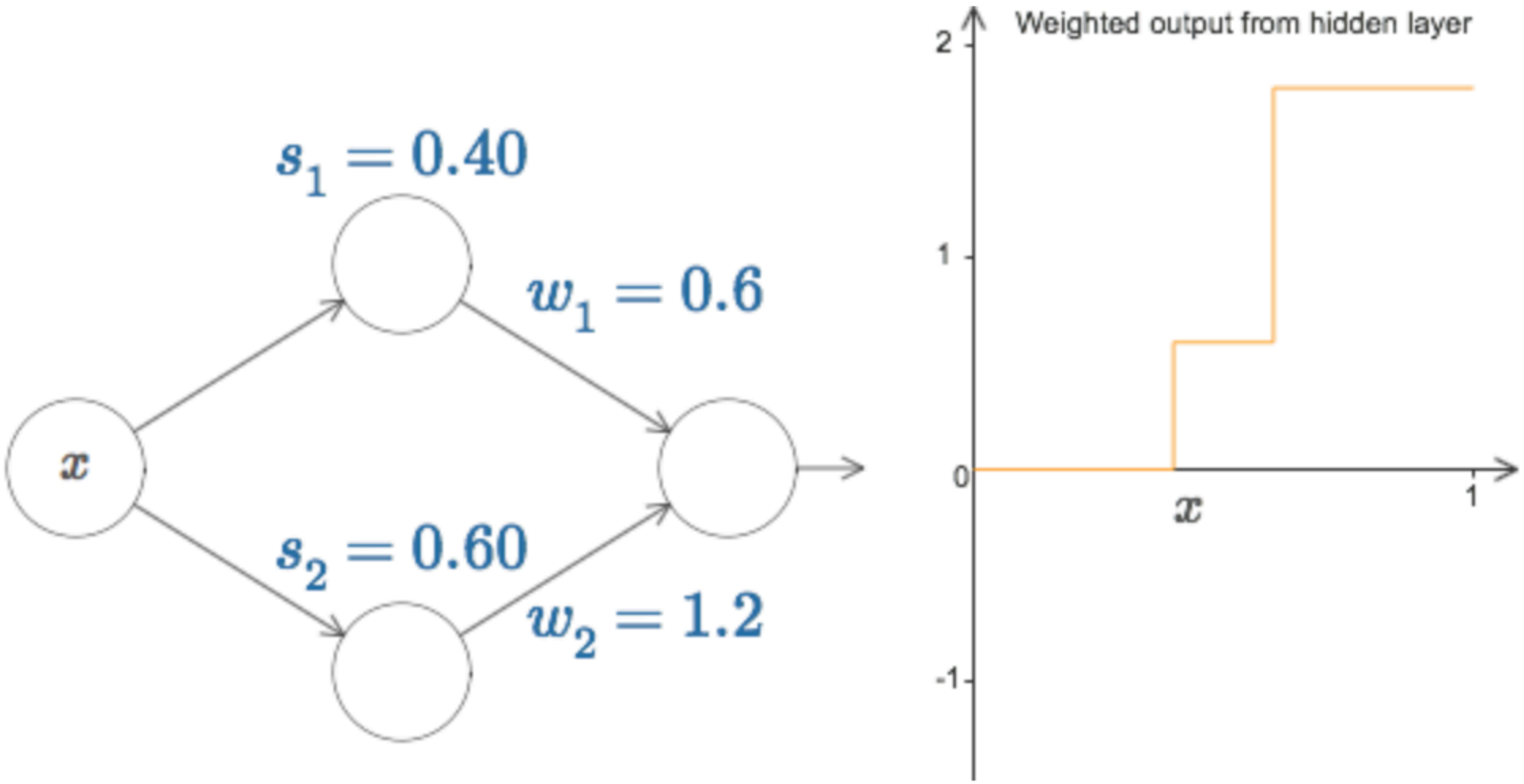
Light Theory: Neural Network as Universal Approximator

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



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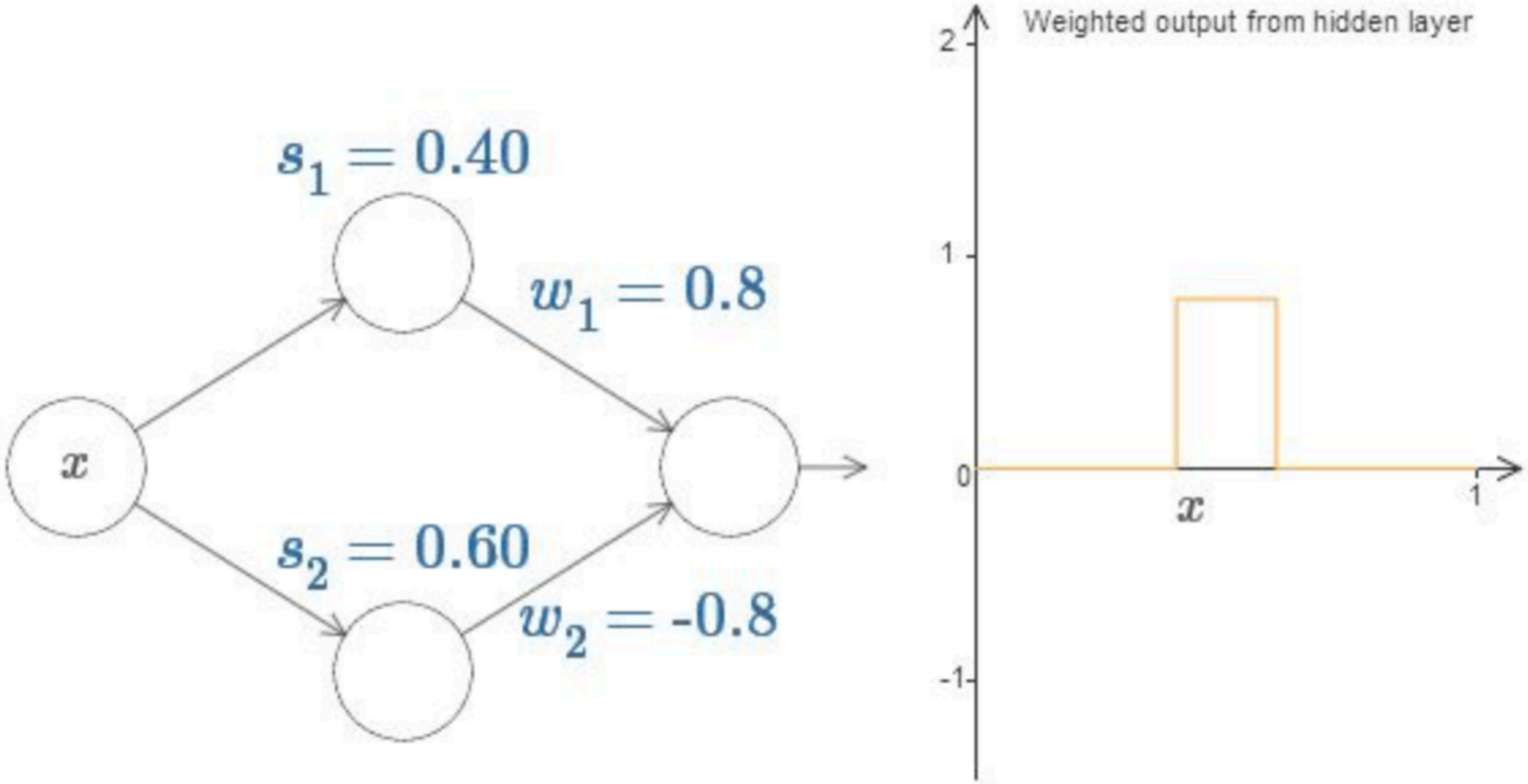

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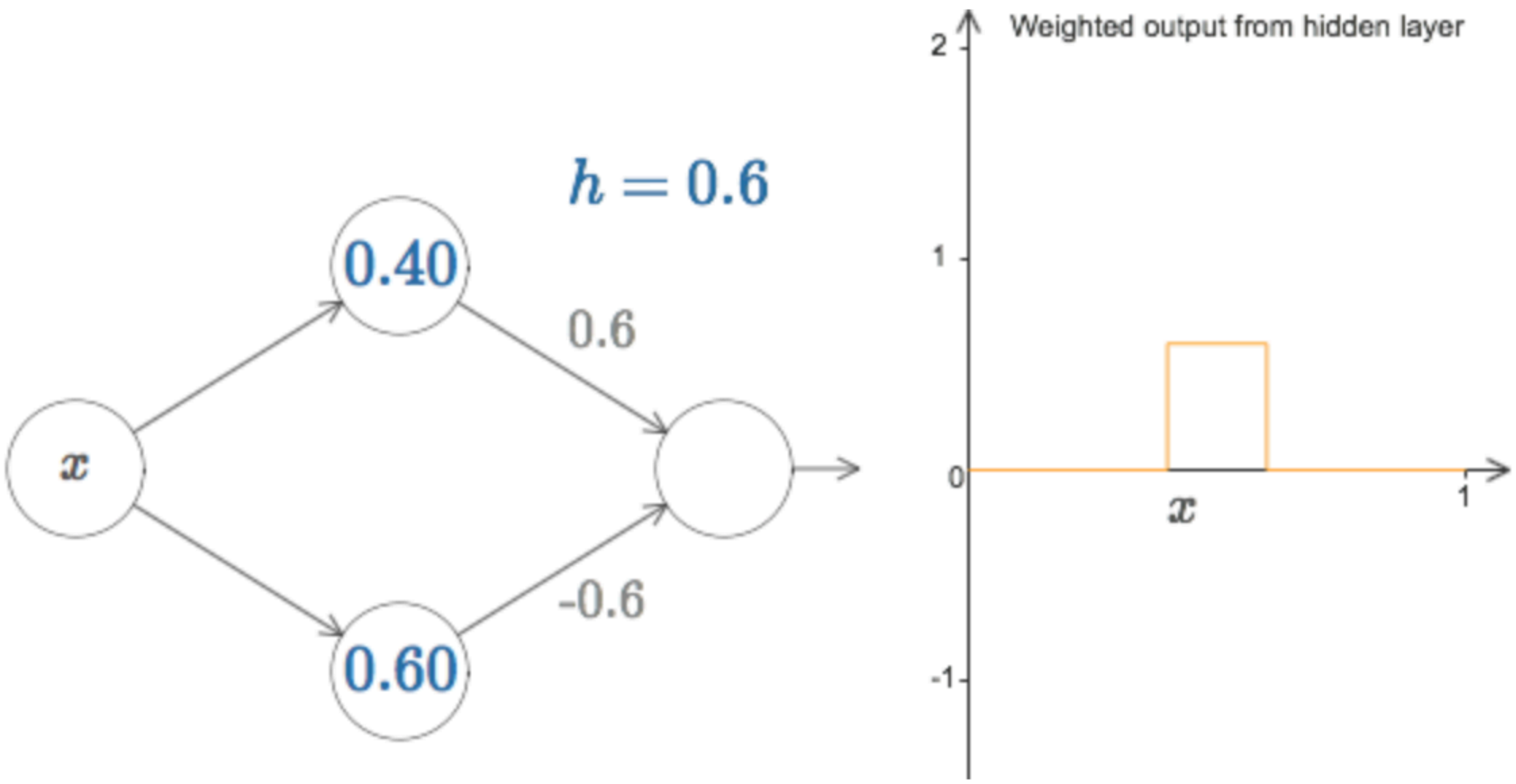

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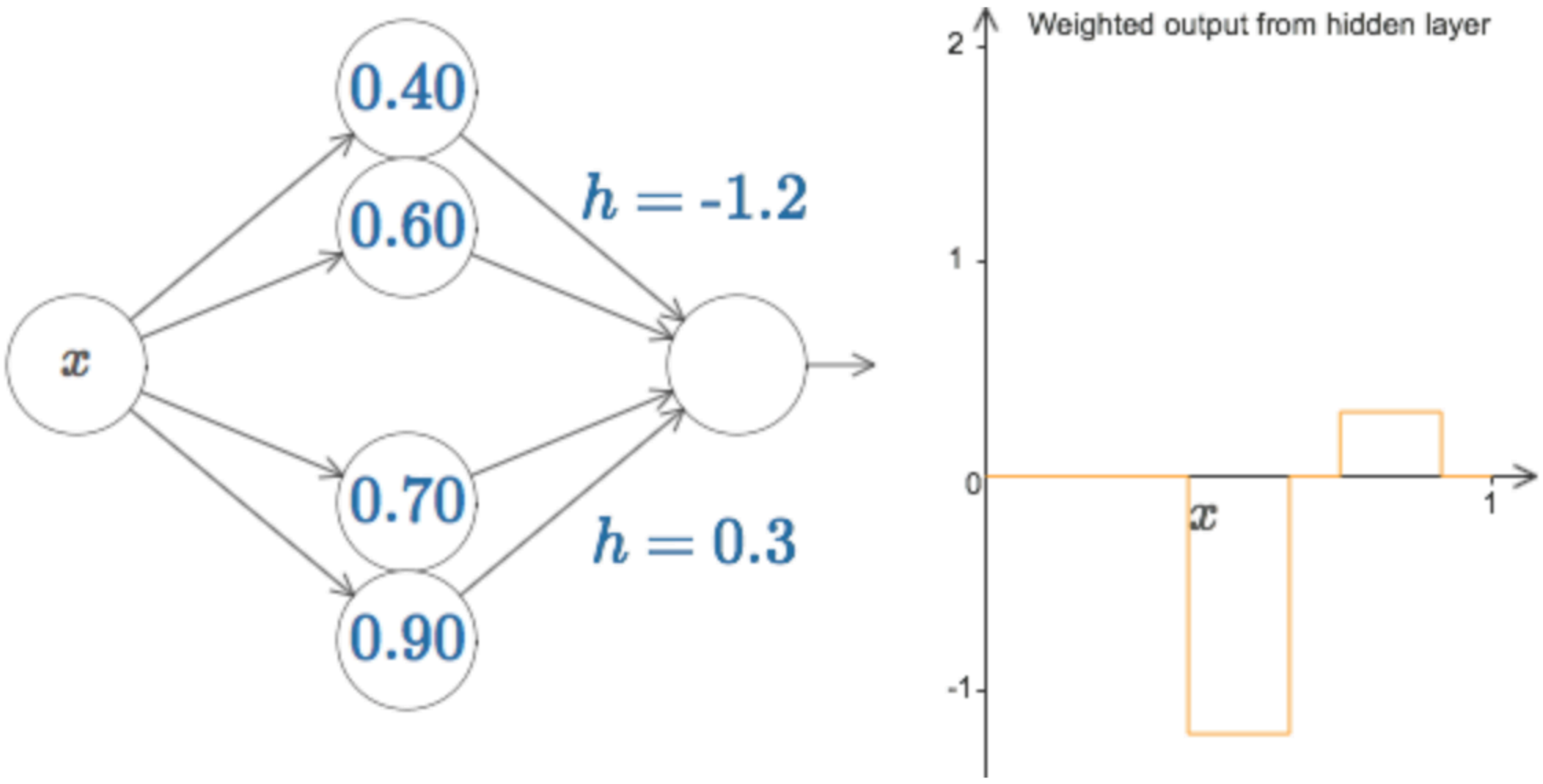

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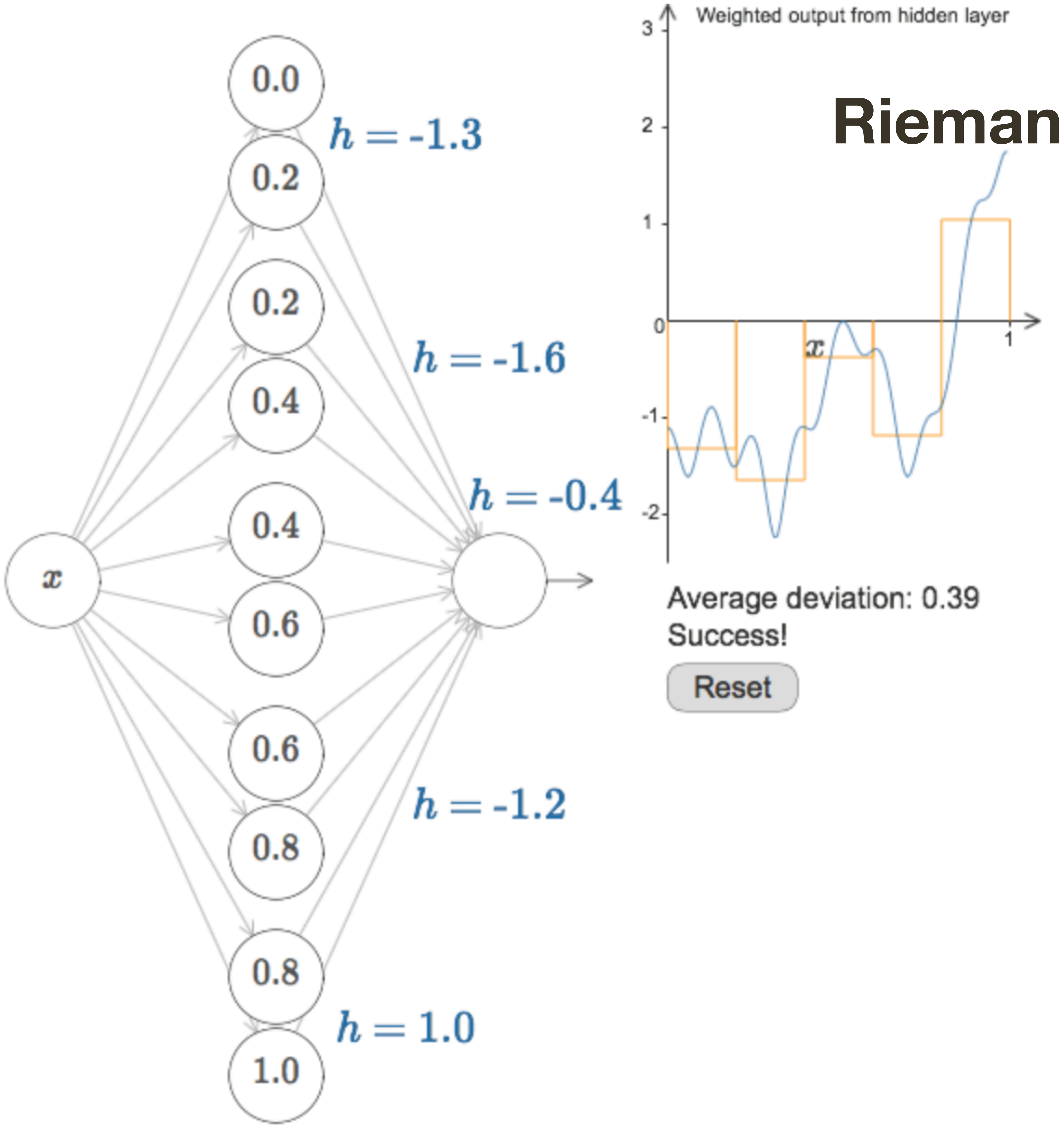

Riemann sum approximation

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Light Theory: Neural Network as Universal Approximator

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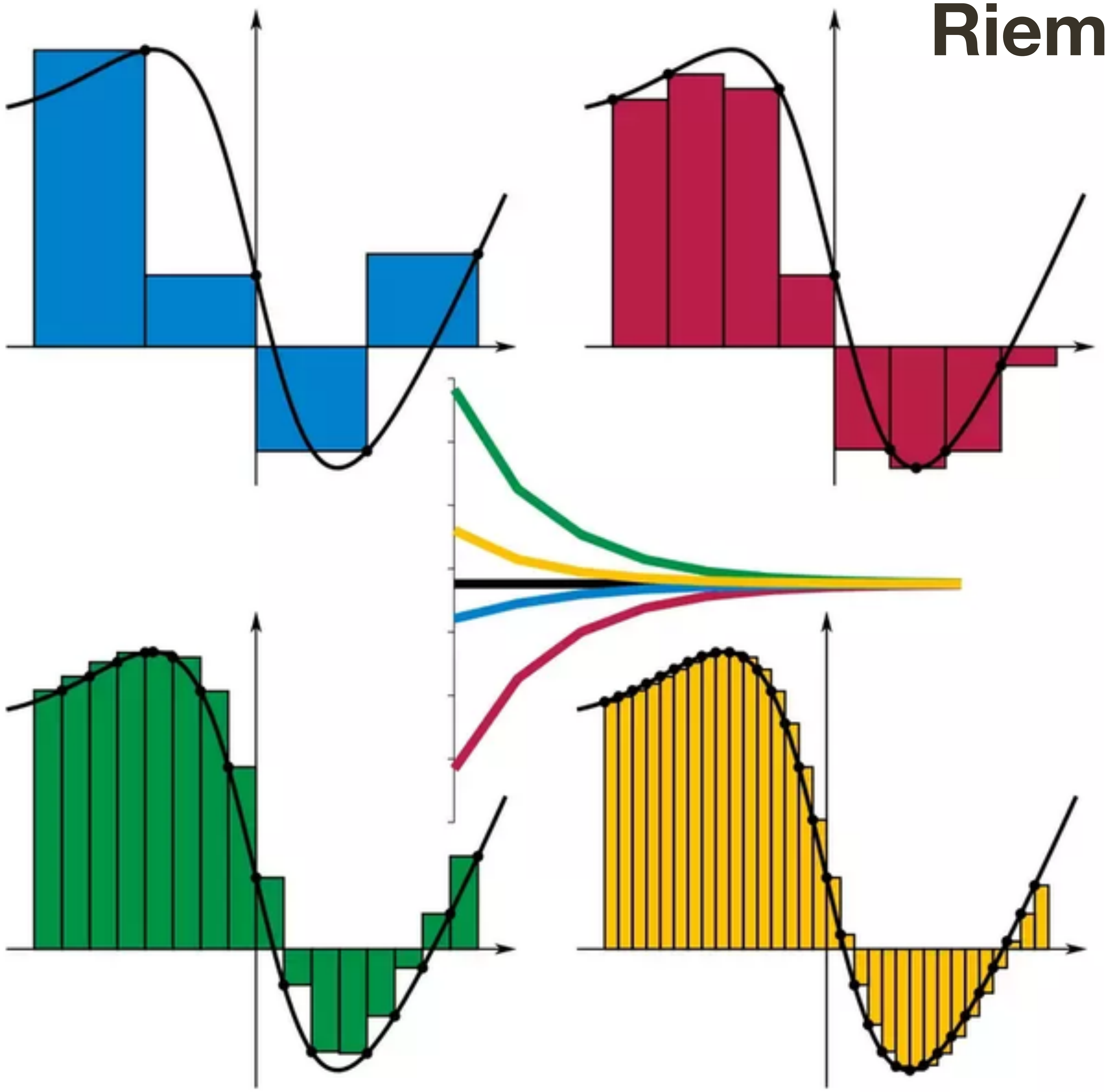

Light Theory: Neural Network as Universal Approximator

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

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

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

$$A \neq B$$

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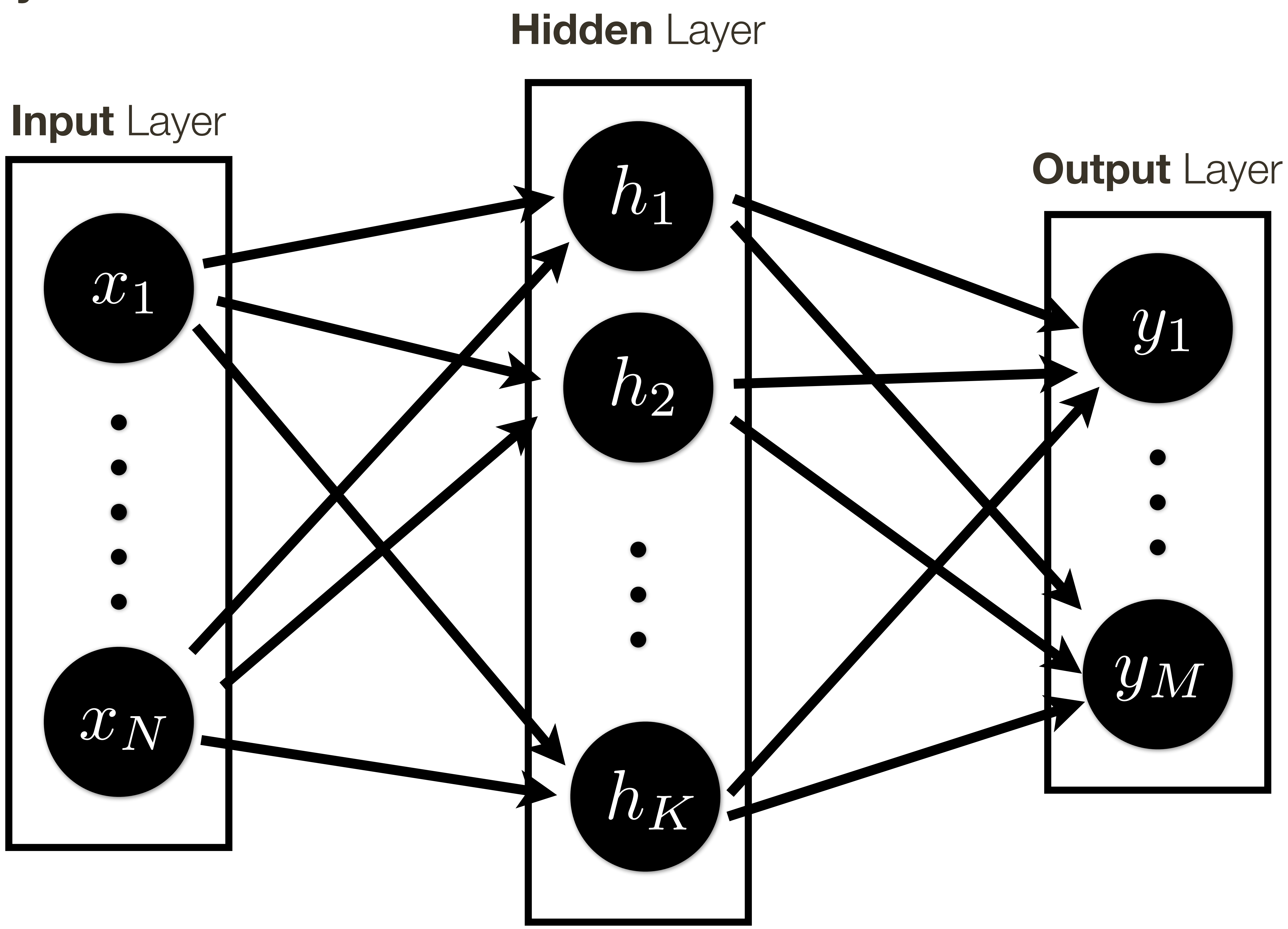
Note: This gives us another way to provably say that linear activation function cannot produce a neural network which is an universal approximator.

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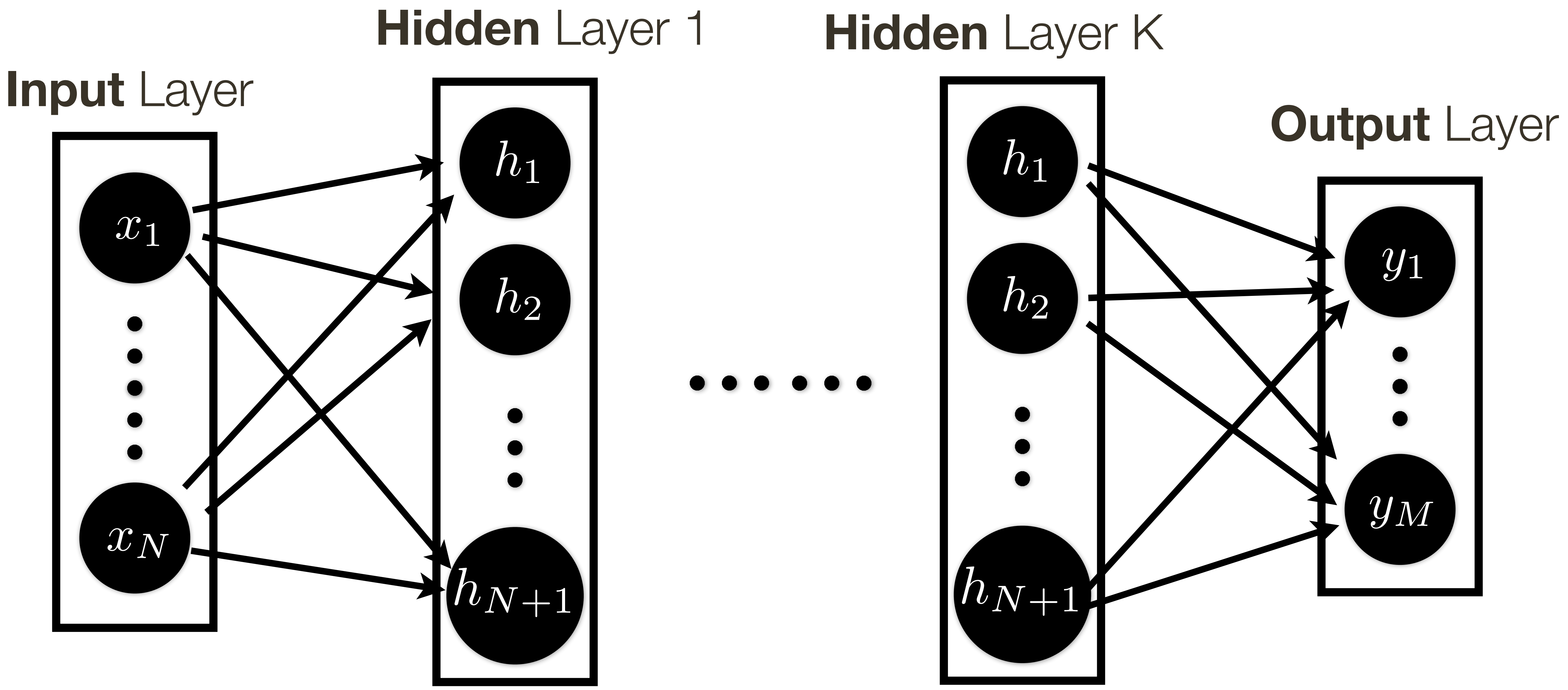
Universal Approximation Theorem (revised): A network of infinite depth with a hidden layer of size $d+1$ neurons, where d is the dimension of the input space, can approximate any continuous function.

[Lu *et al*., NIPS 2017]



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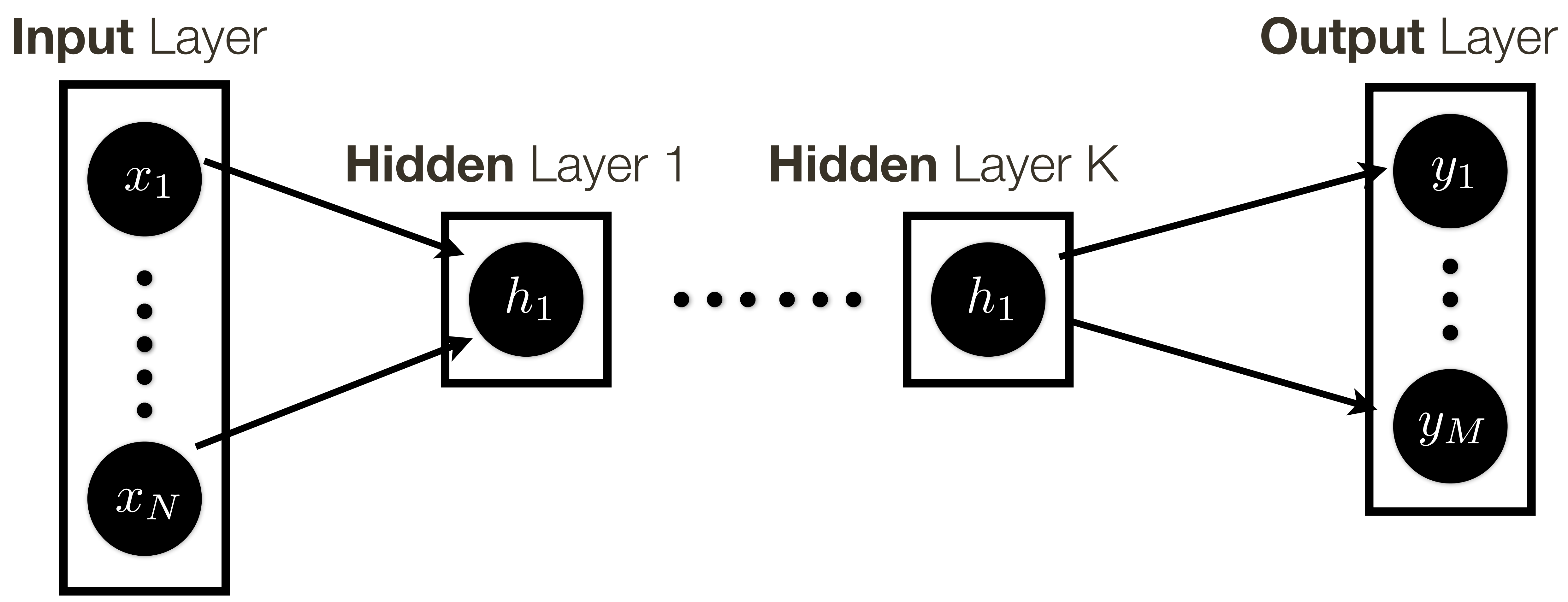

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[Lin and Jegelka, NIPS 2018]

Practical **Observations**

Neural Network represents a function using a **piece-wise linear** approximation

Expressivity (theoretic quality) of NN = the number of piece-wise linear regions

— Number of regions is a polynomial function of units per layer (breadth of NN)

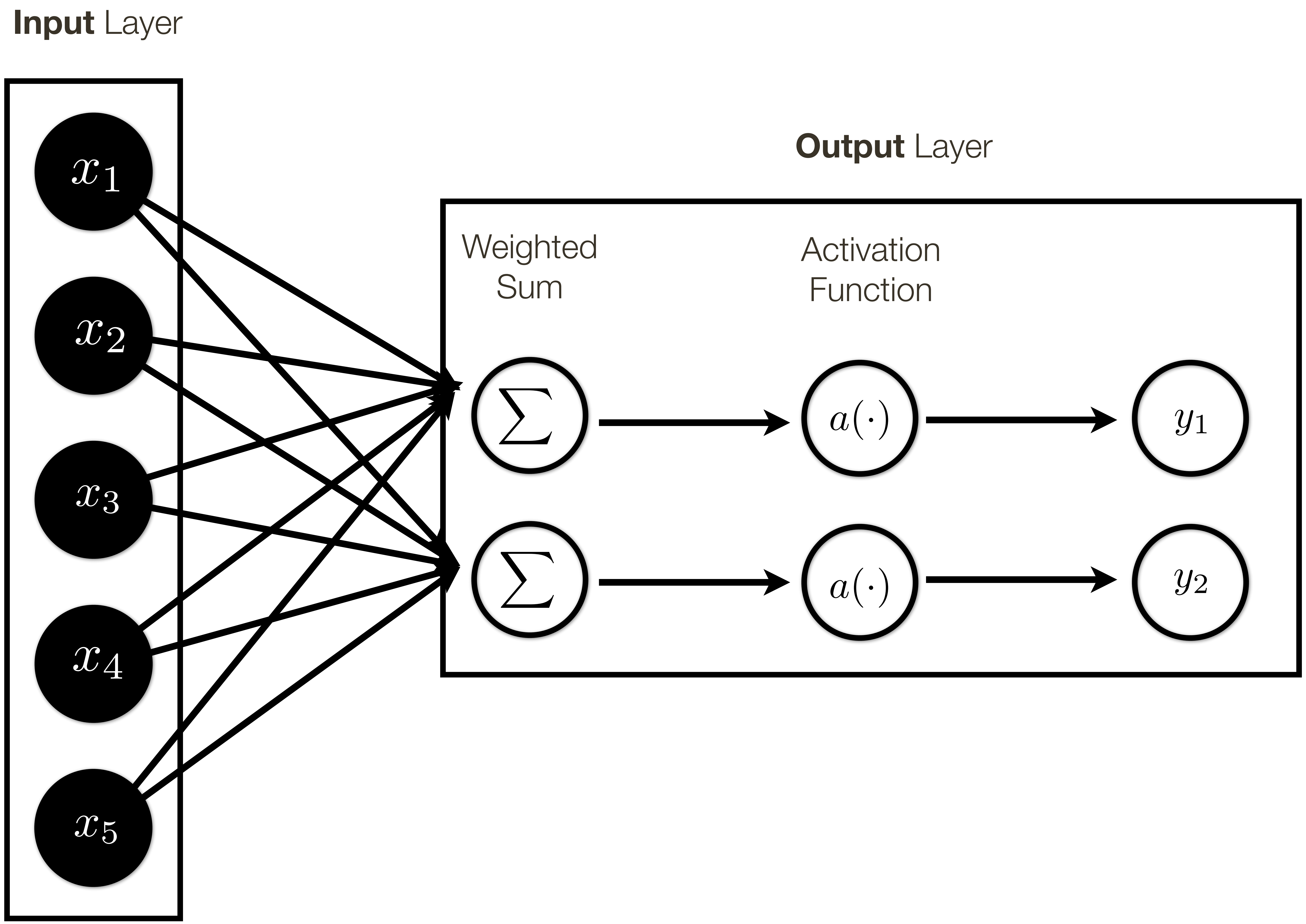
— Number of regions is an exponential function of layers (depth of NN)

Effectiveness (practical quality) of the NN is also a function of optimization

— Deep networks are generally harder to optimize

Note: in recent literature the # of parameters have been used as a proxy for expressiveness of NN, this is not a great practice, because it ignores topology.

One-layer **Neural Network**



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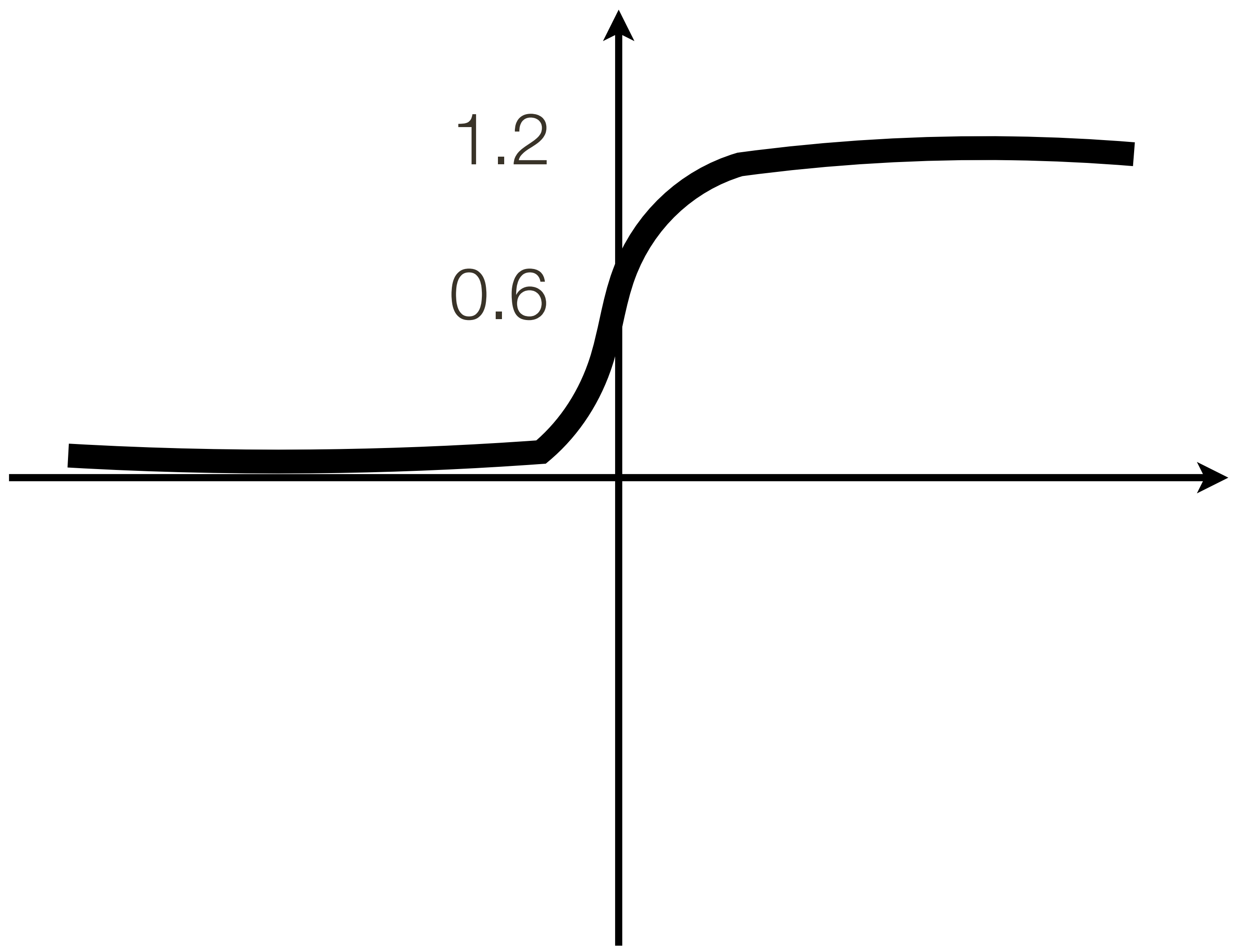

Sigmoid Activation

Learning Parameters of One-layer Neural Network

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

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

*slide adopted from V. Ordonex

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Solution:

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

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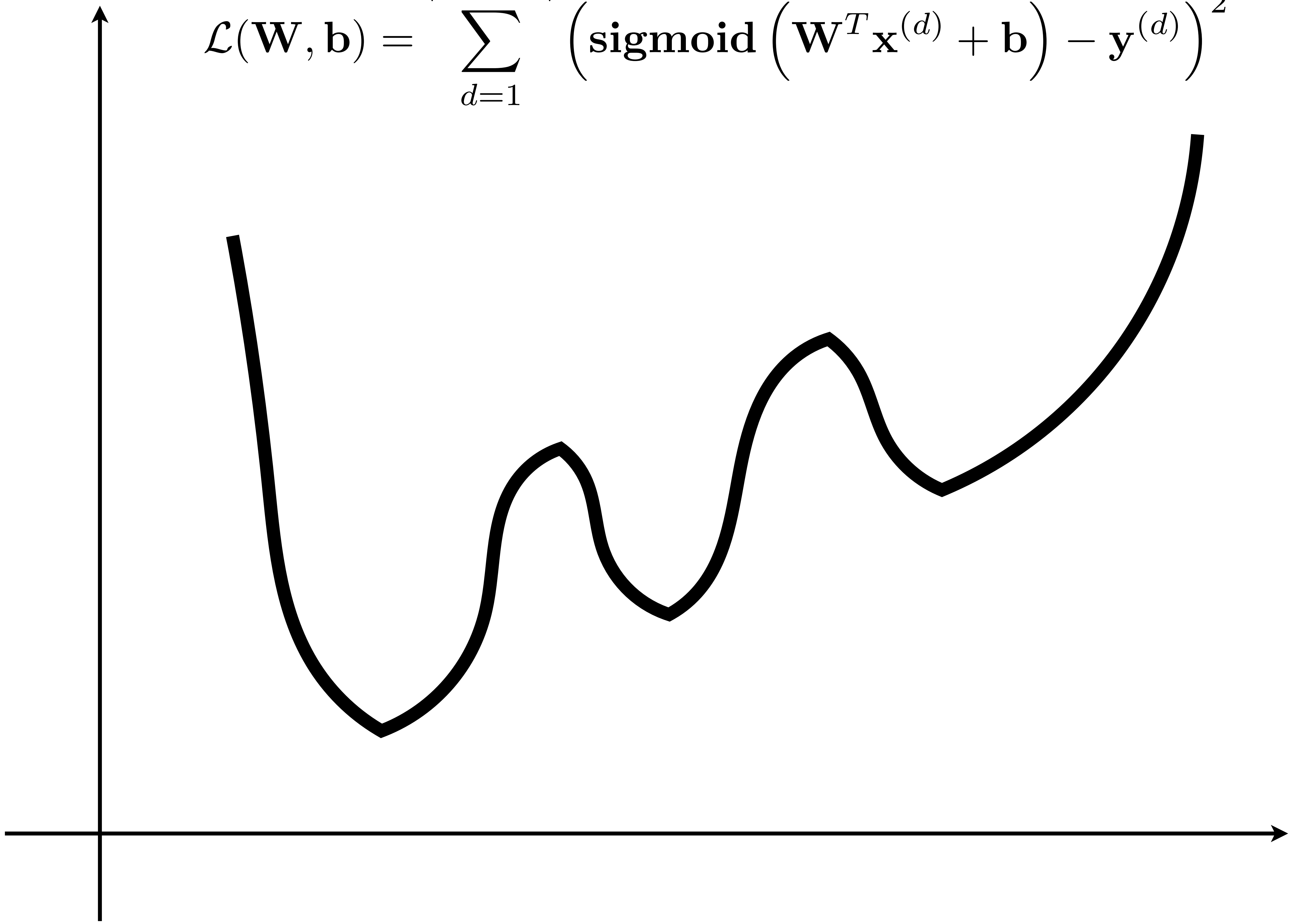
Problem: No closed form solution $\frac{\partial \mathcal{L}(\mathbf{W}, \mathbf{b})}{\partial w_{ji}} = 0$

*slide adopted from V. Ordonex

Gradient Descent (review)

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



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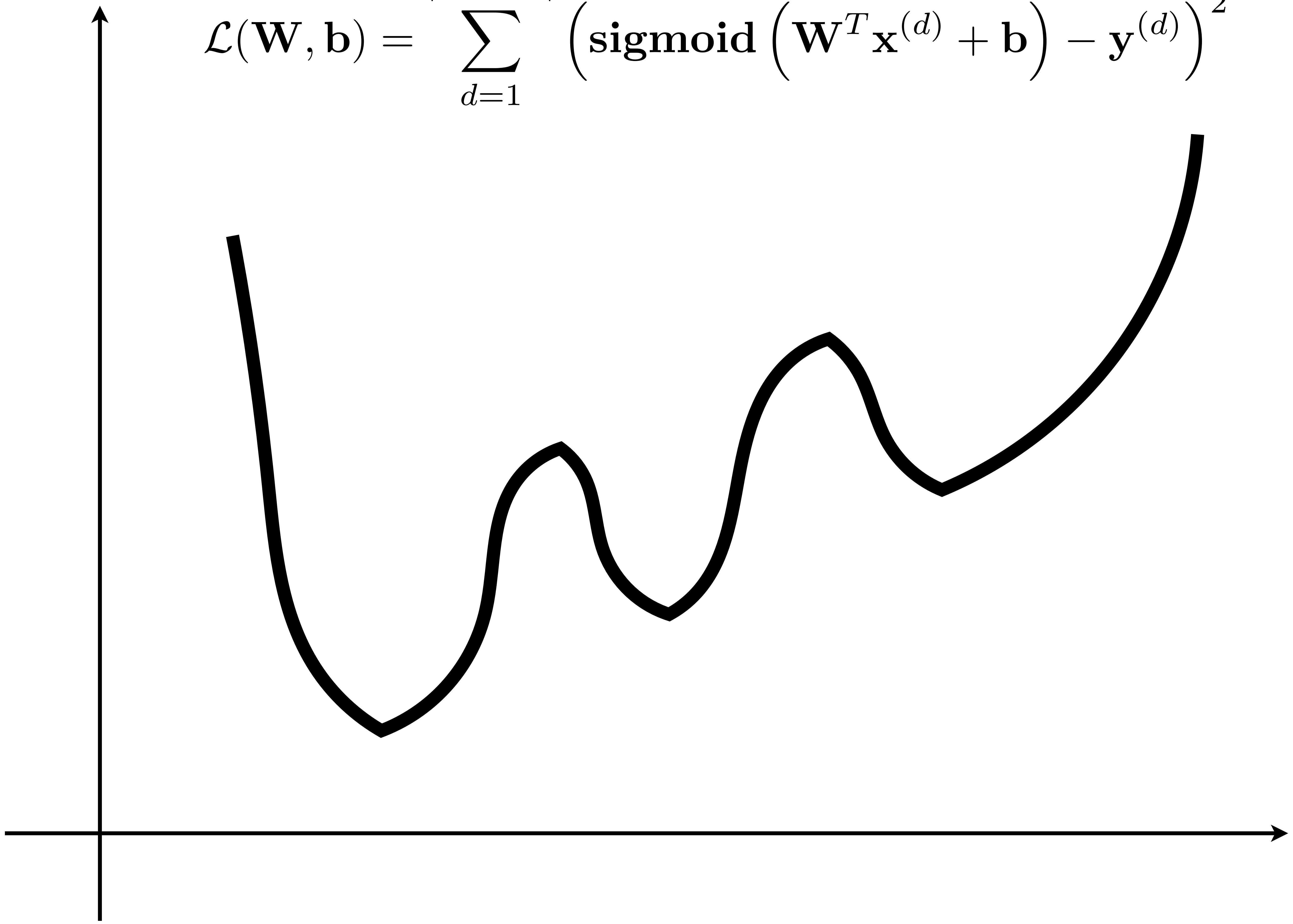

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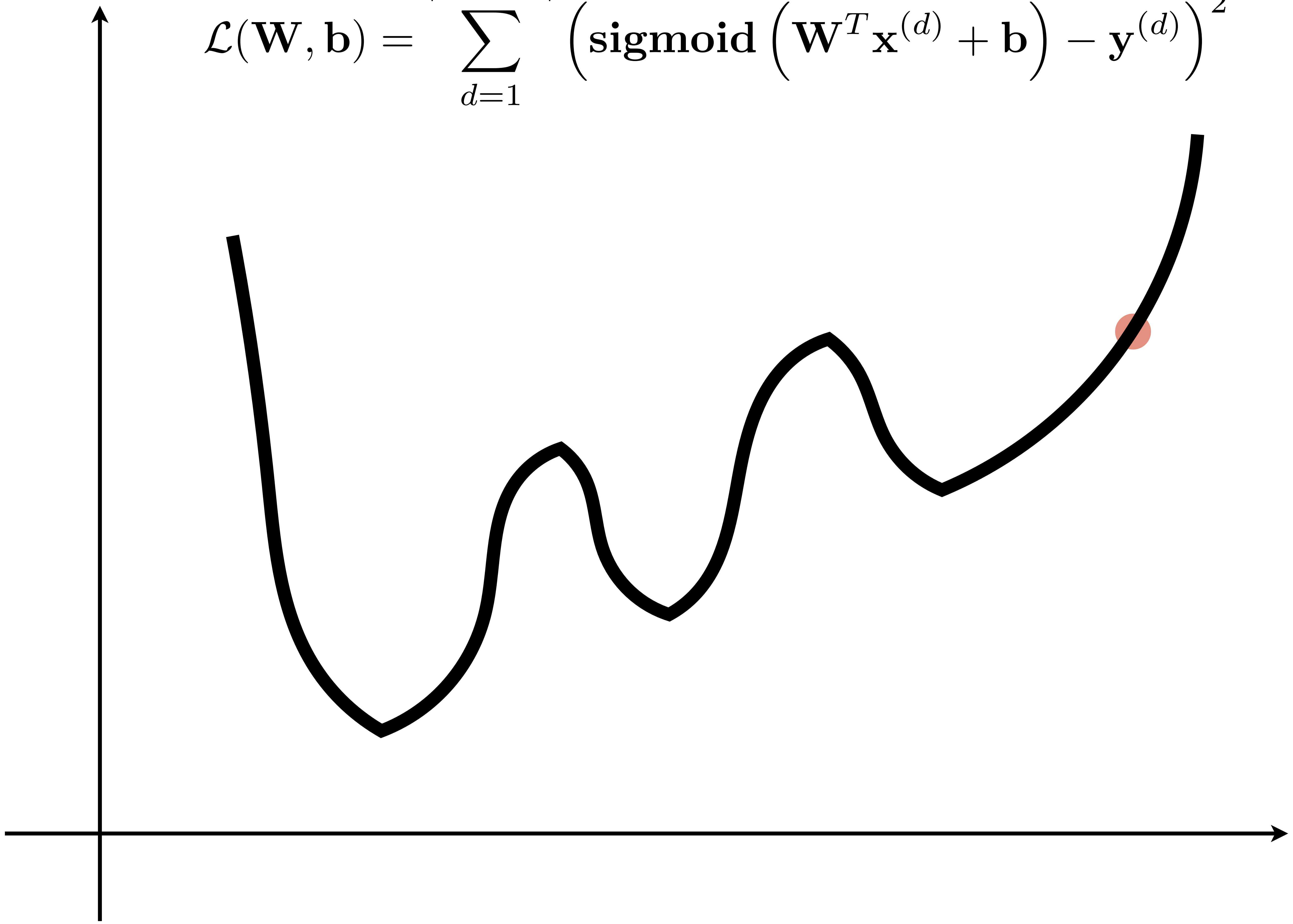

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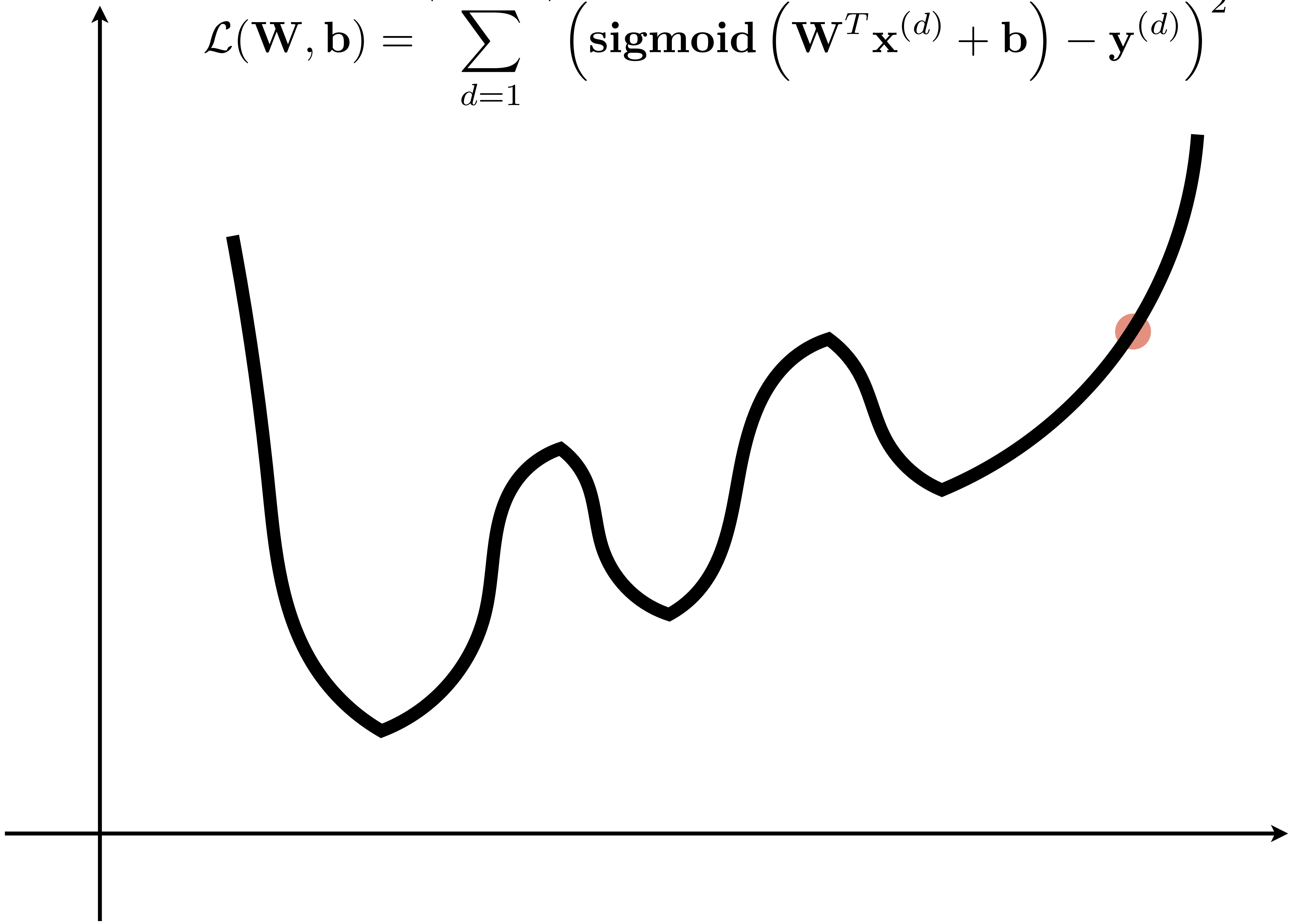

1. Start from random value of $\boxed{\mathbf{W}_0, \mathbf{b}_0}$

For $k = 0$ to max number of iterations

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

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

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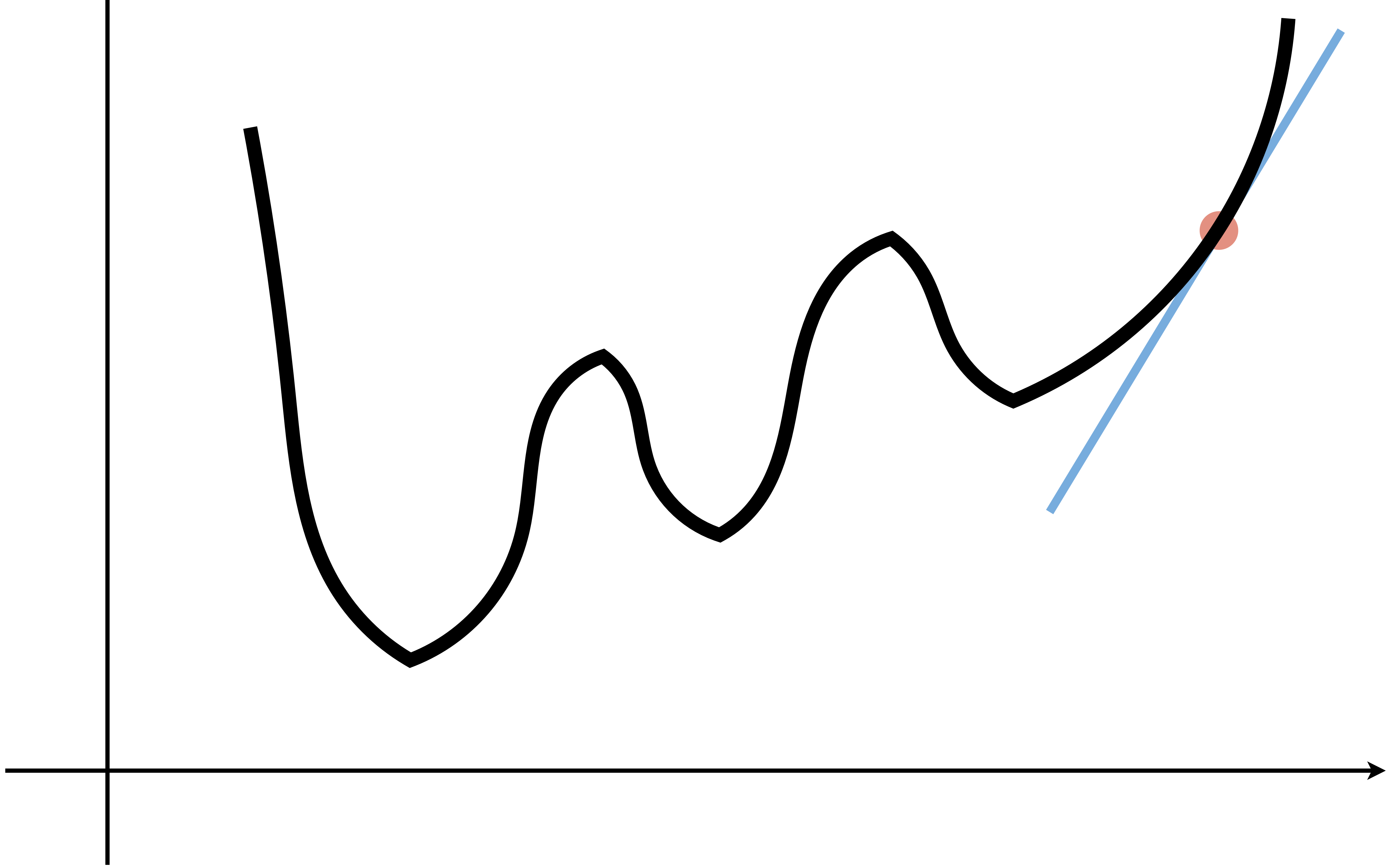

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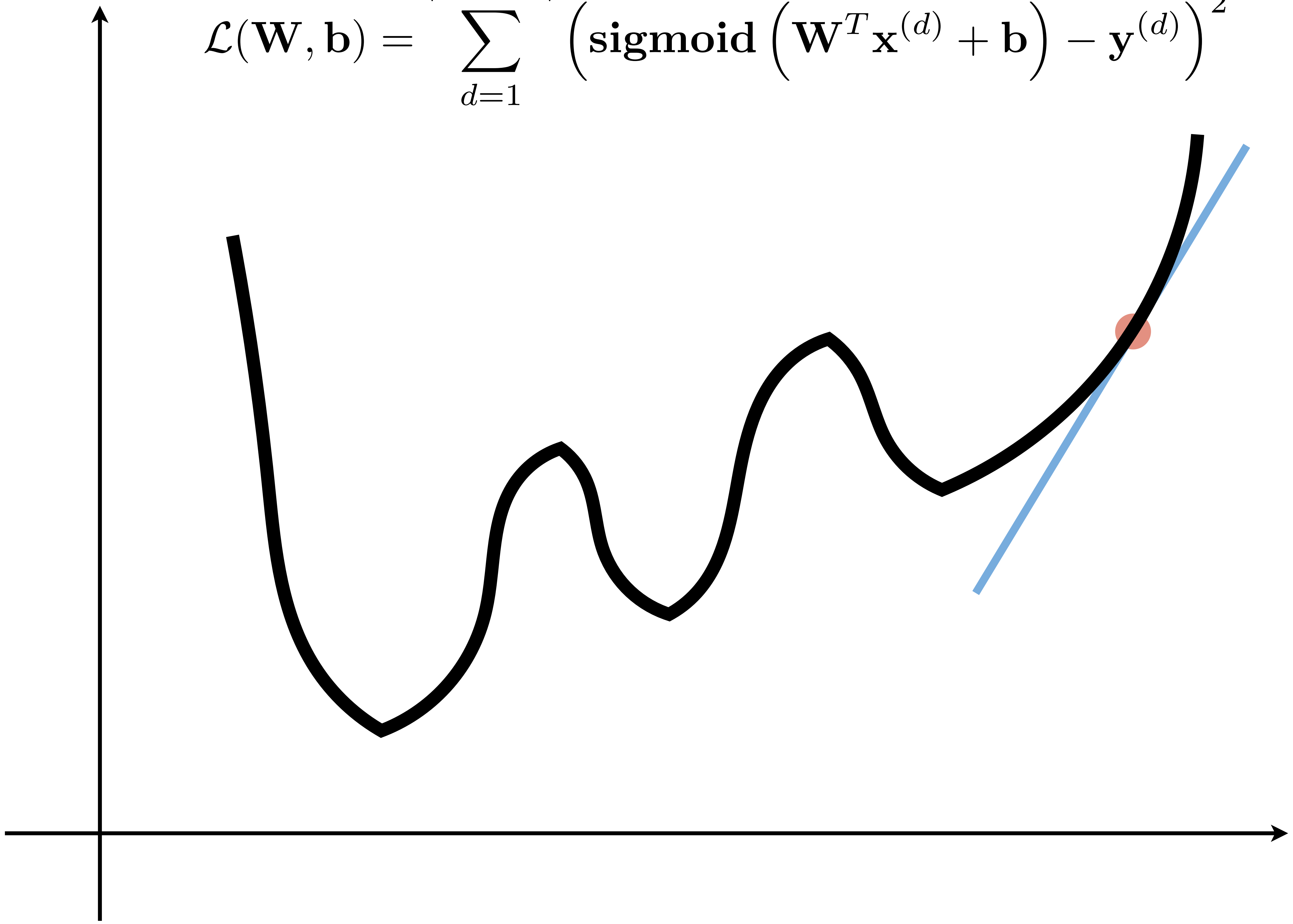

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3. Re-estimate the parameters

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

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

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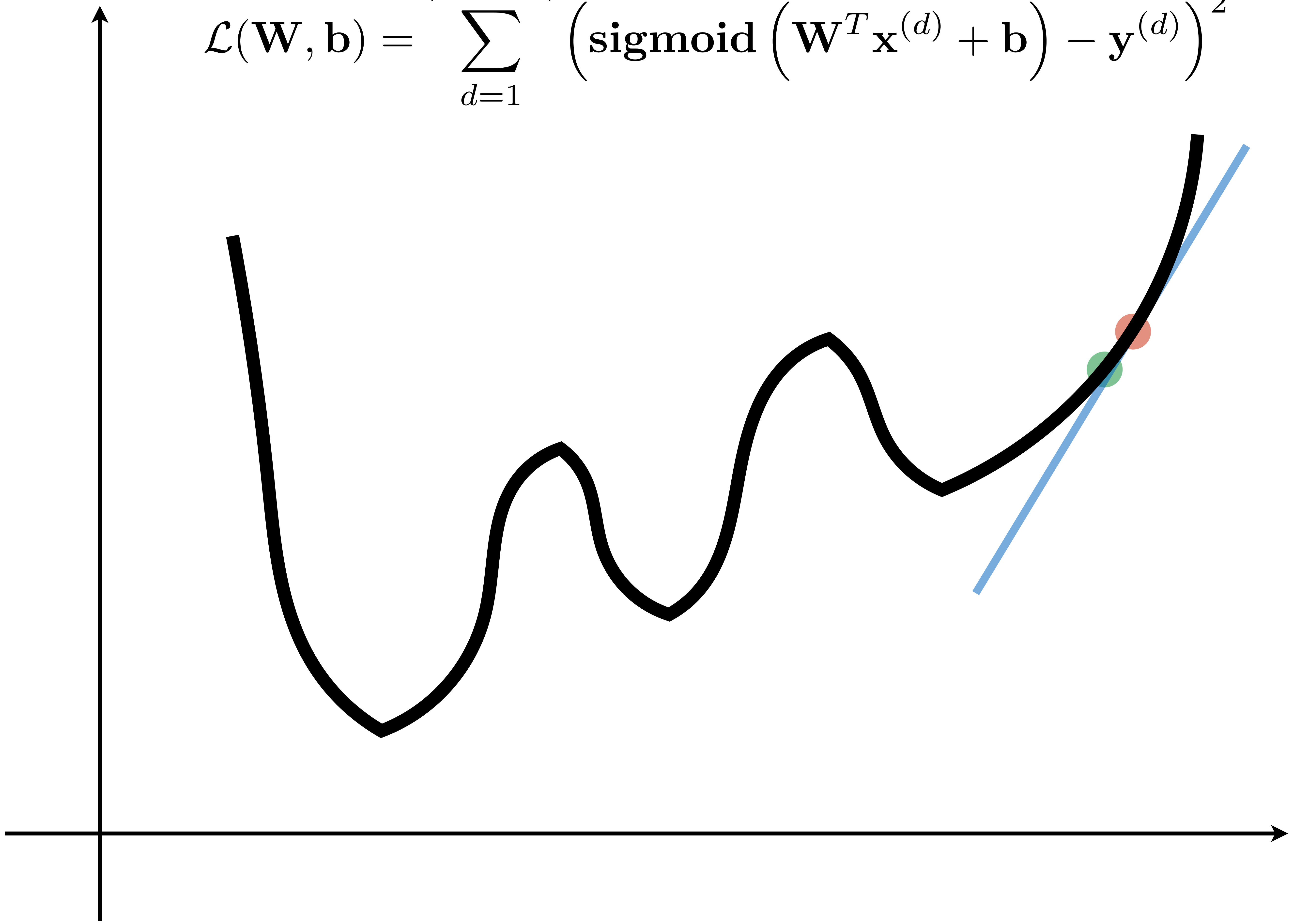


1. Start from random value of $\mathbf{W}_0, \mathbf{b}_0$

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

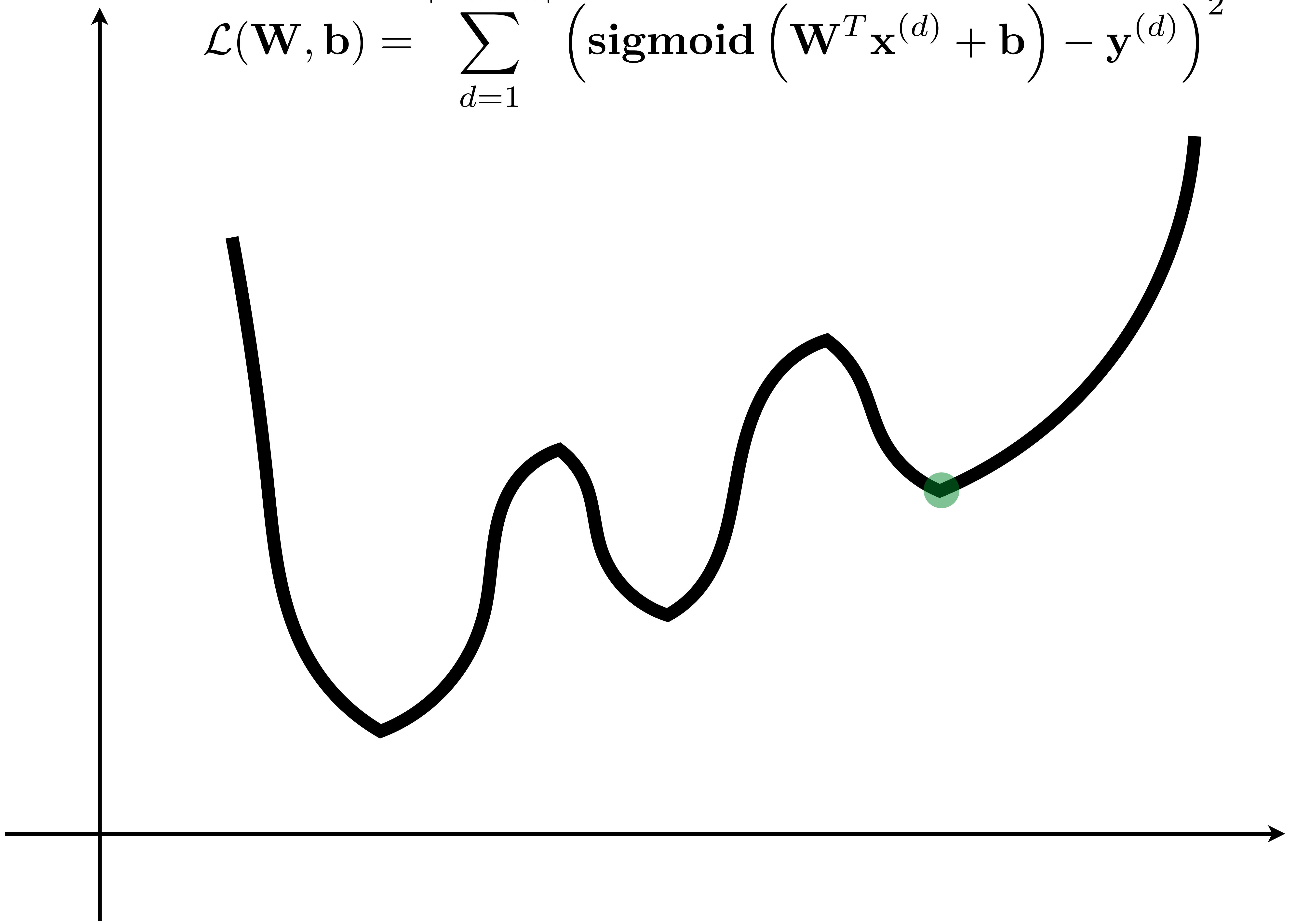
$$\mathbf{W}_{k+1} = \mathbf{W}_k - \lambda \frac{\partial \mathcal{L}(\mathbf{W}, \mathbf{b})}{\partial \mathbf{W}}\bigg|_{\mathbf{W}=\mathbf{W}_k, \mathbf{b}=\mathbf{b}_k}$$

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

*slide adopted from V. Ordonex

Gradient Descent (review)

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



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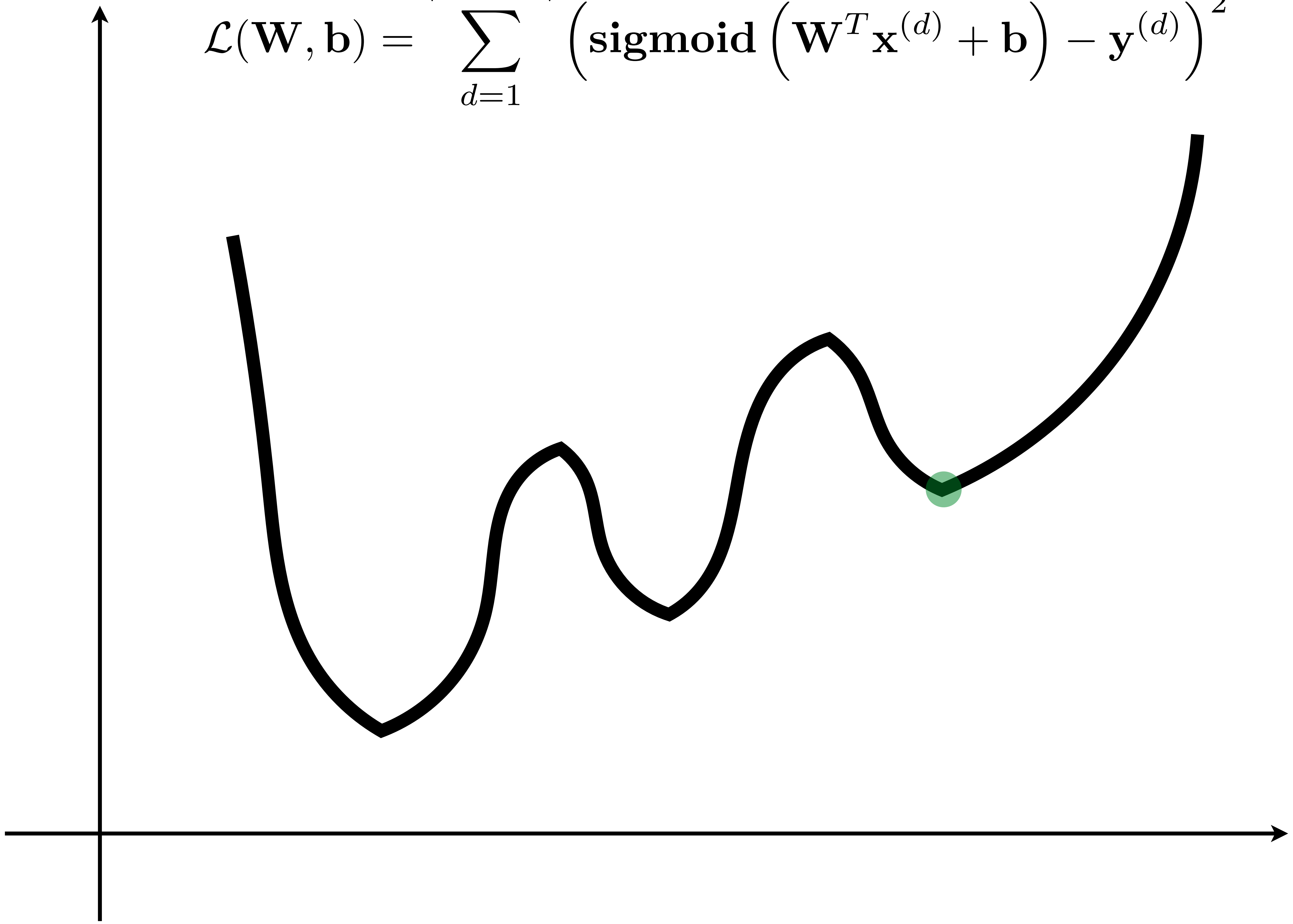

λ - is the learning rate

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

For $k = 0$ to max number of iterations

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

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

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*slide adopted from V. Ordonex

Stochastic Gradient Descent (review)

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

Stochastic Gradient Descent (review)

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

Problem: For large datasets computing sum is expensive

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)

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

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Even better, we can use central differencing:

$$\frac{\partial f(\mathbf{x})}{\partial x_i} \approx \lim_{h \to 0} \frac{f(\mathbf{x} + h\mathbf{1}_i) - f(\mathbf{x} - h\mathbf{1}_i)}{2h}$$

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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 $h = 0.000001$).

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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:

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

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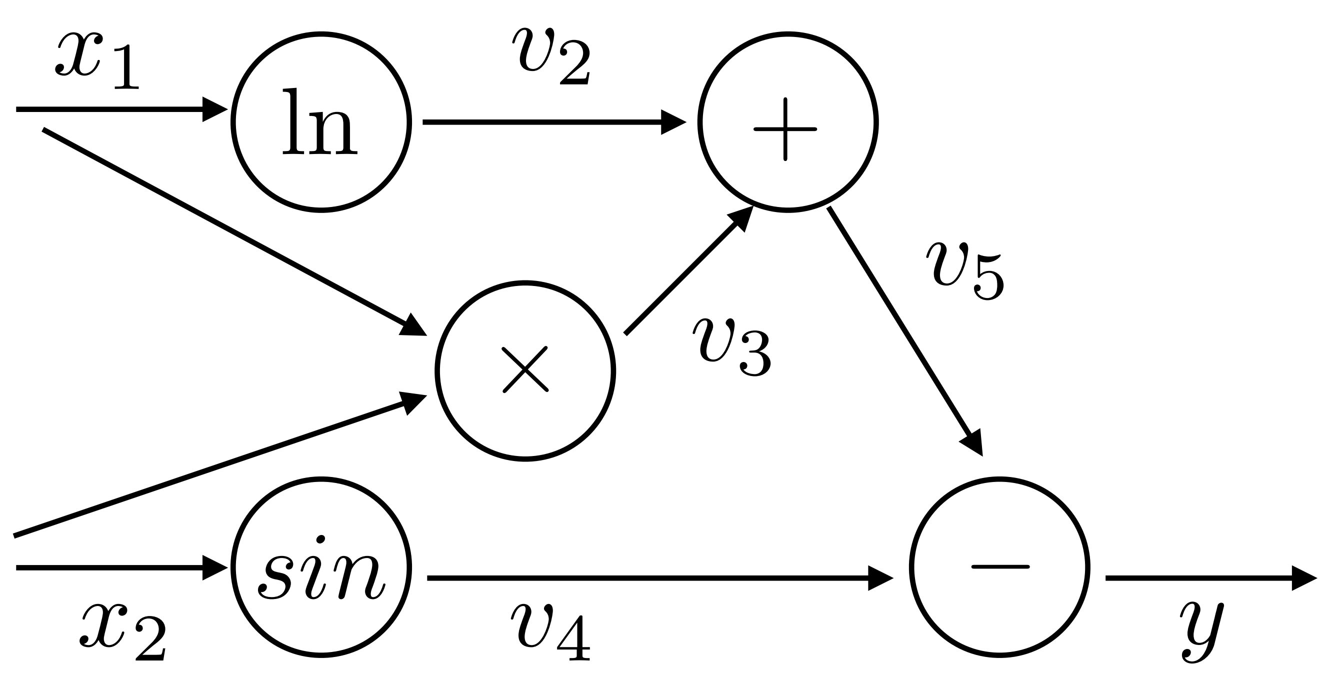
$$\frac{\partial \mathcal{L}(\mathbf{W}, \mathbf{b})}{\partial w_{ij}} \approx \lim_{h \to 0} \frac{\mathcal{L}(\mathbf{W} + h\mathbf{1}_{ij}, \mathbf{b}) - \mathcal{L}(\mathbf{W} + h\mathbf{1}_{ij}, \mathbf{b})}{2h} \qquad \frac{\partial \mathcal{L}(\mathbf{W}, \mathbf{b})}{\partial b_j} \approx \lim_{h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

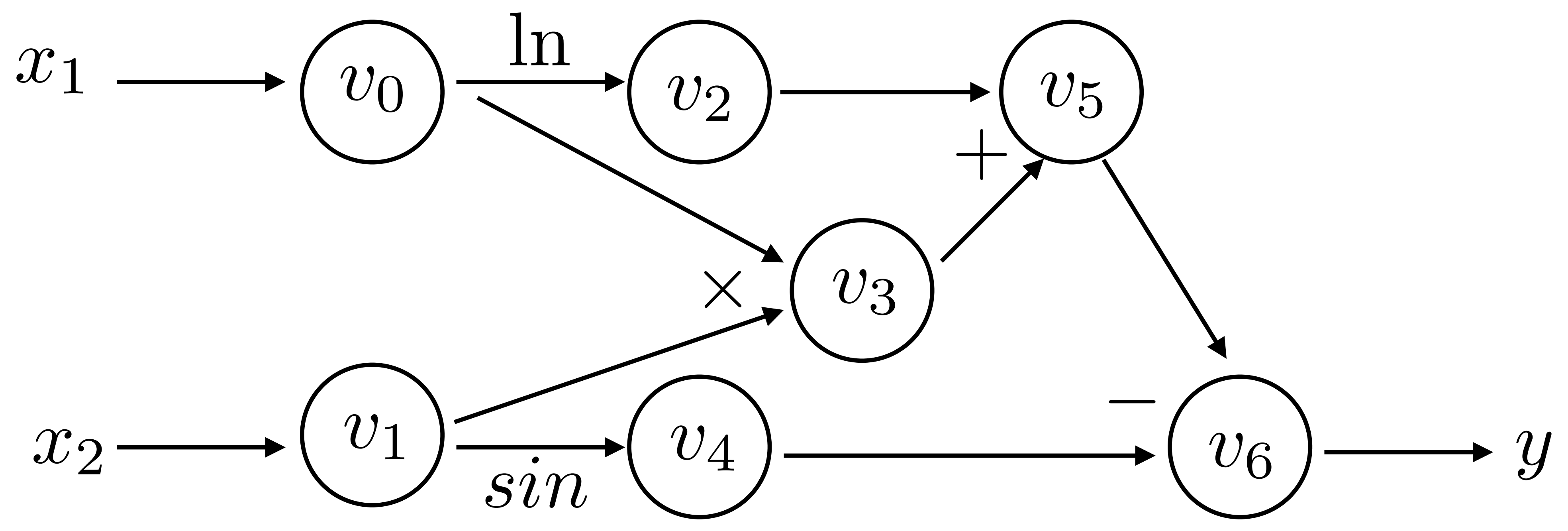
However, both of theses suffer from rounding errors and are not good enough for learning (they are very good tools for checking the correctness of implementation though, e.g., use $h = 0.000001$).

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

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

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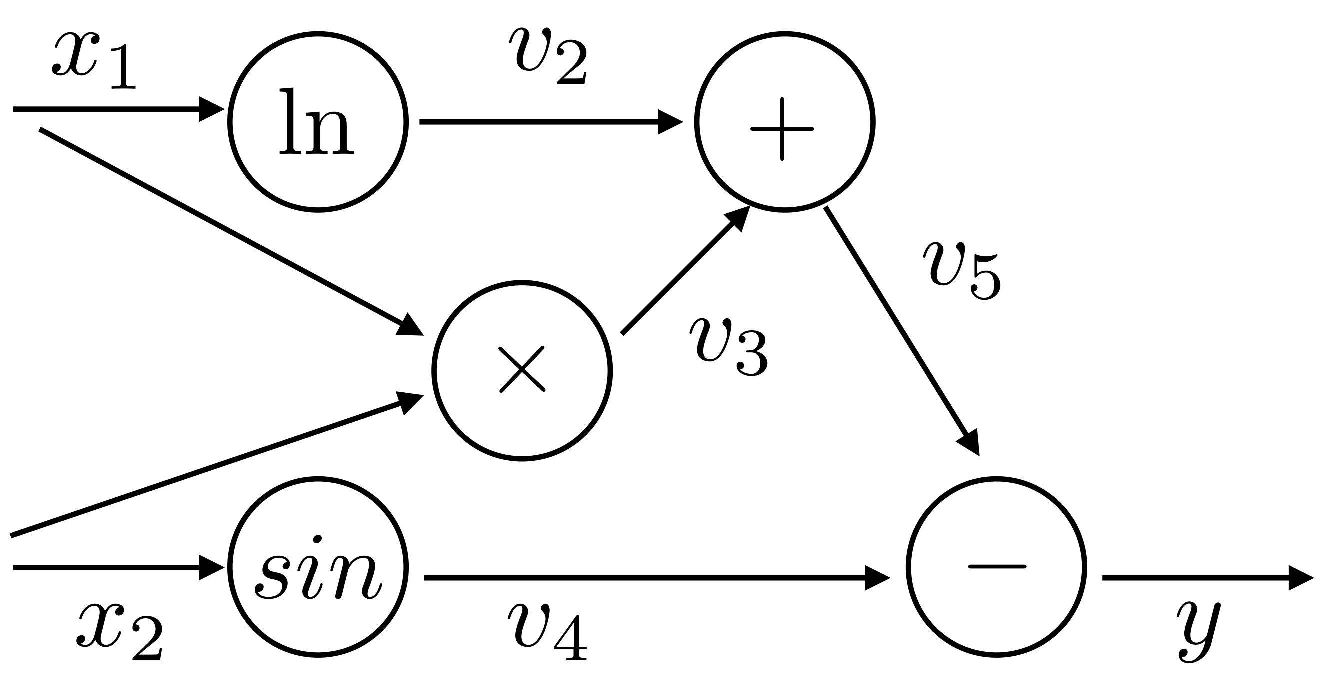

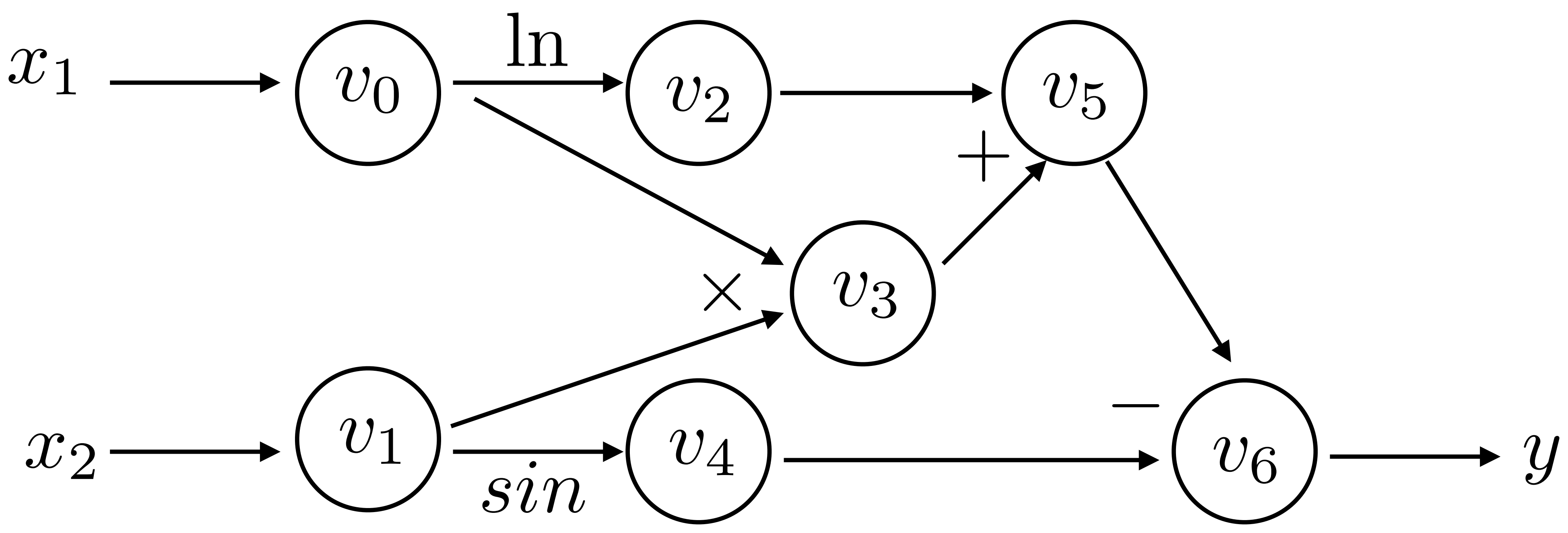

Implements differentiation rules for composite functions:

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

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

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

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

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)

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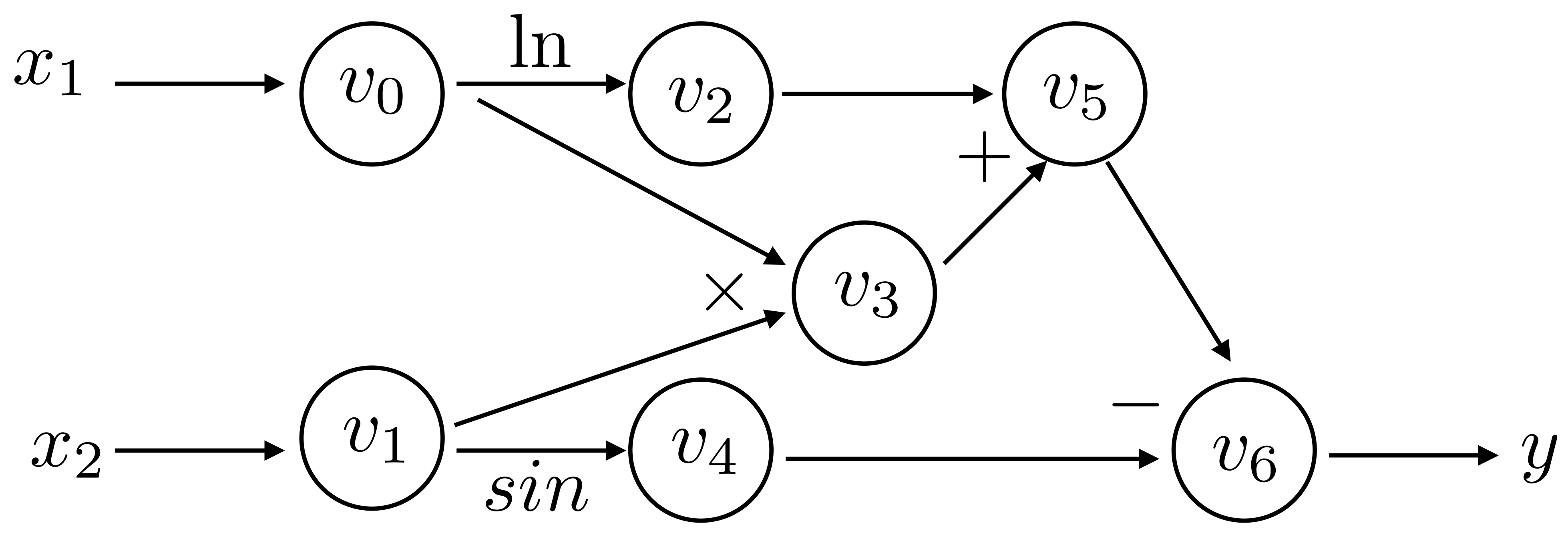

Each **node** is an input, intermediate, or output variable

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

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

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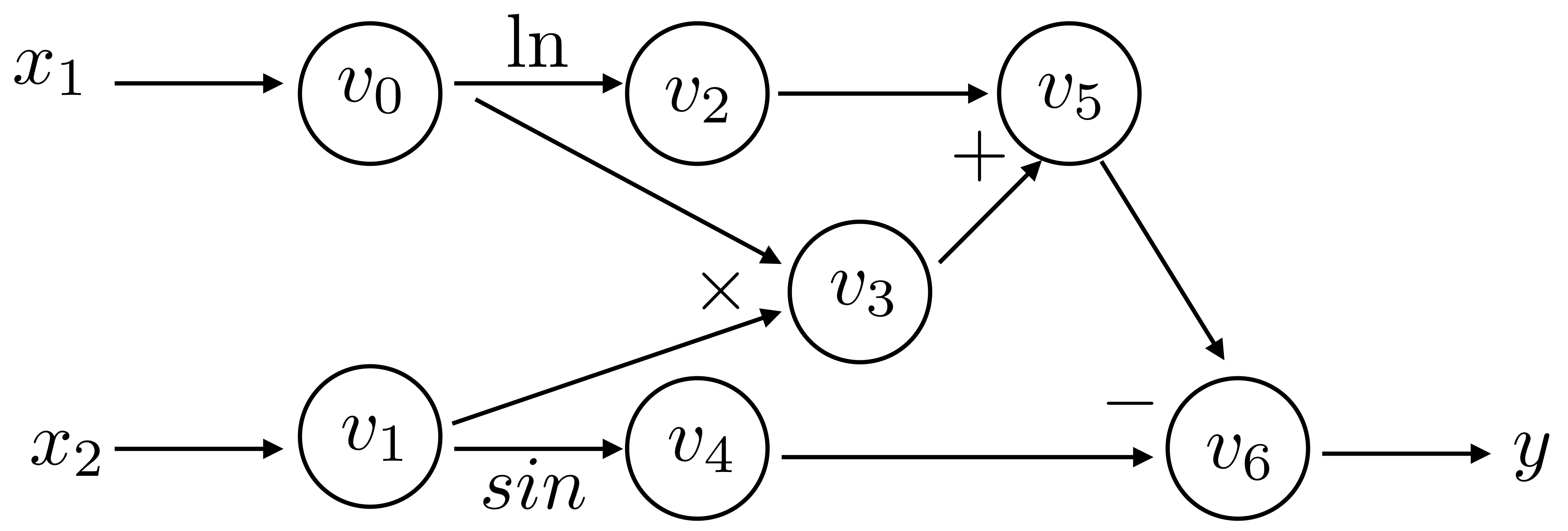

Computational graph is governed by these equations

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

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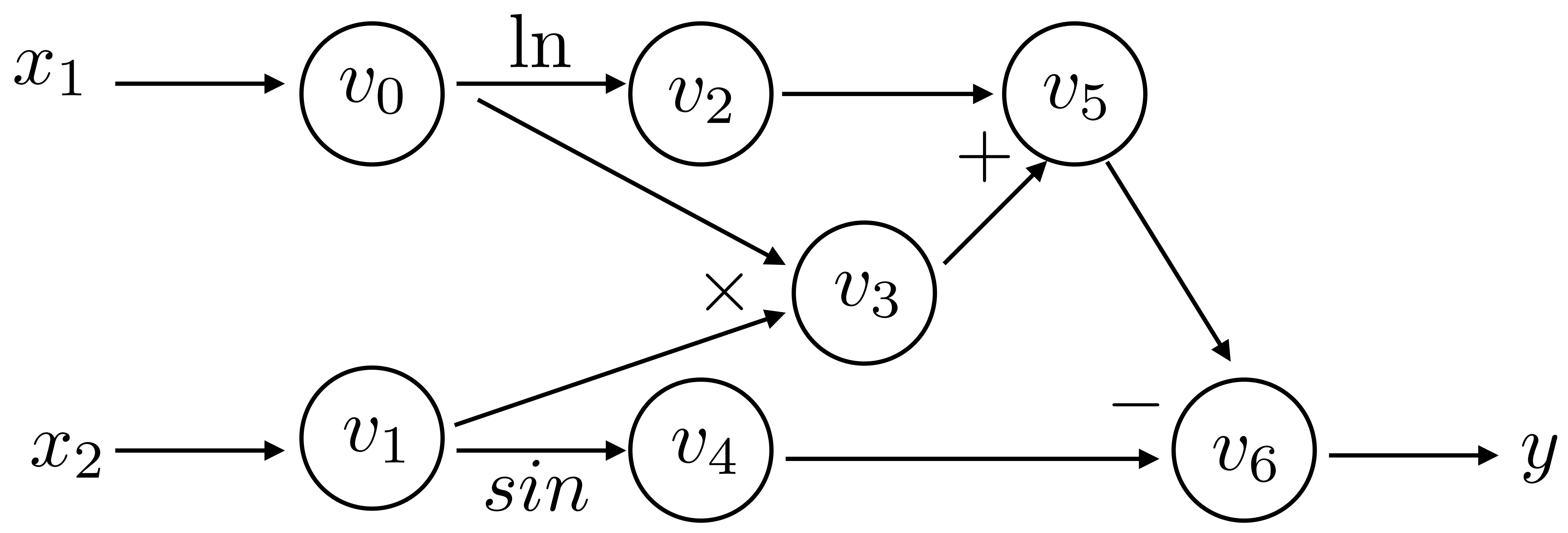

Lets see how we can **evaluate a function** using computational graph (DNN inferences)

Computational graph is governed by these equations

$$v_0 = x_1$$
$$v_1 = x_2$$
$$v_2 = \ln(v_0)$$
$$v_3 = v_0 \cdot v_1$$
$$v_4 = sin(v_1)$$
$$v_5 = v_2 + v_3$$
$$v_6 = v_5 - v_4$$
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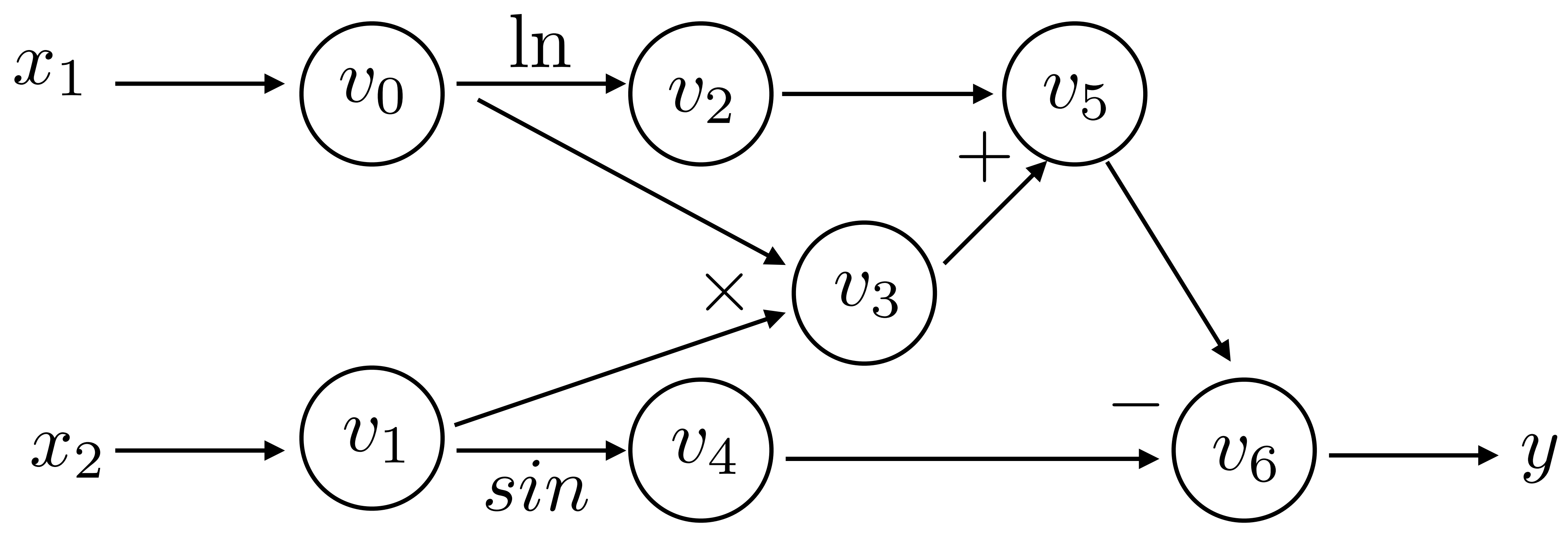

Forward Evaluation Trace:

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

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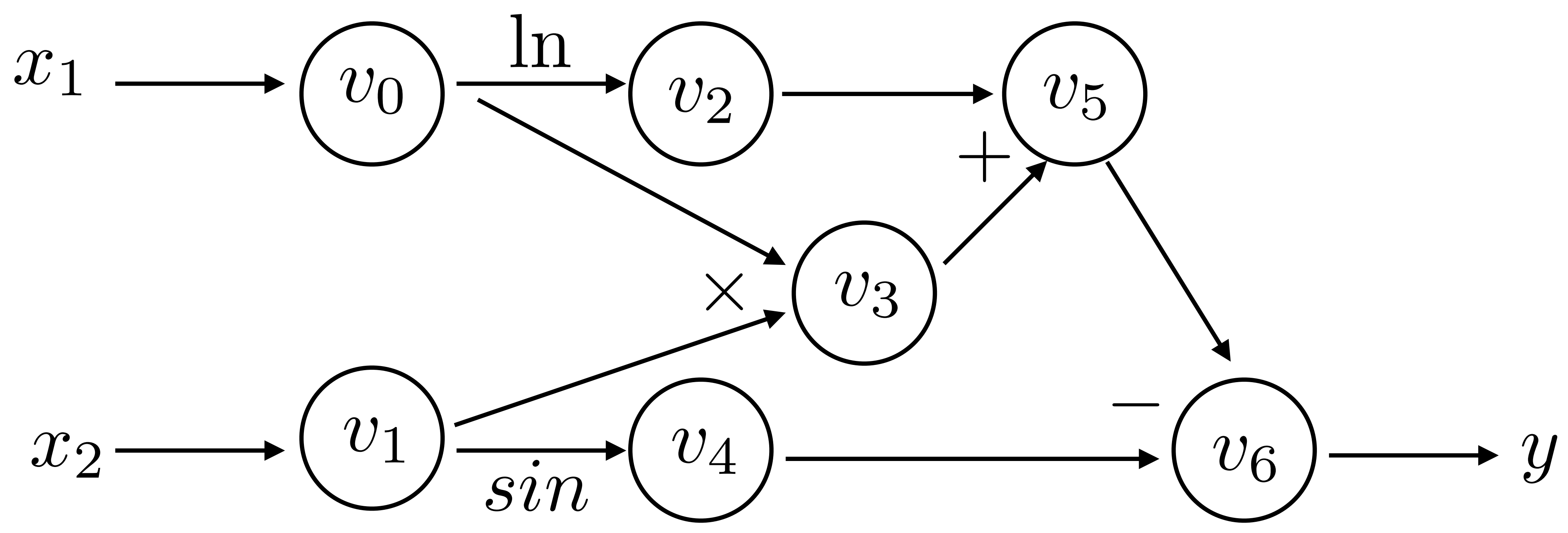

Lets see how we can **evaluate a function** using computational graph (DNN inferences)

Forward Evaluation Trace:

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

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

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

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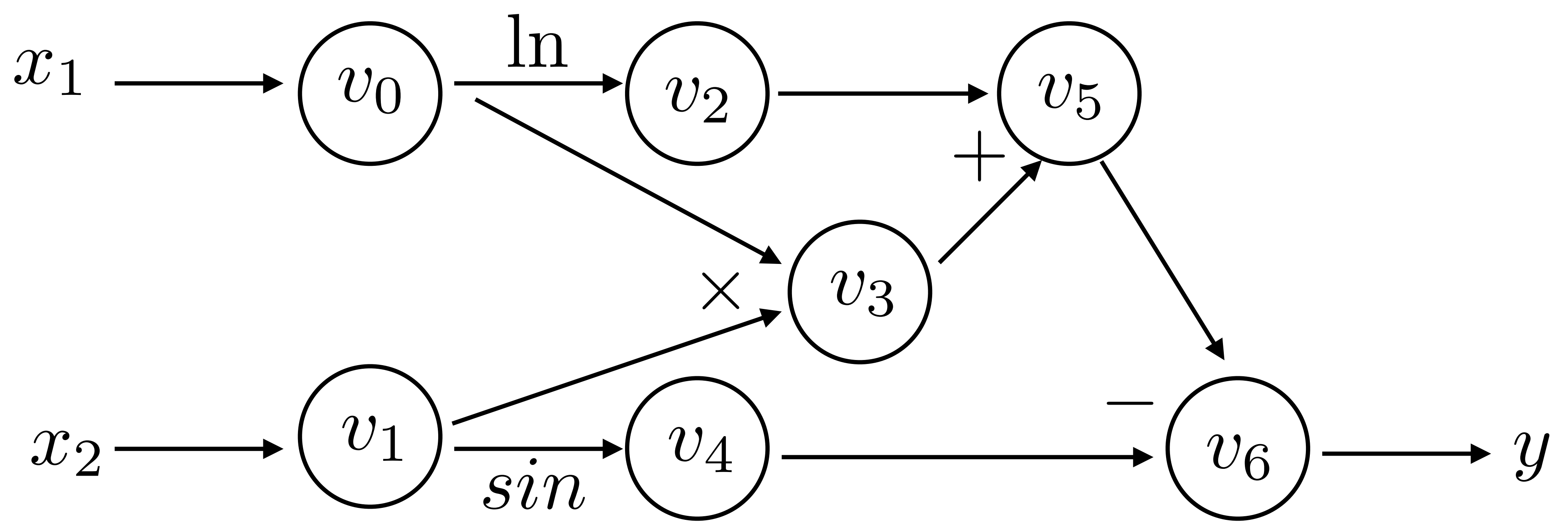

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Each **node** is an input, intermediate, or output variable

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

Forward Evaluation Trace:

	$f(2,5)$
$v_0 = x_1$	2
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$v_2 = \ln(v_0)$	
$v_3 = v_0 \cdot v_1$	
$v_4 = sin(v_1)$	
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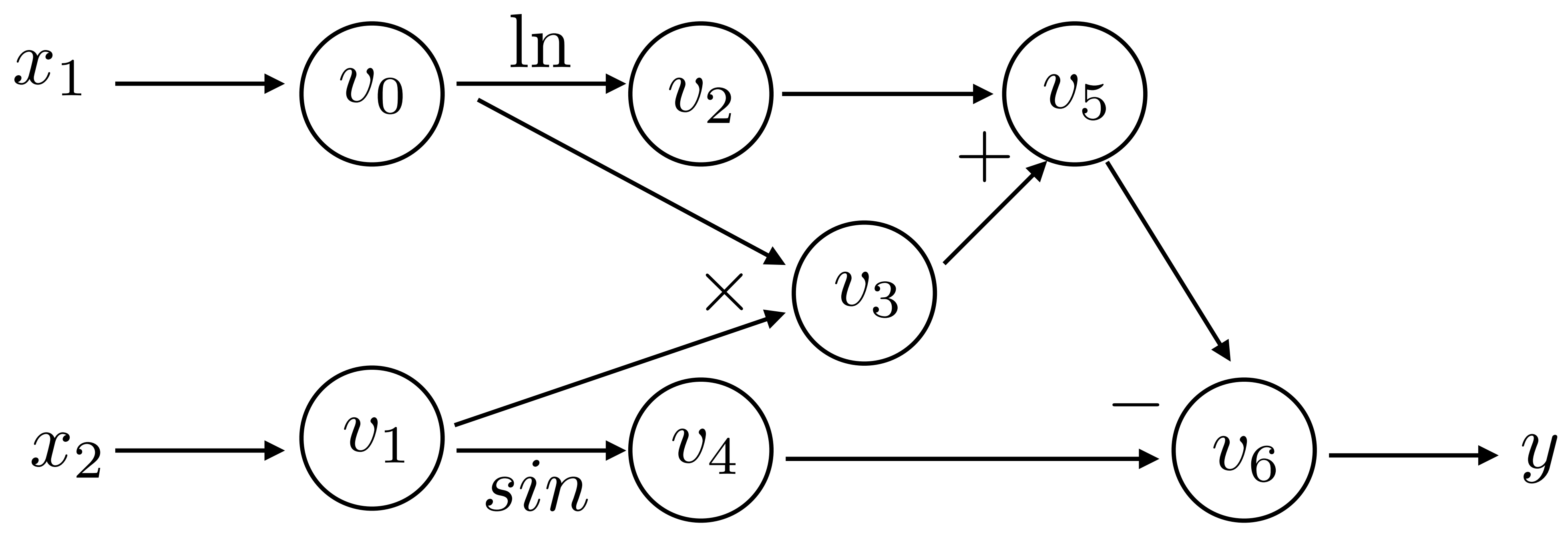

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Computational graph (a DAG) with variable ordering from topological sort.

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
$v_2 = \ln(v_0)$	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)

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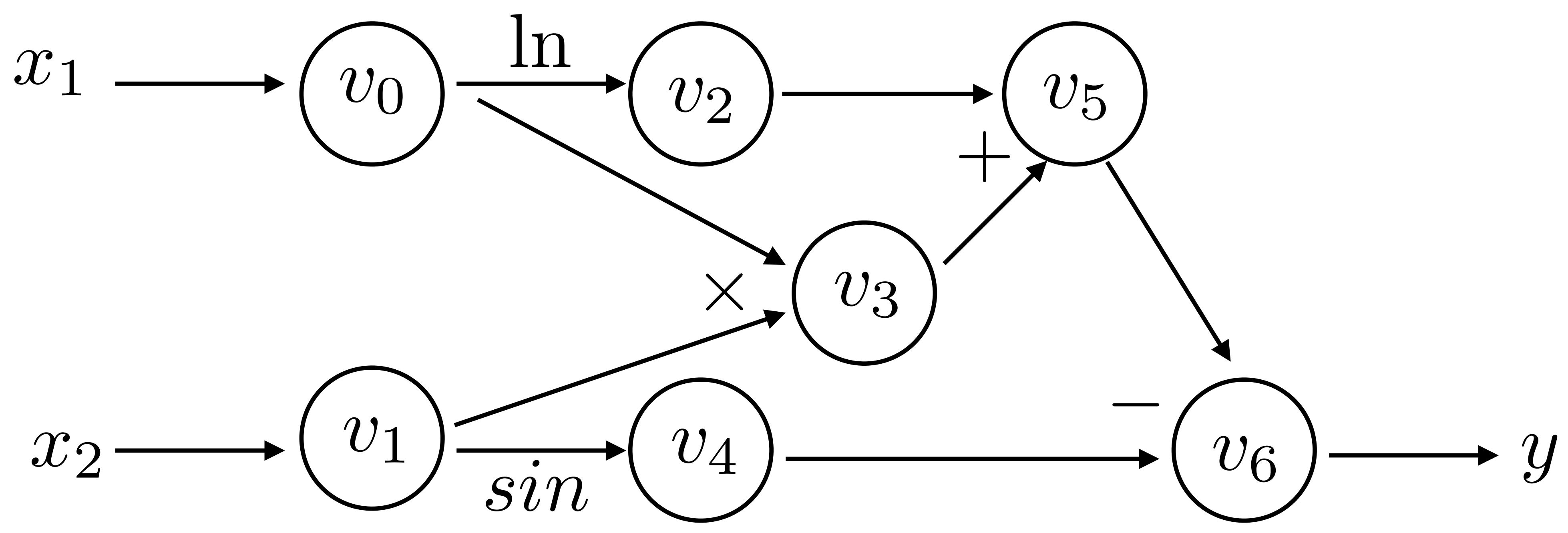
Lets see how we can **evaluate a function** using computational graph (DNN inferences)



Forward Evaluation Trace:

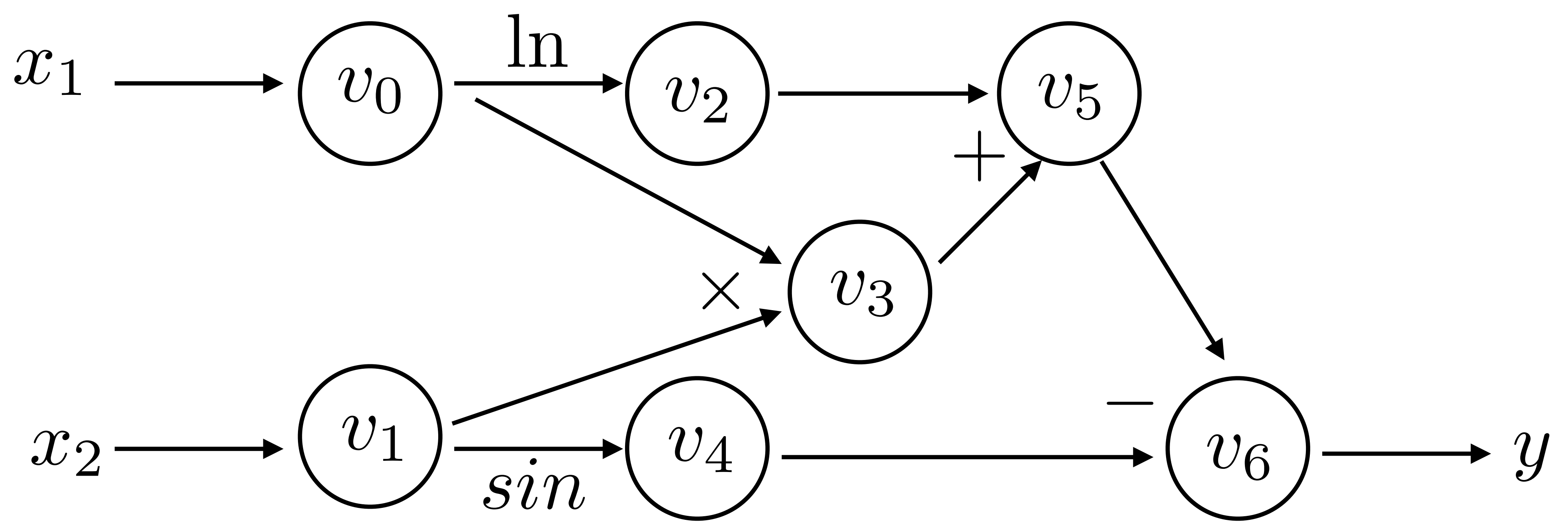
	$f(2,5)$
$v_0 = x_1$	2
$v_1 = x_2$	5
$v_2 = \ln(v_0)$	ln(2) = 0.693
$v_3 = v_0 \cdot v_1$	2 x 5 = 10
$v_4 = sin(v_1)$	sin(5) = 0.959
$v_5 = v_2 + v_3$	0.693 + 10 = 10.693
$v_6 = v_5 - v_4$	10.693 + 0.959 = 11.652
$y = v_6$	11.652

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

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

Automatic Differentiation (AutoDiff)

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



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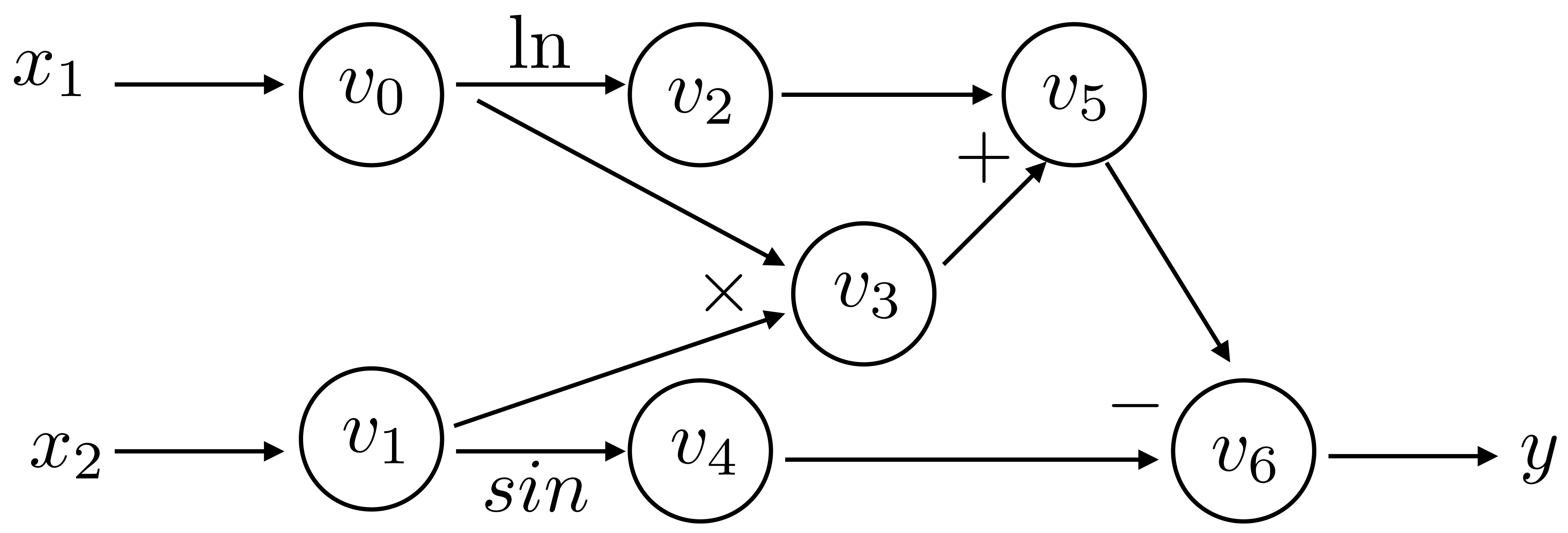

Forward Evaluation Trace:

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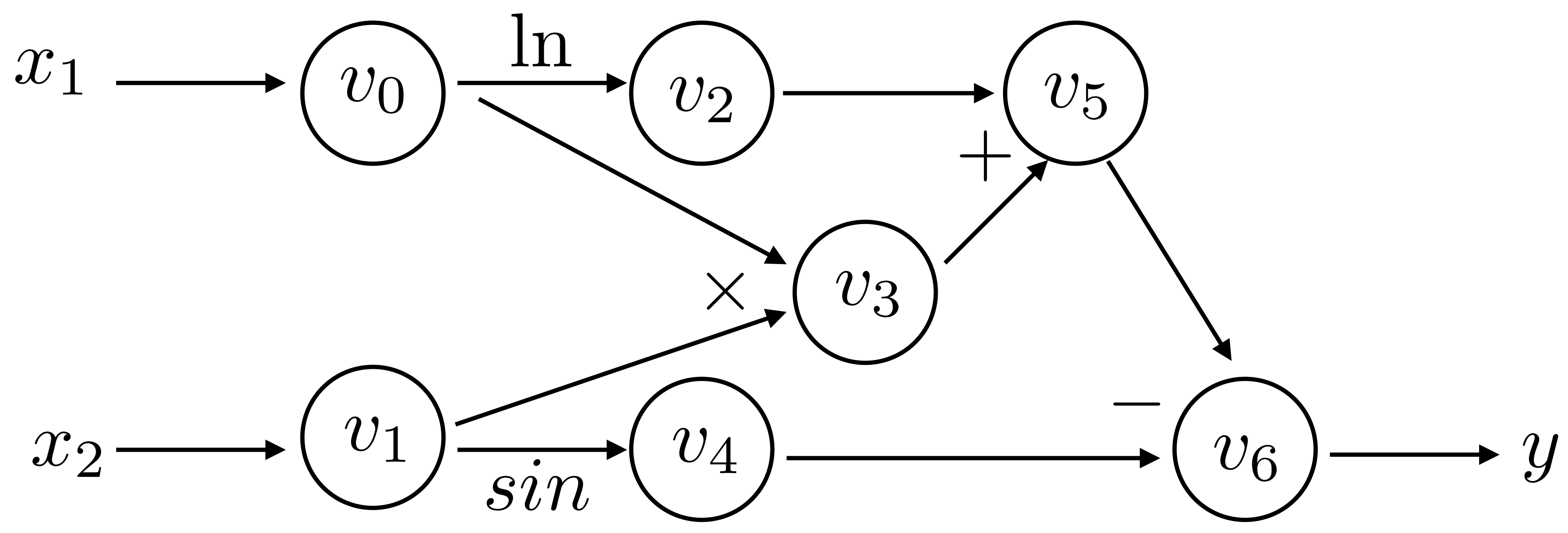
AutoDiff - **Forward Mode**

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



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
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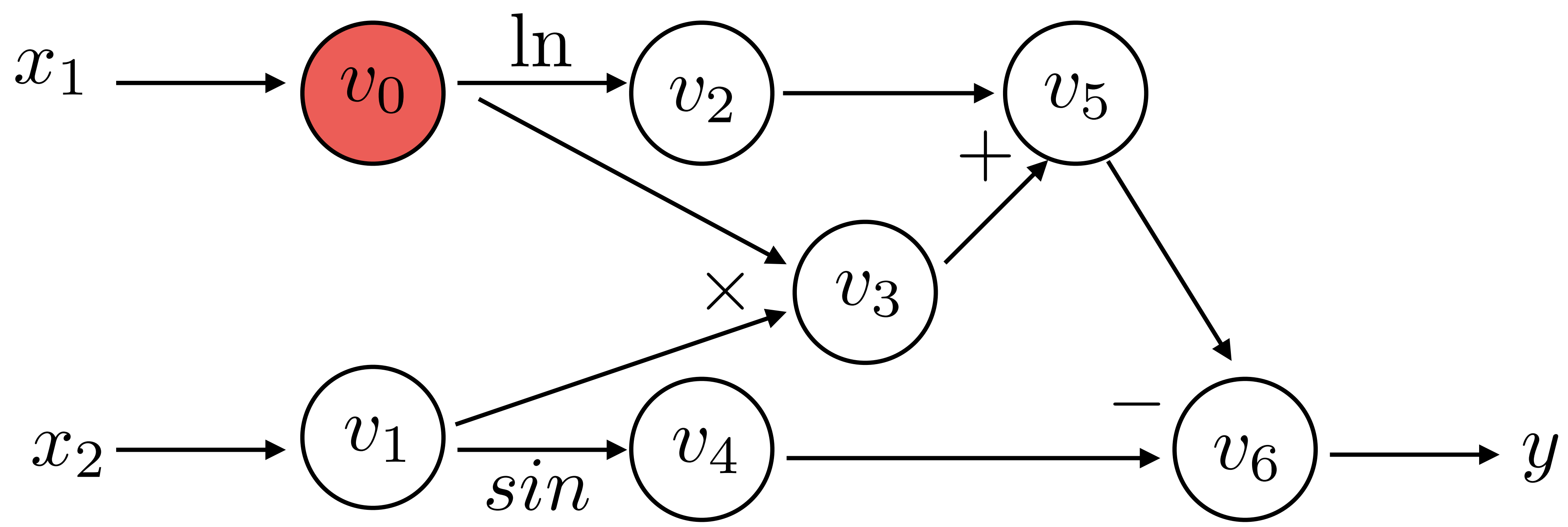
$v_6 = v_5 - v_4$	10.693 + 0.959 = 11.652
$y = v_6$	11.652

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
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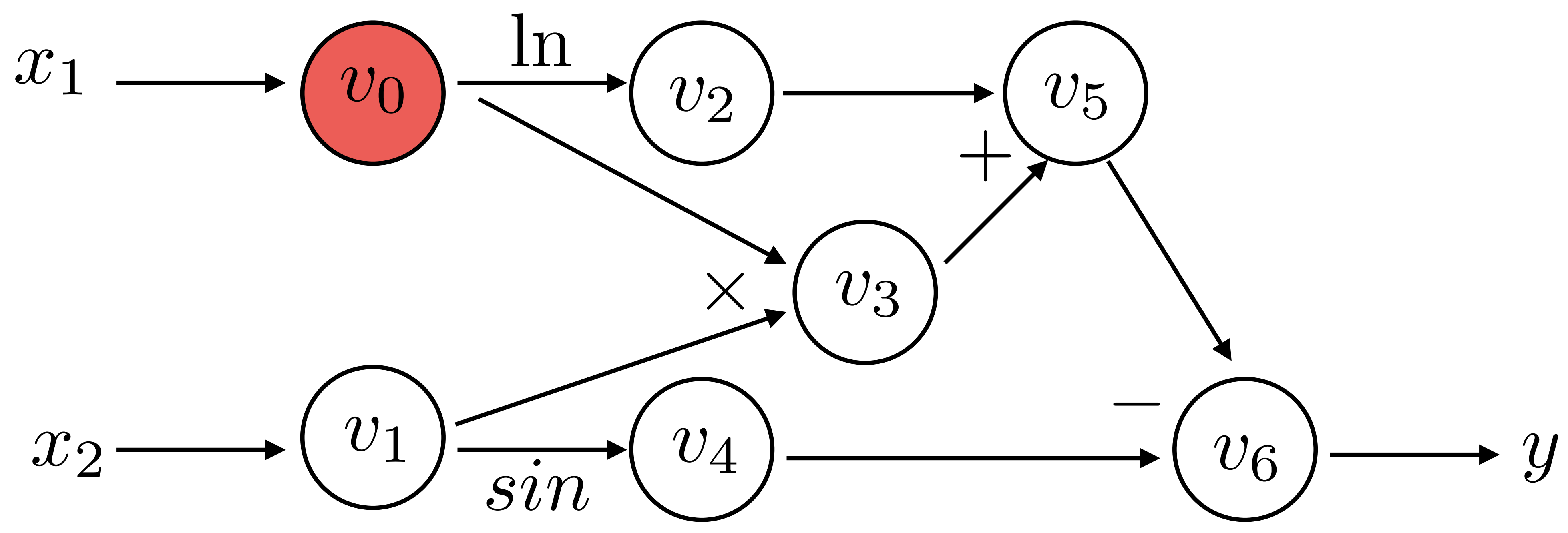
Forward Derivative Trace:

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

AutoDiff - **Forward Mode**

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



Forward Evaluation Trace:

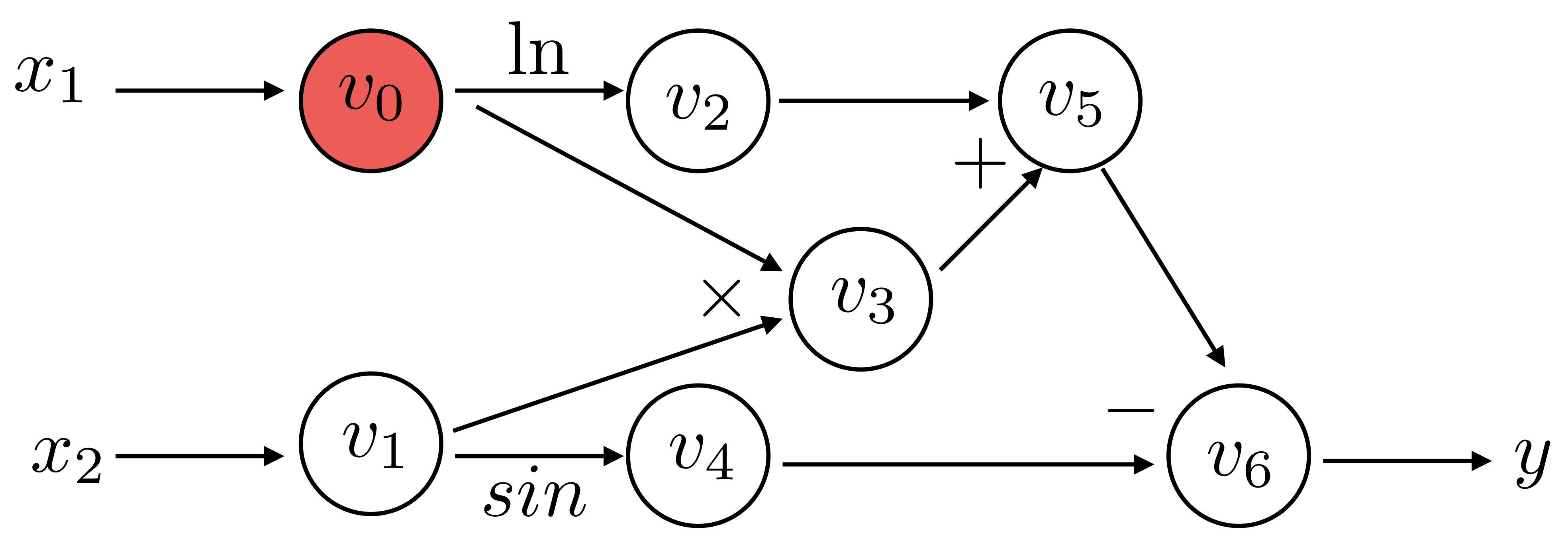
	$f(2,5)$
$v_0 = x_1$	2
$v_1 = x_2$	5
$v_2 = \ln(v_0)$	ln(2) = 0.693
$v_3 = v_0 \cdot v_1$	2 x 5 = 10
$v_4 = sin(v_1)$	sin(5) = 0.959
$v_5 = v_2 + v_3$	0.693 + 10 = 10.693
$v_6 = v_5 - v_4$	10.693 + 0.959 = 11.652
$y = v_6$	11.652

Forward Derivative Trace:

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

AutoDiff - **Forward Mode**

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



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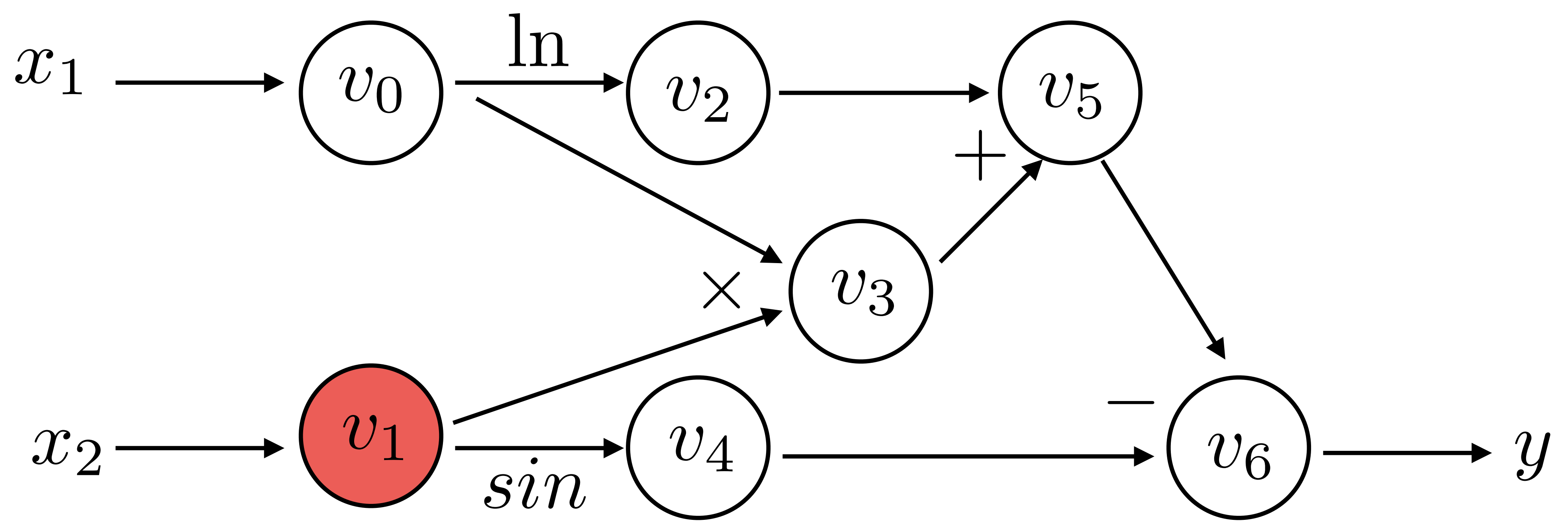
$v_5 = v_2 + v_3$	0.693 + 10 = 10.693
$v_6 = v_5 - v_4$	10.693 + 0.959 = 11.652
$y = v_6$	11.652

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:

	$f(2,5)$
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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
$\frac{\partial v_1}{\partial x_1}$	

AutoDiff - **Forward Mode**

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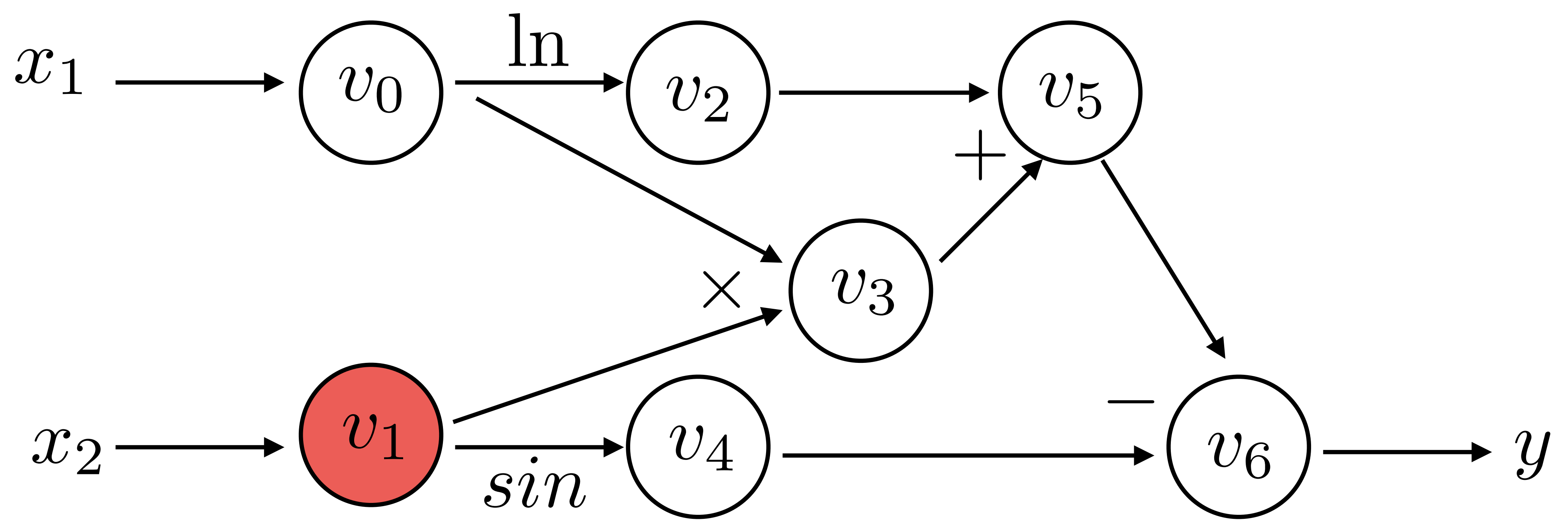

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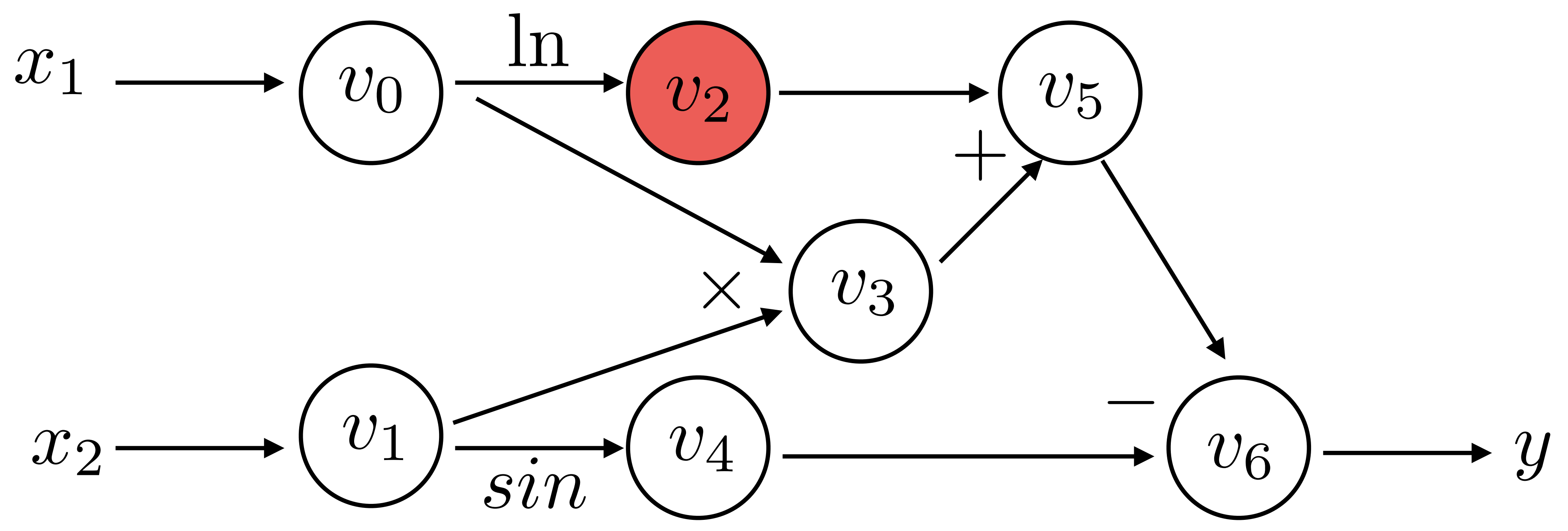
	$\left.\frac{\partial f(x_1, x_2)}{\partial x_1}\right\|_{(x_1=2, x_2=5)}$
$\frac{\partial v_0}{\partial x_1}$	1
$\frac{\partial v_1}{\partial x_1}$	0

AutoDiff - **Forward Mode**

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



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$\frac{\partial v_2}{\partial x_1}$	

AutoDiff - **Forward Mode**

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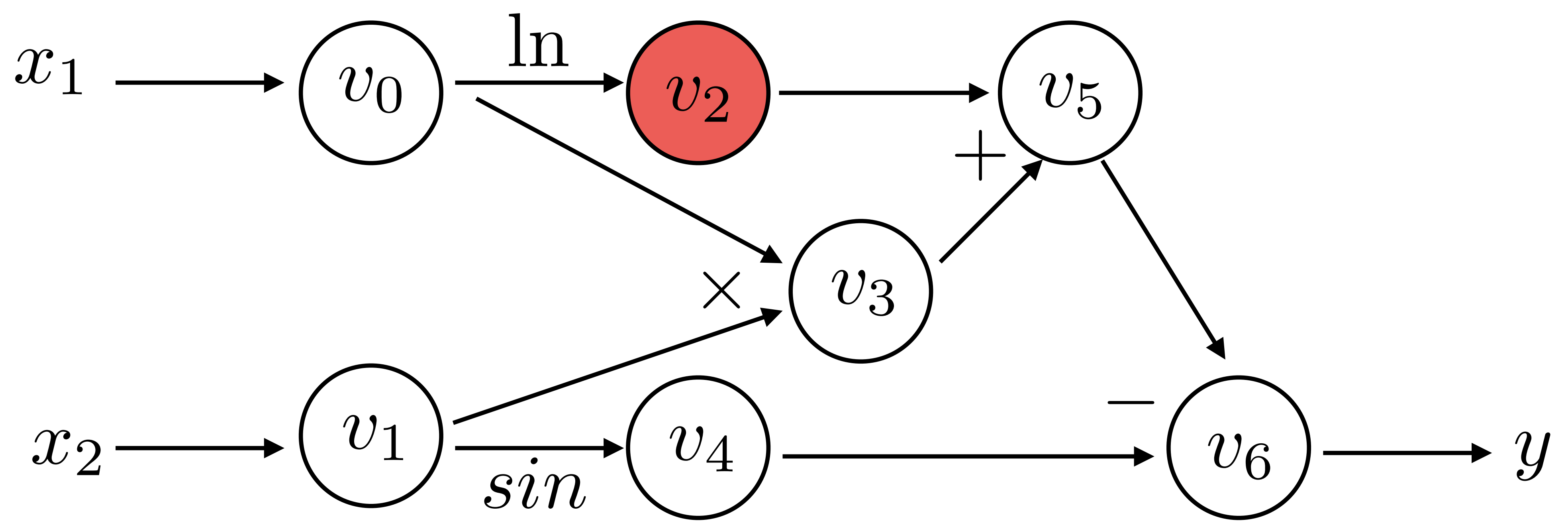

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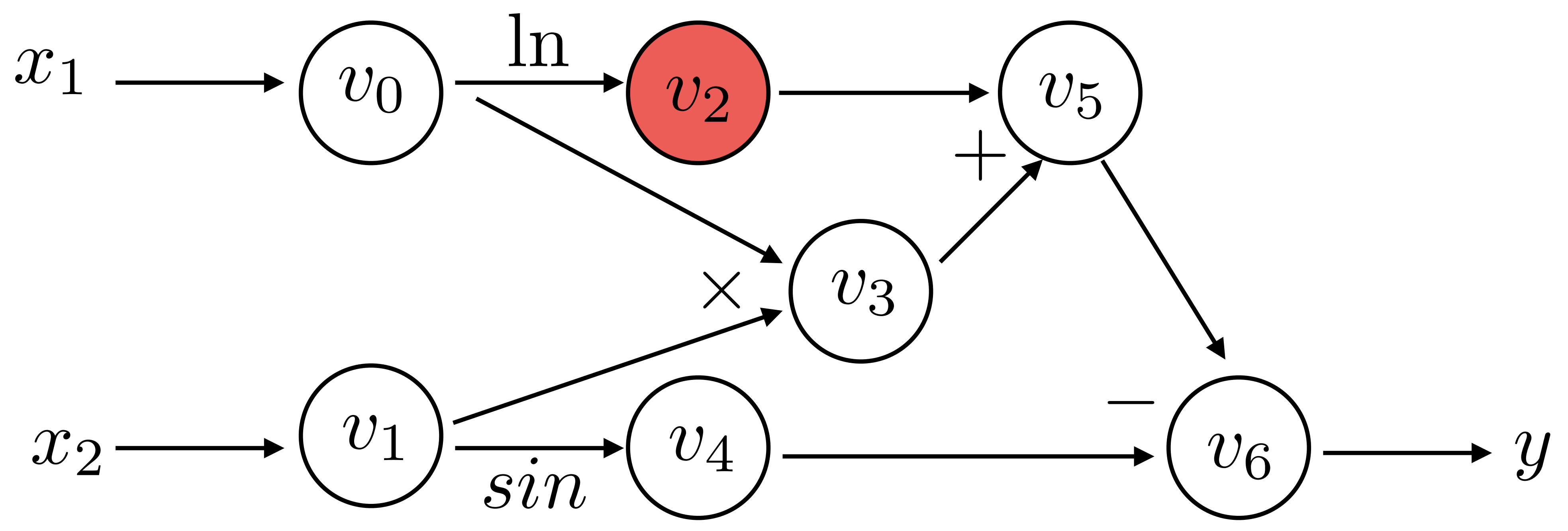
$\frac{\partial v_1}{\partial x_1}$	0
$\frac{\partial v_2}{\partial x_1}$	
Chain Rule	

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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$v_1 = x_2$	5
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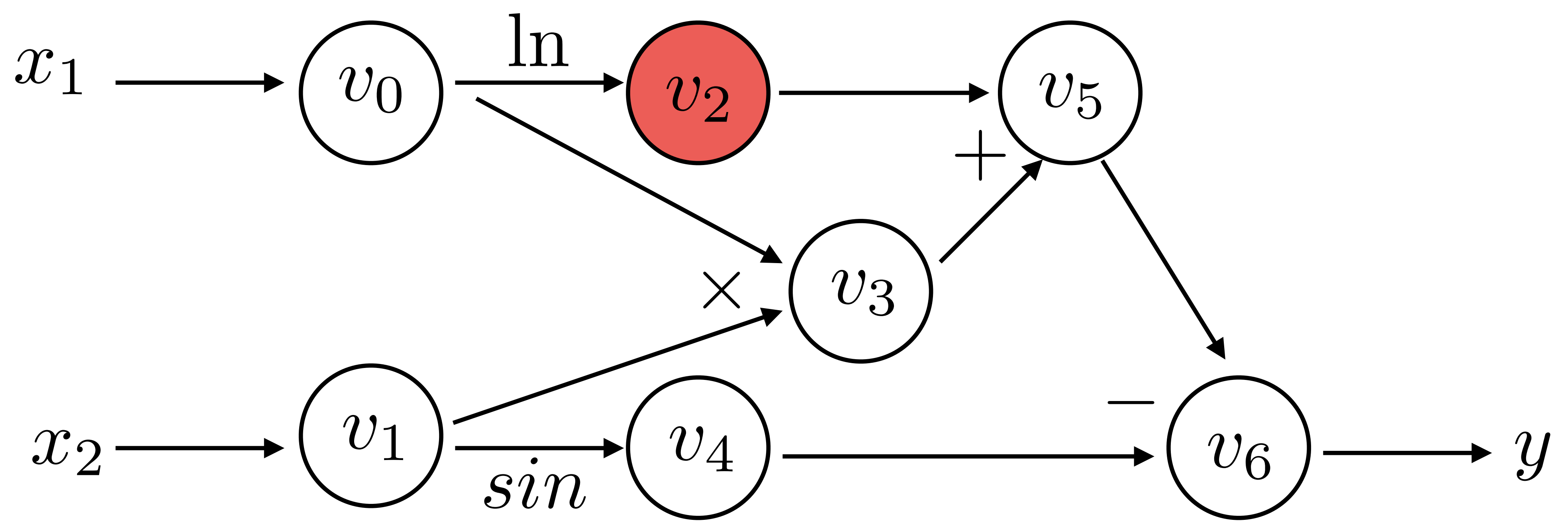
Forward Derivative Trace:

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

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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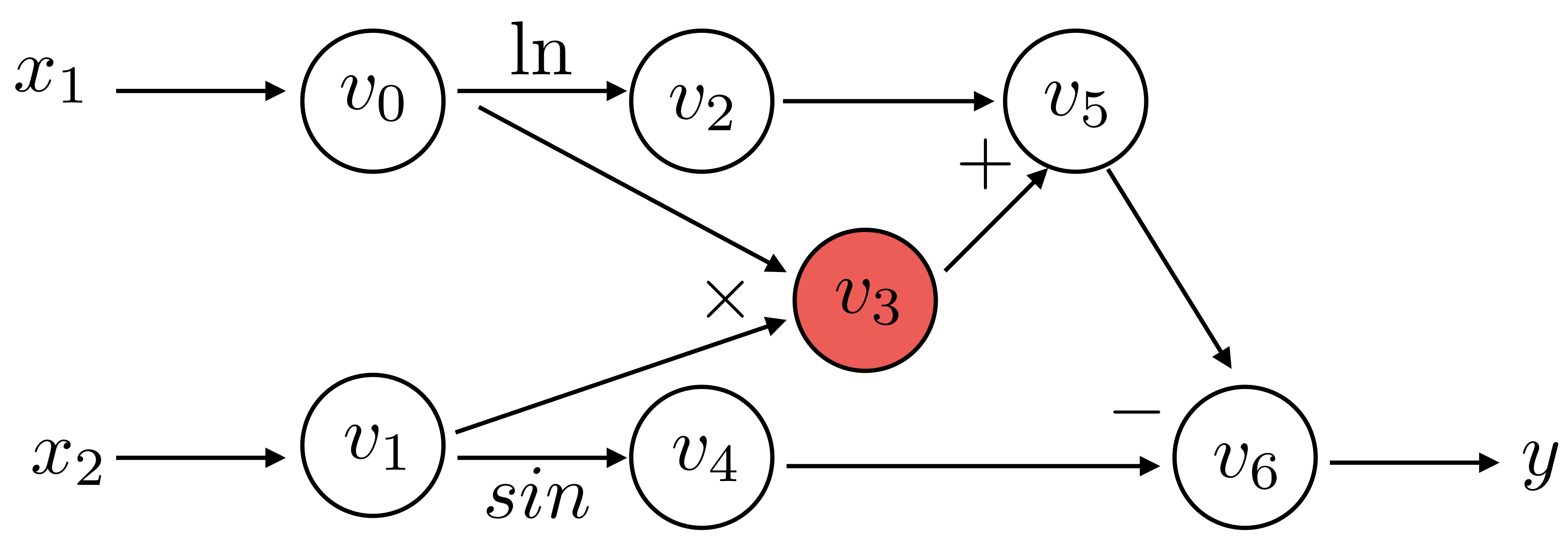
Forward Derivative Trace:

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

Chain Rule

AutoDiff - **Forward Mode**

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



Forward Evaluation Trace:

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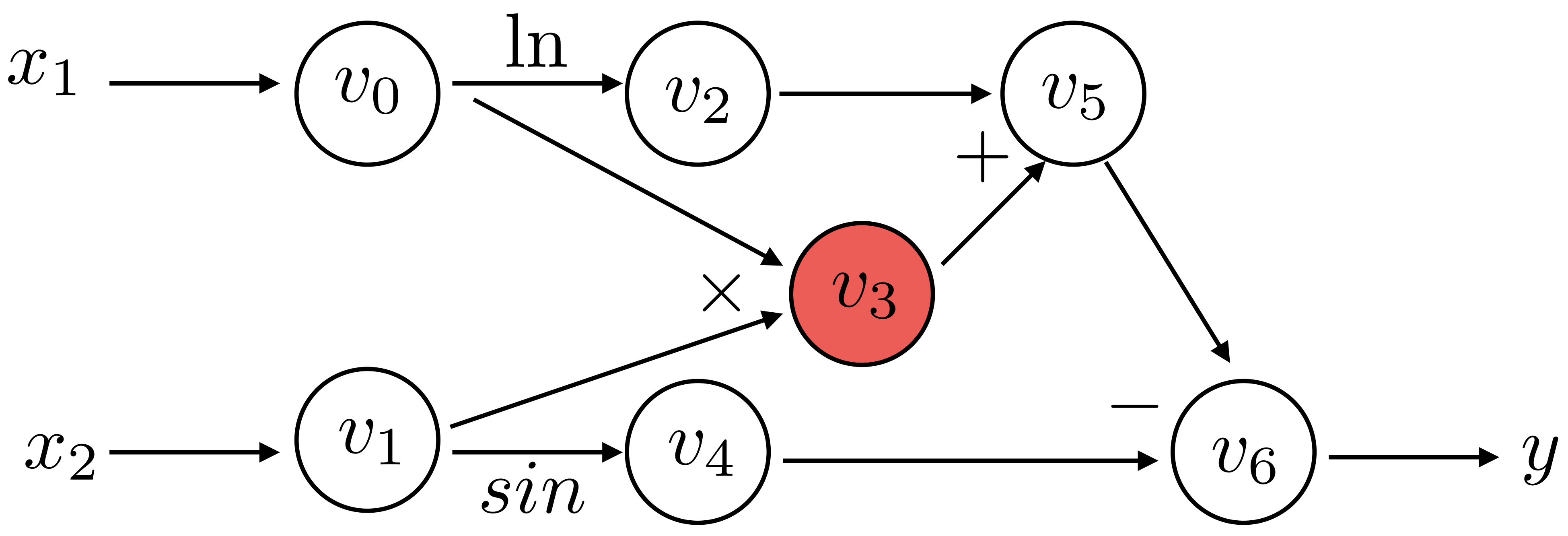
$y = v_6$	11.652

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
$\frac{\partial v_3}{\partial x_1}$	

AutoDiff - **Forward Mode**

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



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$v_0 = x_1$	2
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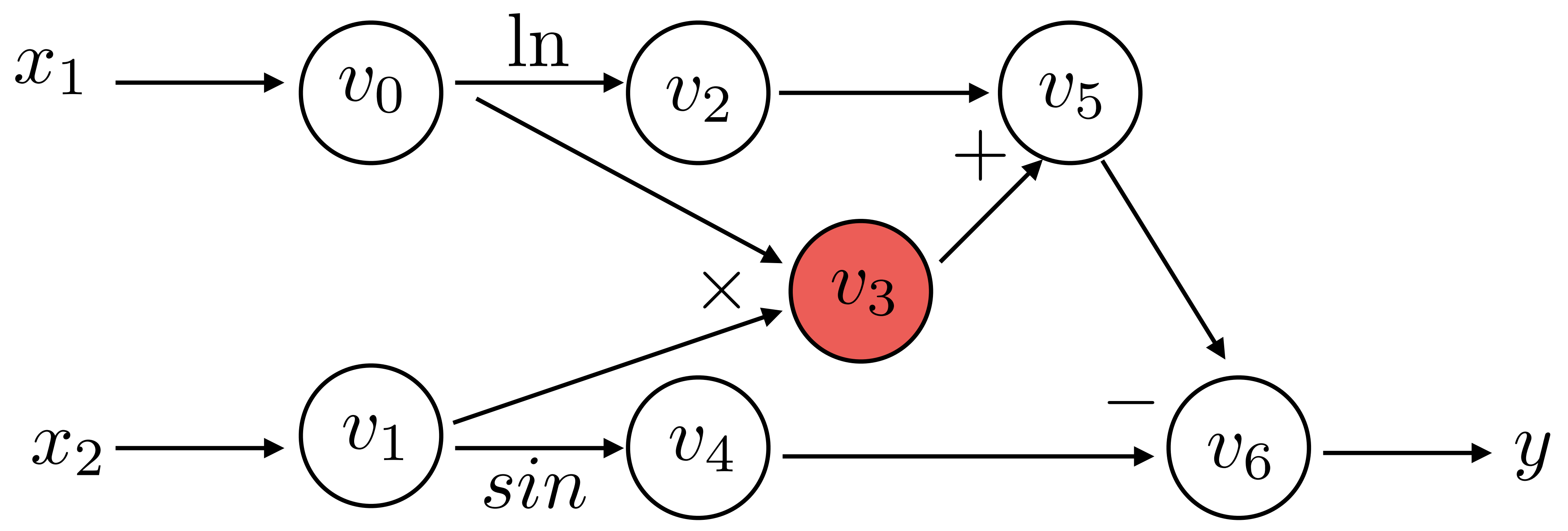
Forward Derivative Trace:

	$\left.\frac{\partial f(x_1,x_2)}{\partial x_1}\right\|_{(x_1=2,x_2=5)}$
$\frac{\partial v_0}{\partial x_1}$	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
$\frac{\partial v_3}{\partial x_1}$	
Product Rule	

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
$\underline{v_3 = v_0 \cdot v_1}$	2 x 5 = 10
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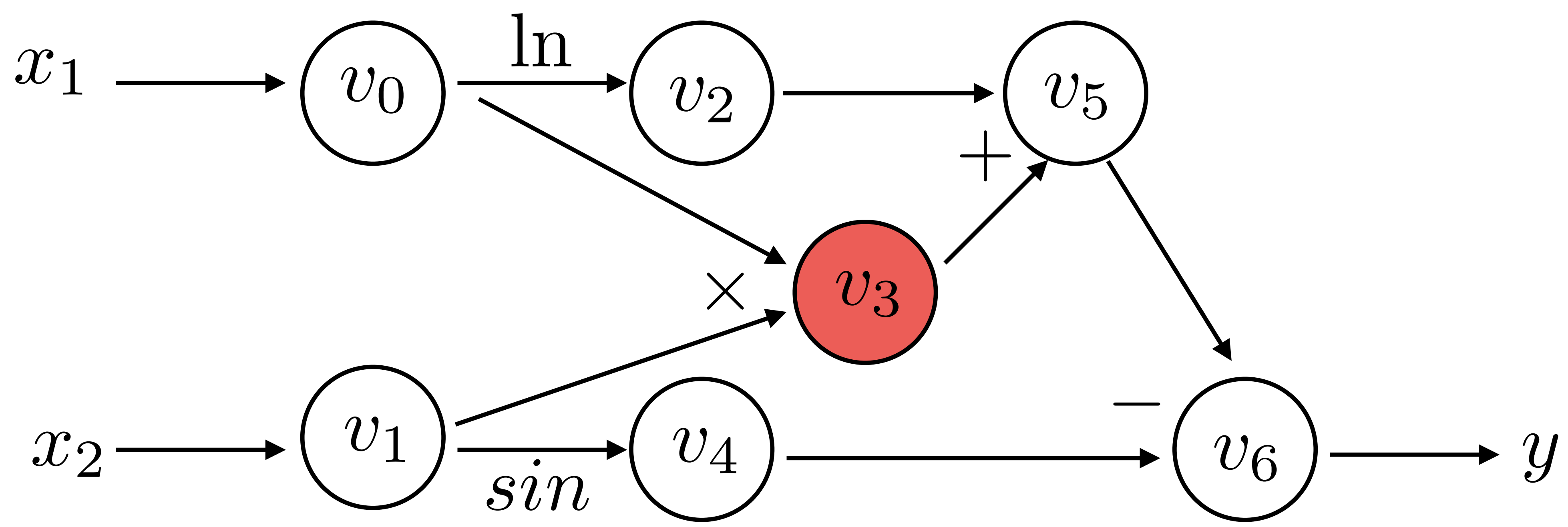
Forward Derivative Trace:

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

AutoDiff - **Forward Mode**

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



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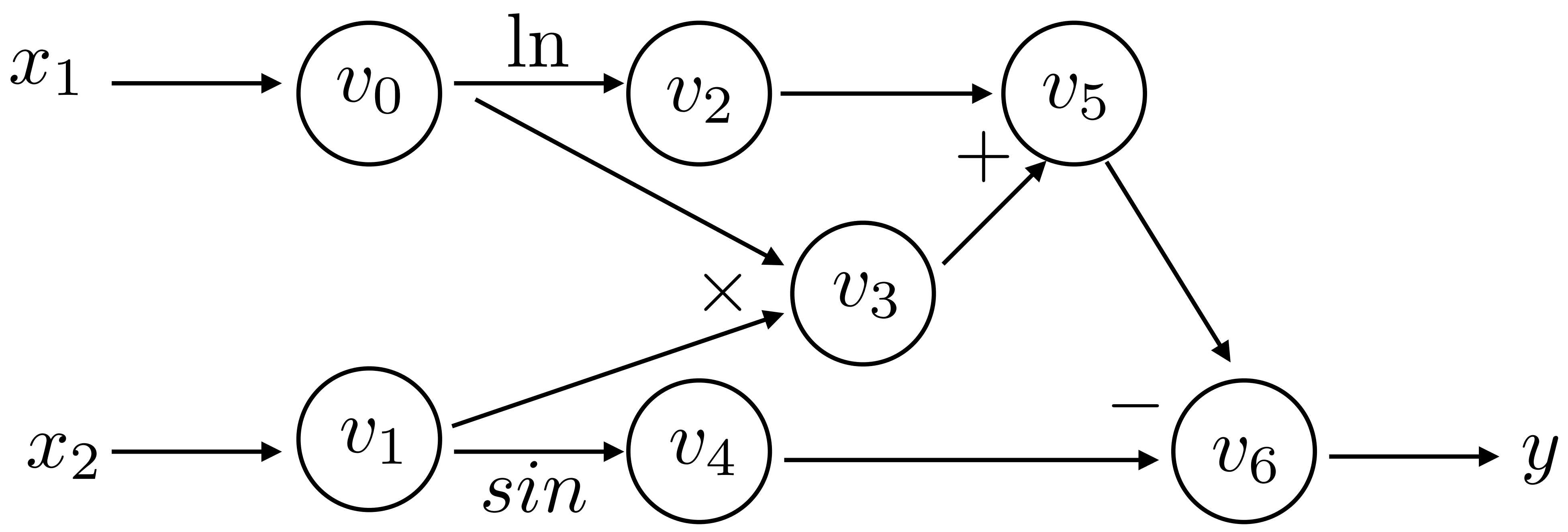
Forward Derivative Trace:

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

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



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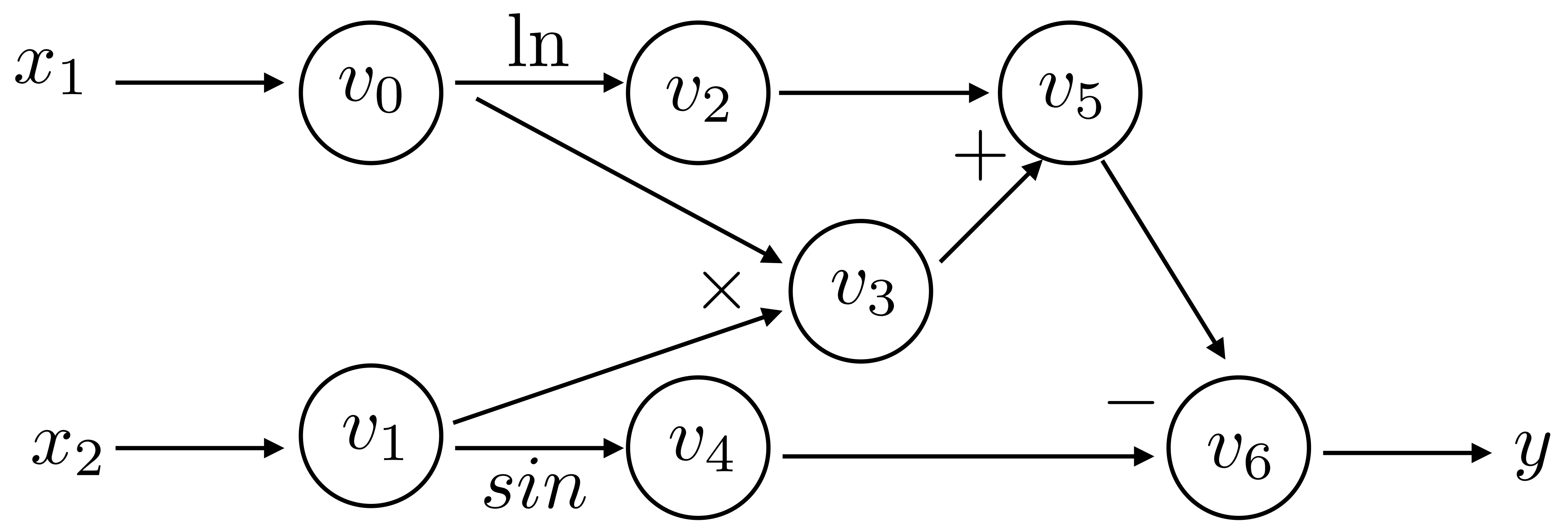
Forward Derivative Trace:

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

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



Forward Derivative Trace:

	$\left.\dfrac{\partial f(x_1, x_2)}{\partial x_1}\right\|_{(x_1=2, x_2=5)}$
$\dfrac{\partial v_0}{\partial x_1}$	1
$\dfrac{\partial v_1}{\partial x_1}$	0
$\dfrac{\partial v_2}{\partial x_1} = \dfrac{1}{v_0}\dfrac{\partial v_0}{\partial x_1}$	1/2 * 1 = 0.5
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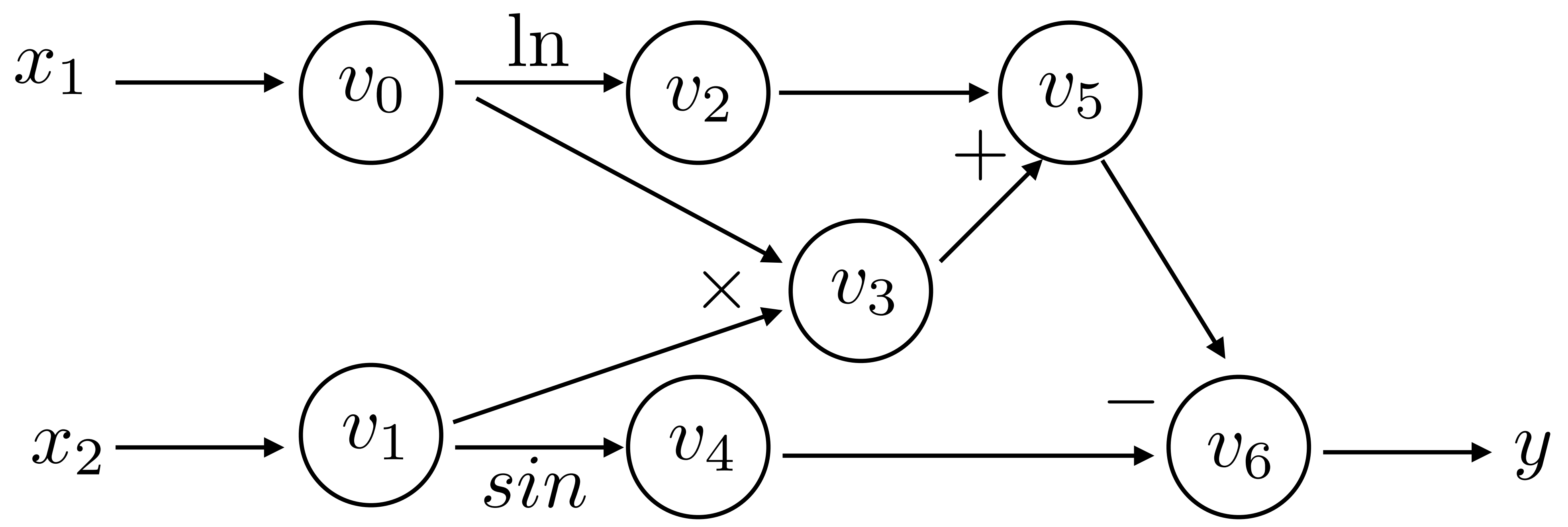
$\dfrac{\partial y}{\partial x_1} = \dfrac{\partial v_6}{\partial x_1}$	5.5

We now have:

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

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:

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$\frac{\partial v_0}{\partial x_1}$	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
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$\frac{\partial v_5}{\partial x_1} = \frac{\partial v_2}{\partial x_1} + \frac{\partial v_3}{\partial x_1}$	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

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

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

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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 $n = 1$)

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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?**

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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

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

Problem: DNN typically has large number of inputs:

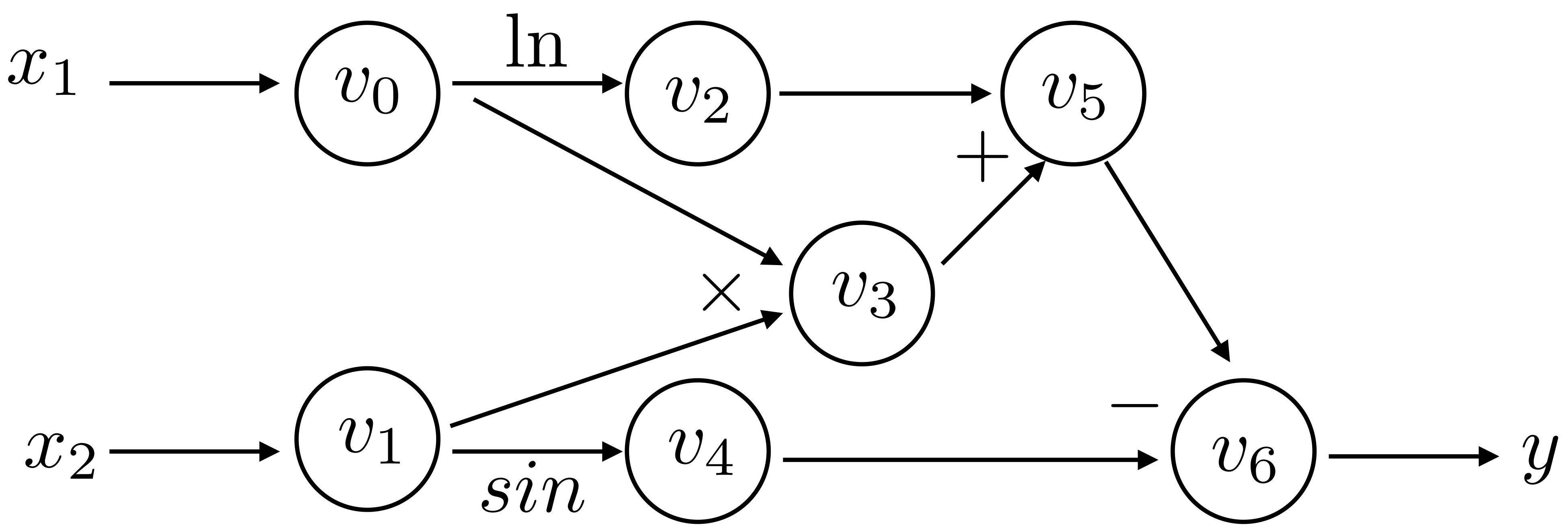
image as an input, plus all the weights and biases of layers = millions of inputs!

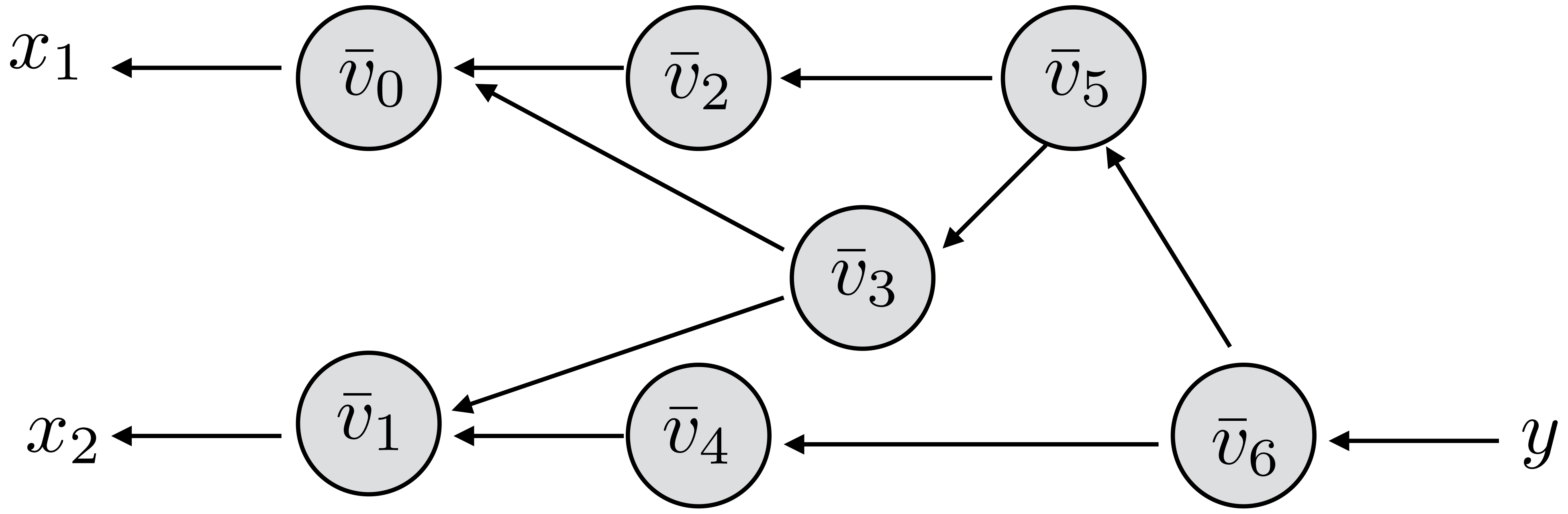
and very few outputs (many DNNs have $n = 1$)

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**





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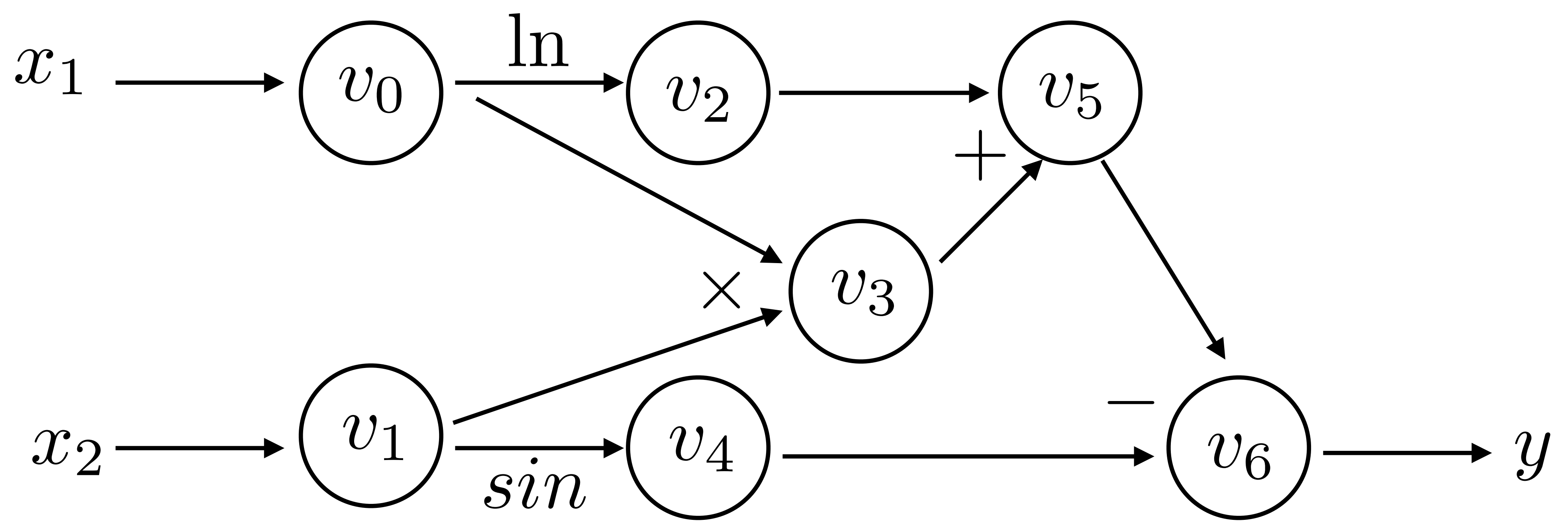
$v_6 = v_5 - v_4$	10.693 + 0.959 = 11.652
$y = v_6$	11.652

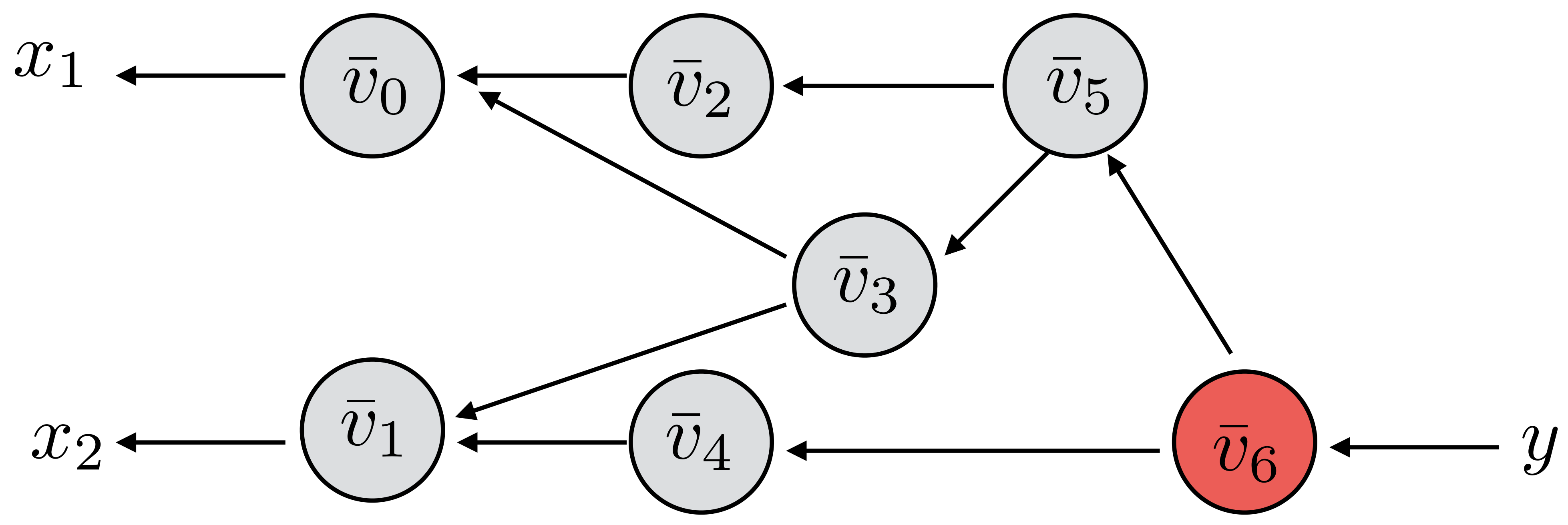
Traverse the original graph in the *reverse* topological order and for each node in the original graph introduce an **adjoint node**, which computes derivative of the output with respect to the local node (using Chain rule):

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

"**local**" derivative

AutoDiff - **Reverse Mode**





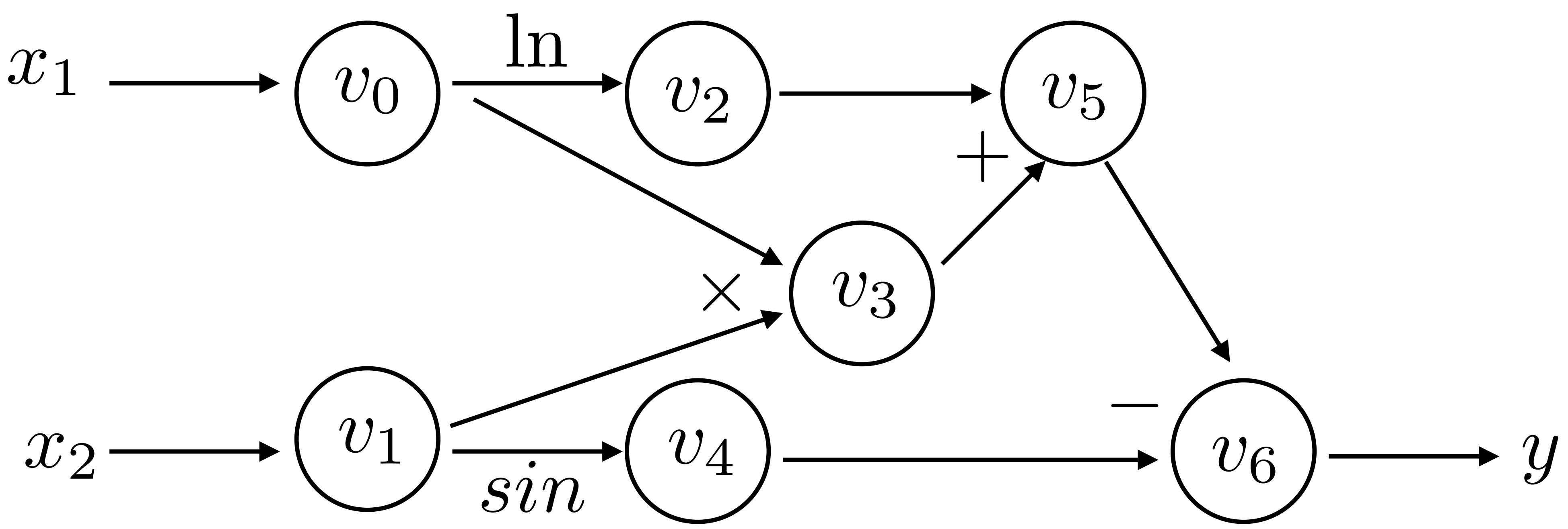
Forward Evaluation Trace:

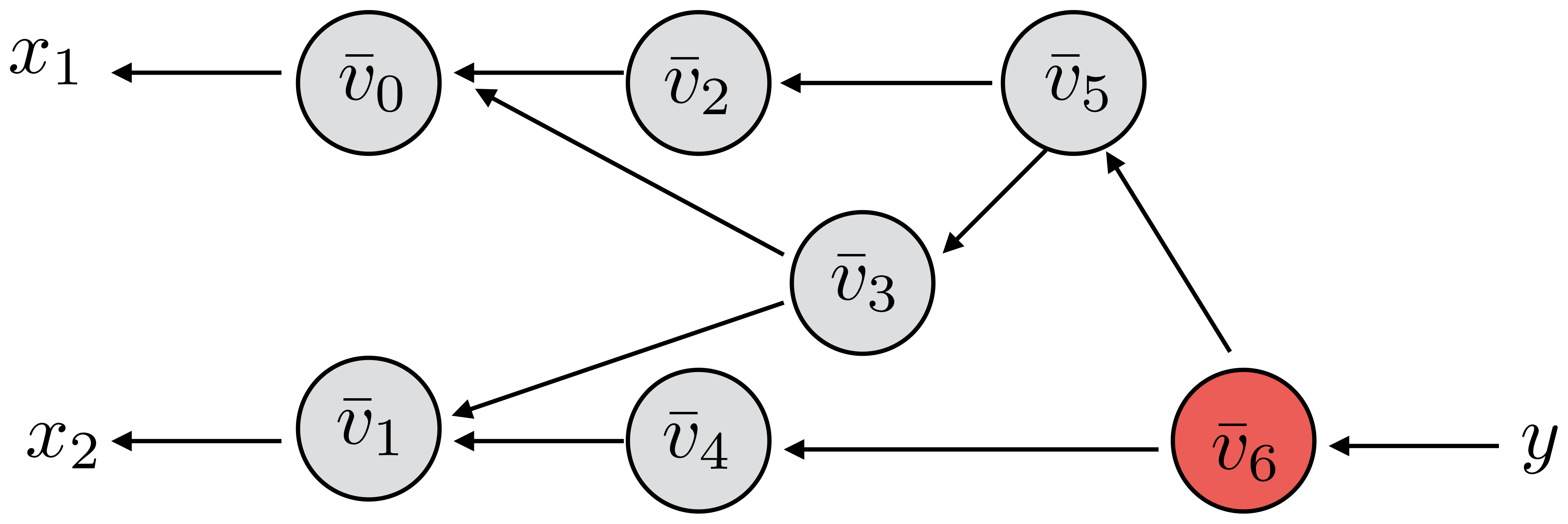
	$f(2,5)$
$v_0 = x_1$	2
$v_1 = x_2$	5
$v_2 = \ln(v_0)$	ln(2) = 0.693
$v_3 = v_0 \cdot v_1$	2 x 5 = 10
$v_4 = sin(v_1)$	sin(5) = 0.959
$v_5 = v_2 + v_3$	0.693 + 10 = 10.693
$v_6 = v_5 - v_4$	10.693 + 0.959 = 11.652
$y = v_6$	11.652

Backwards Derivative Trace:

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

AutoDiff - **Reverse Mode**





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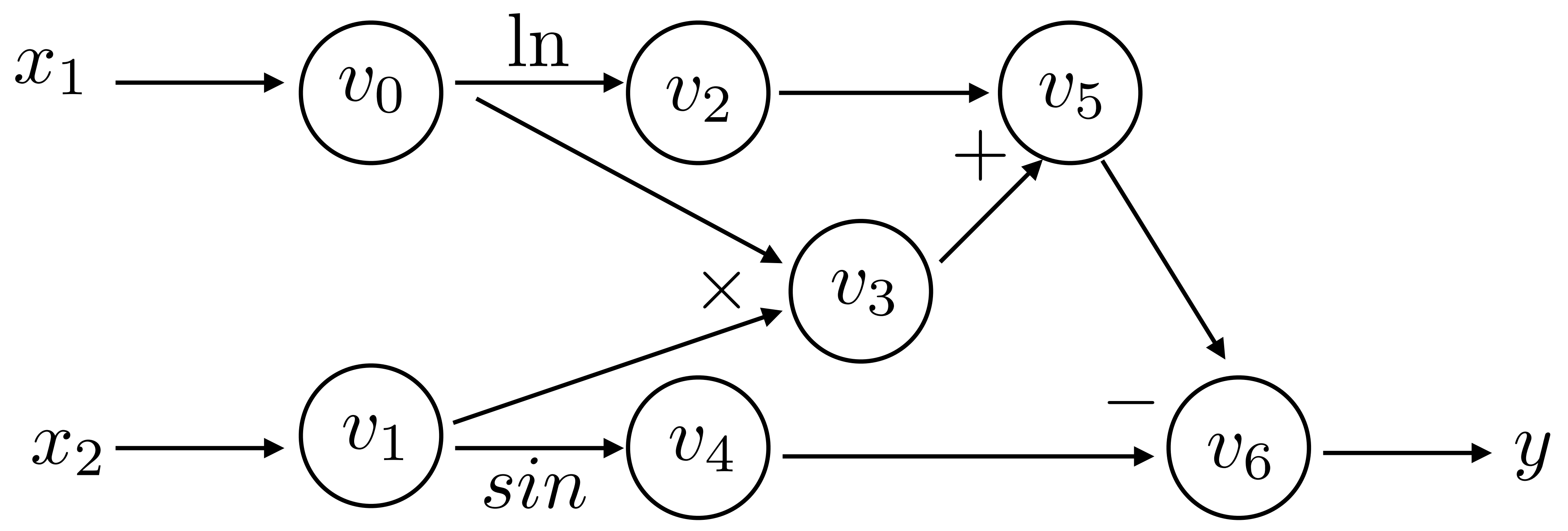
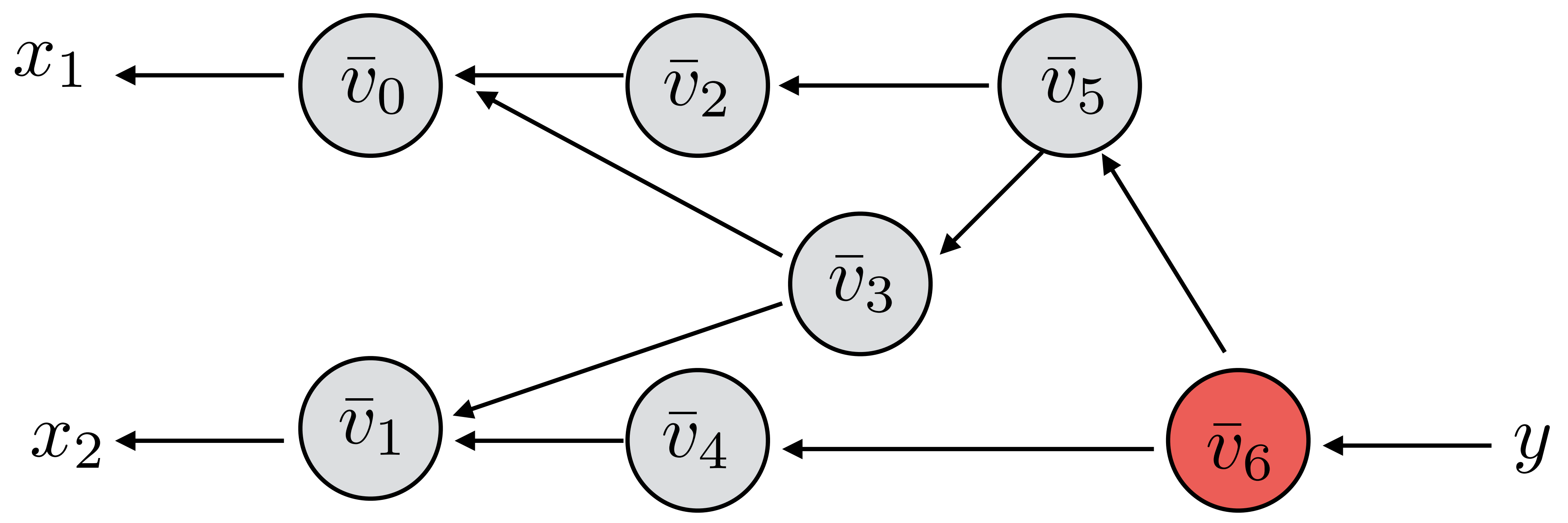
$$\bar{v}_6 = \frac{\partial y}{\partial v_6}$$

AutoDiff - **Reverse Mode**





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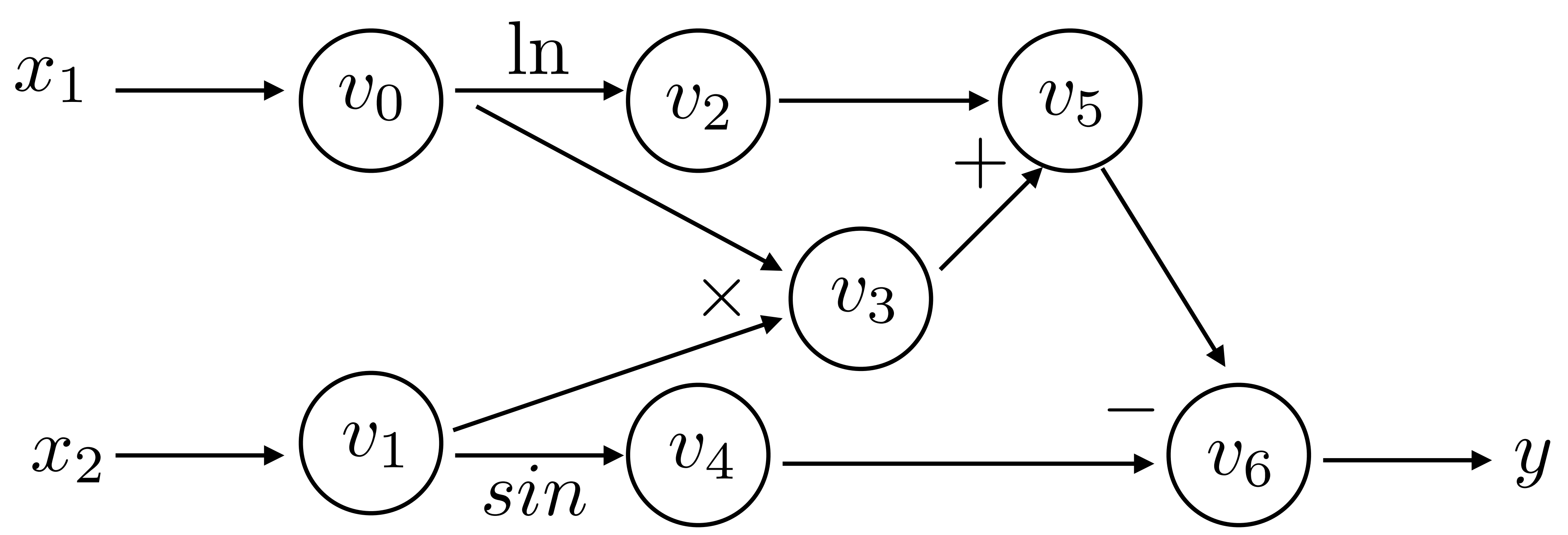
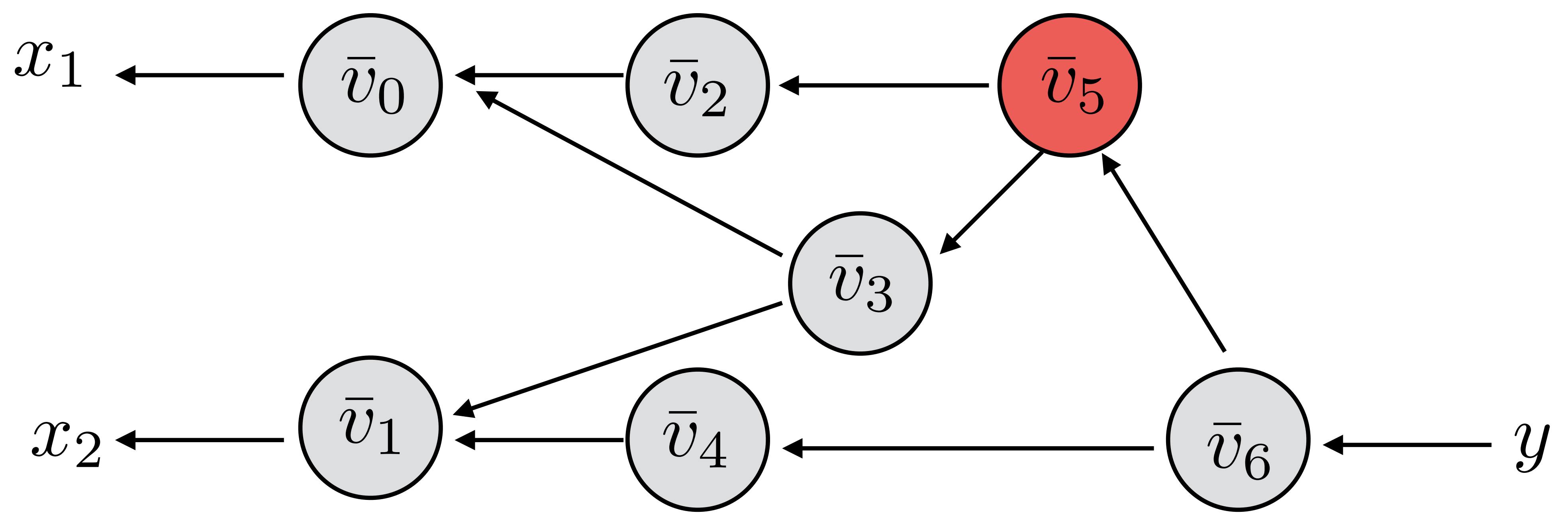
$y = v_6$	11.652

Backwards Derivative Trace:

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

AutoDiff - **Reverse Mode**





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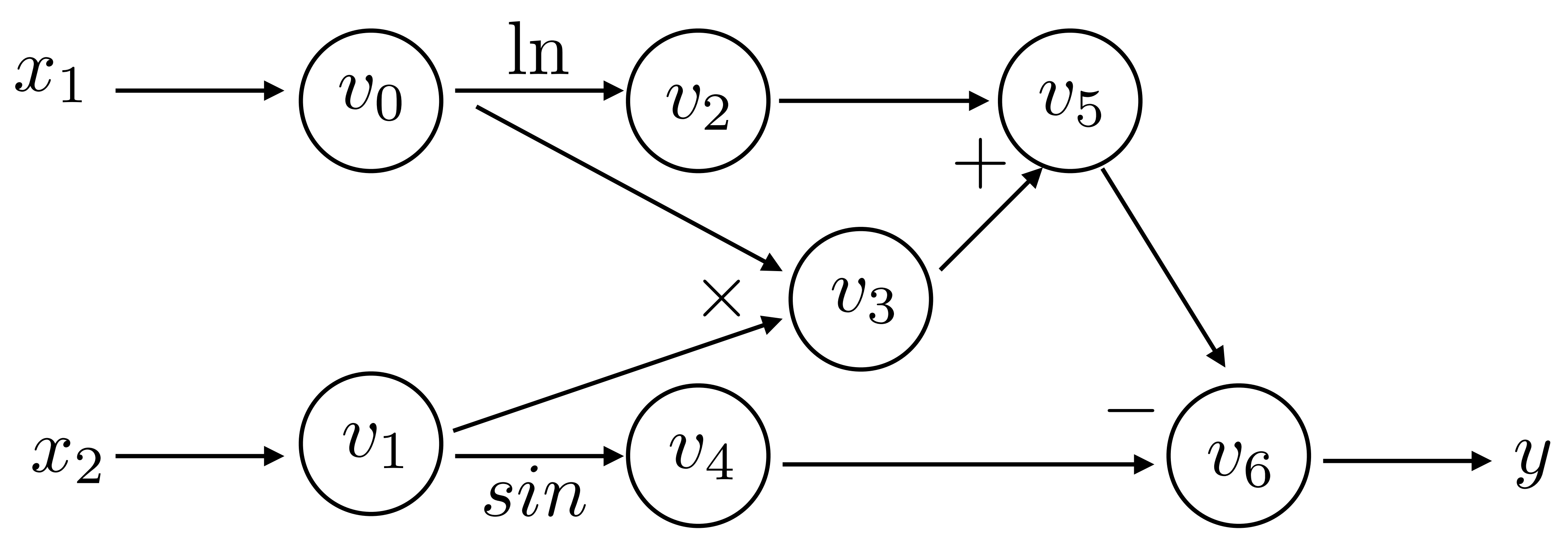
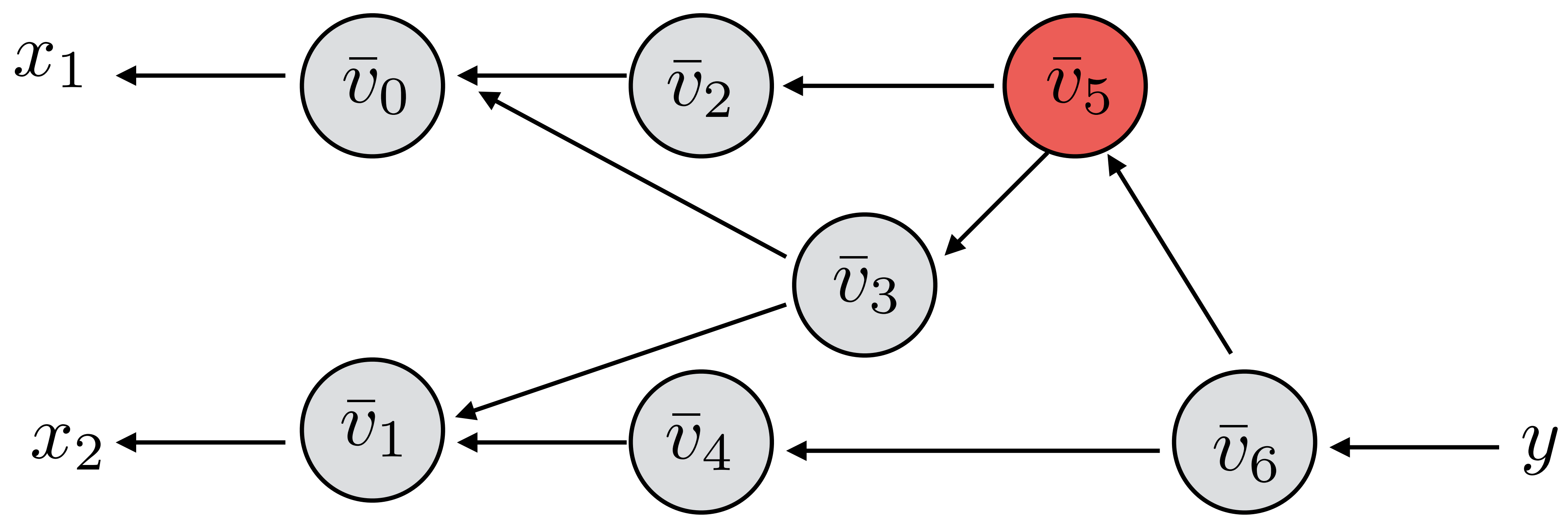
$y = v_6$	11.652

Backwards Derivative Trace:

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

AutoDiff - **Reverse Mode**





Backwards Derivative Trace:

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

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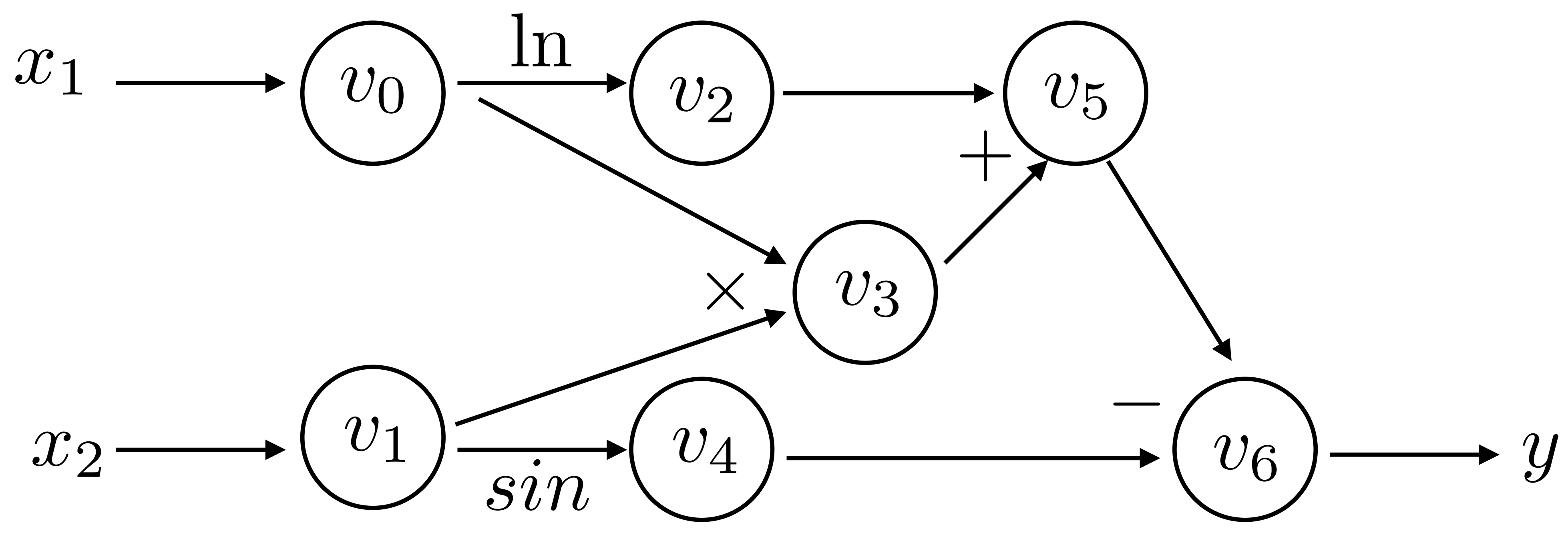
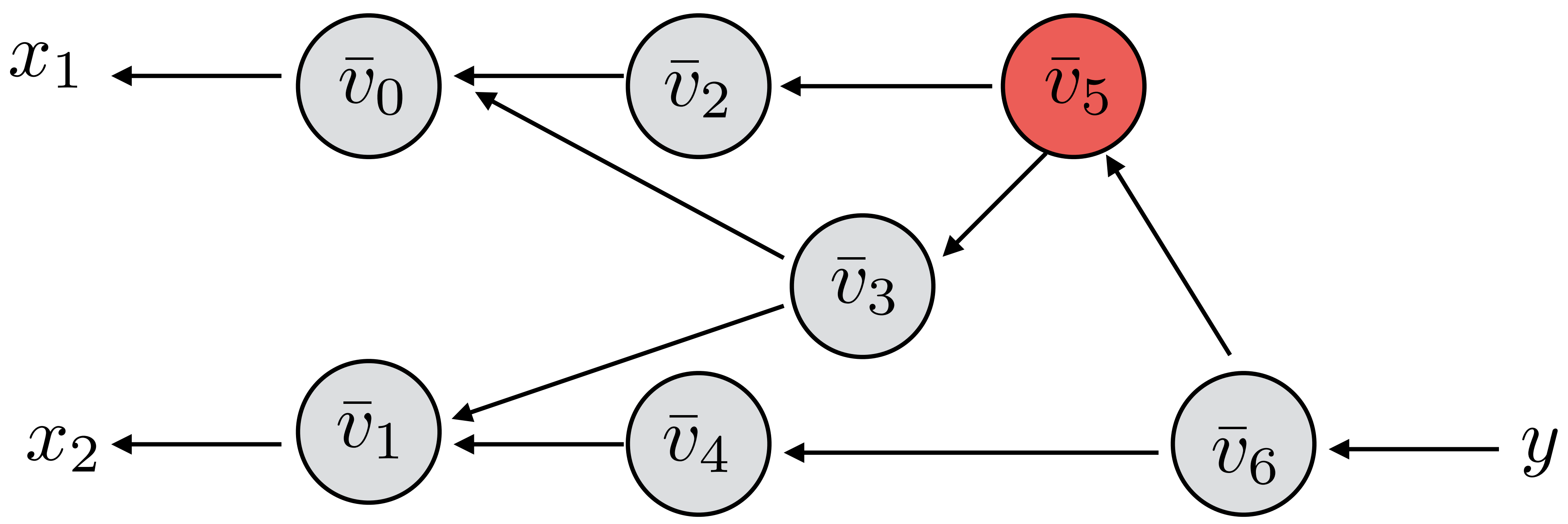
AutoDiff - **Reverse Mode**





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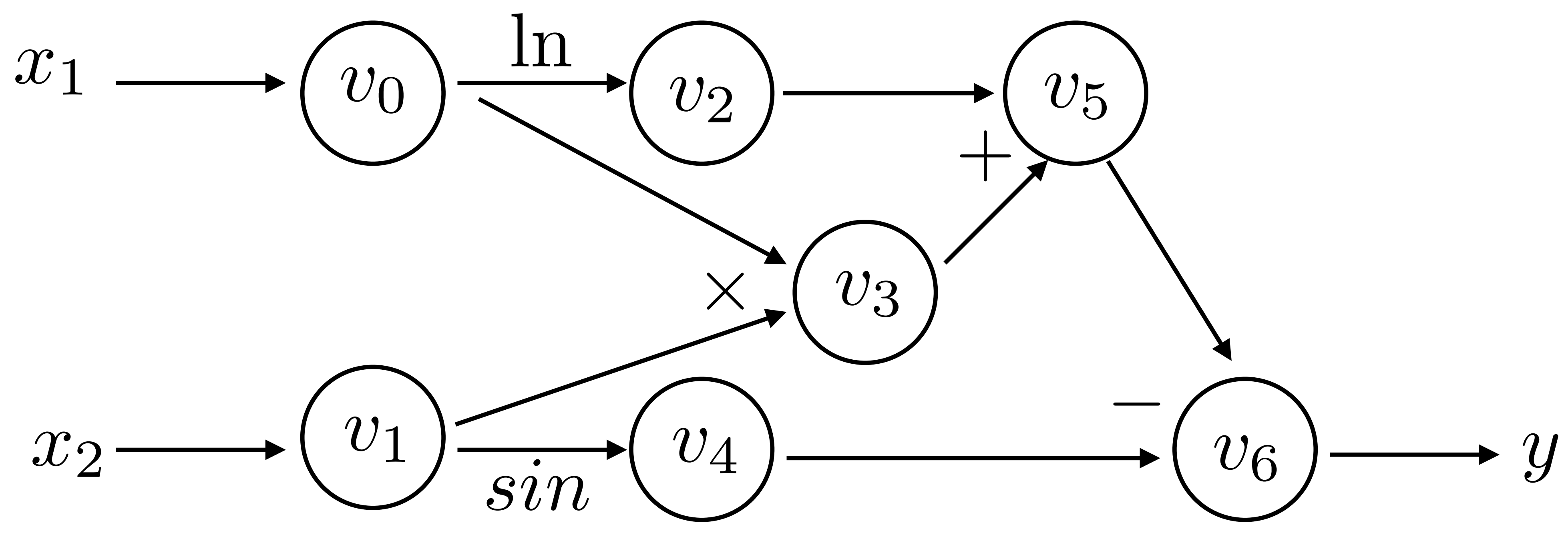
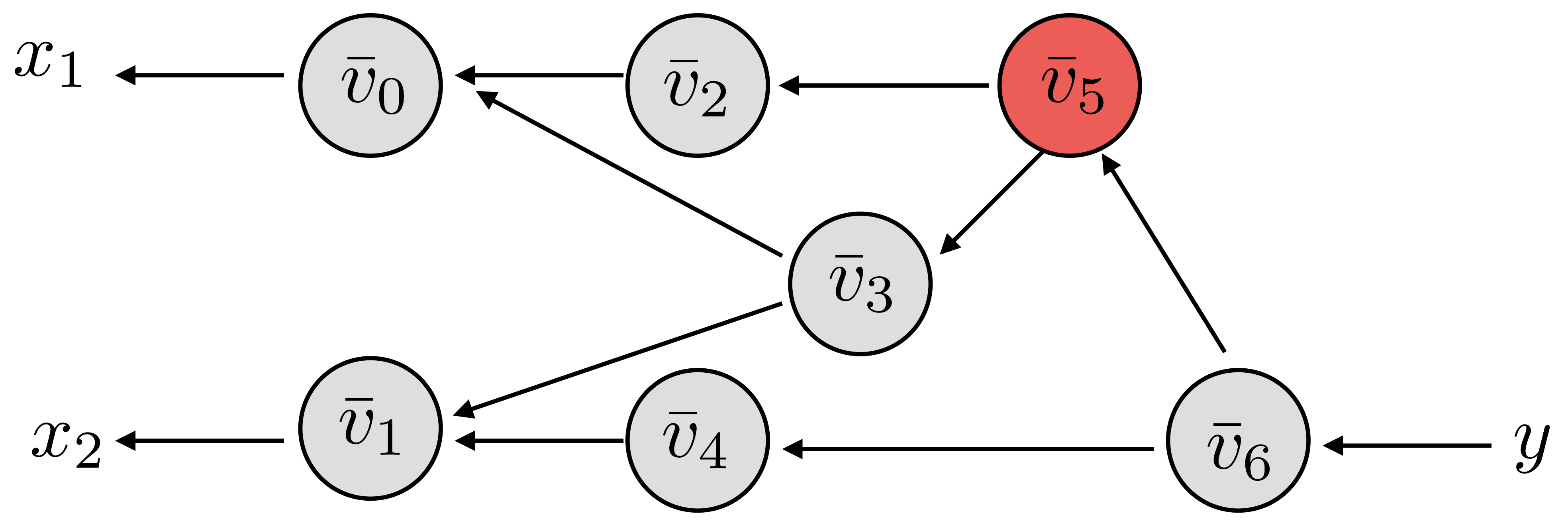
$y = v_6$	11.652

Backwards Derivative Trace:

$\bar{v}_5 = \bar{v}_6 \dfrac{\partial v_6}{\partial v_5} = \bar{v}_6 \cdot 1$	
$\bar{v}_6 = \dfrac{\partial y}{\partial v_6}$	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
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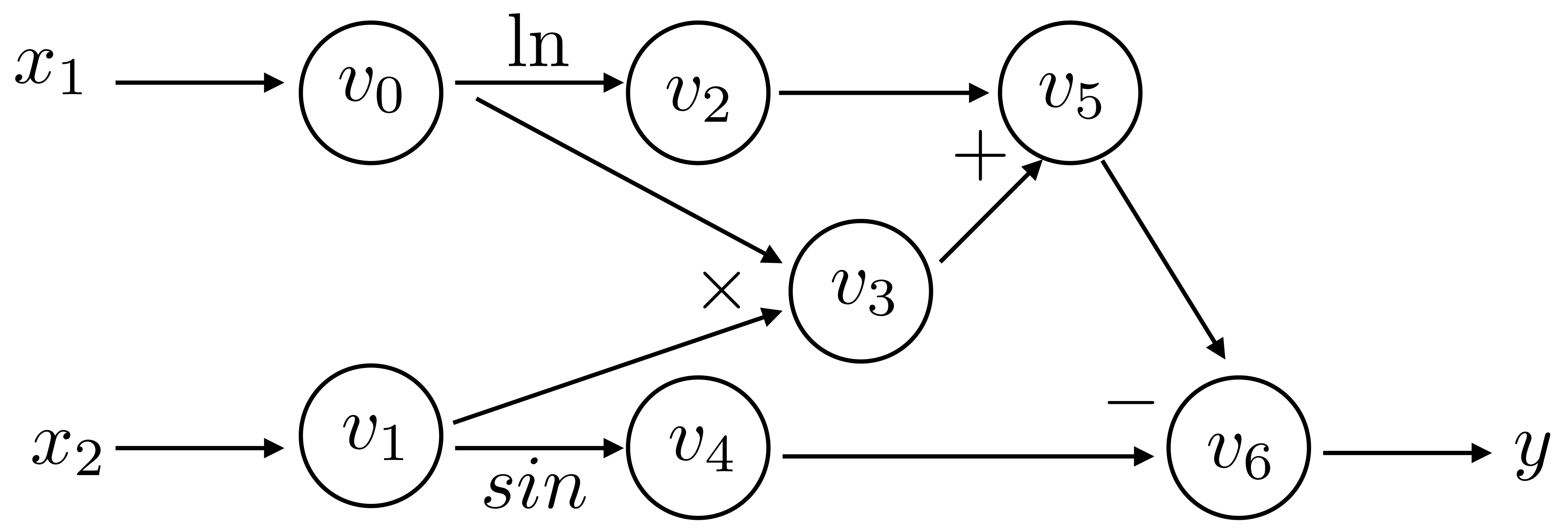
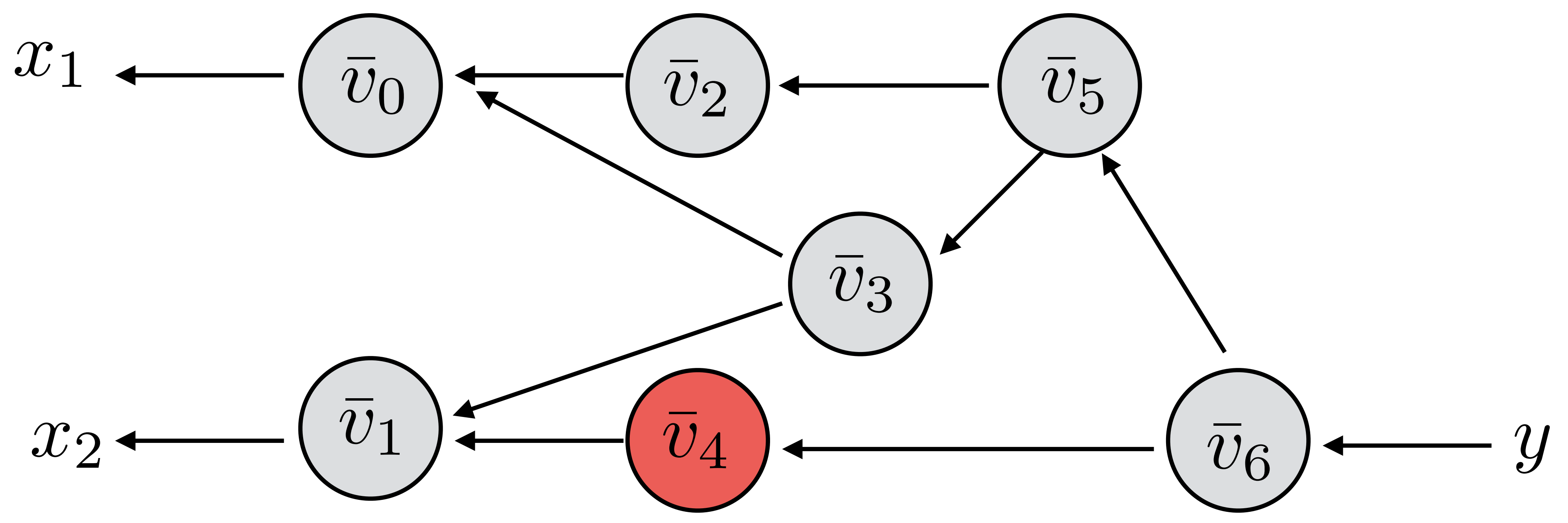
AutoDiff - **Reverse Mode**





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$v_2 = \ln(v_0)$	ln(2) = 0.693
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Backwards Derivative Trace:

$\bar{v}_4 = \bar{v}_6 \dfrac{\partial v_6}{\partial v_4}$	
$\bar{v}_5 = \bar{v}_6 \dfrac{\partial v_6}{\partial v_5} = \bar{v}_6 \cdot 1$	1x1 = 1
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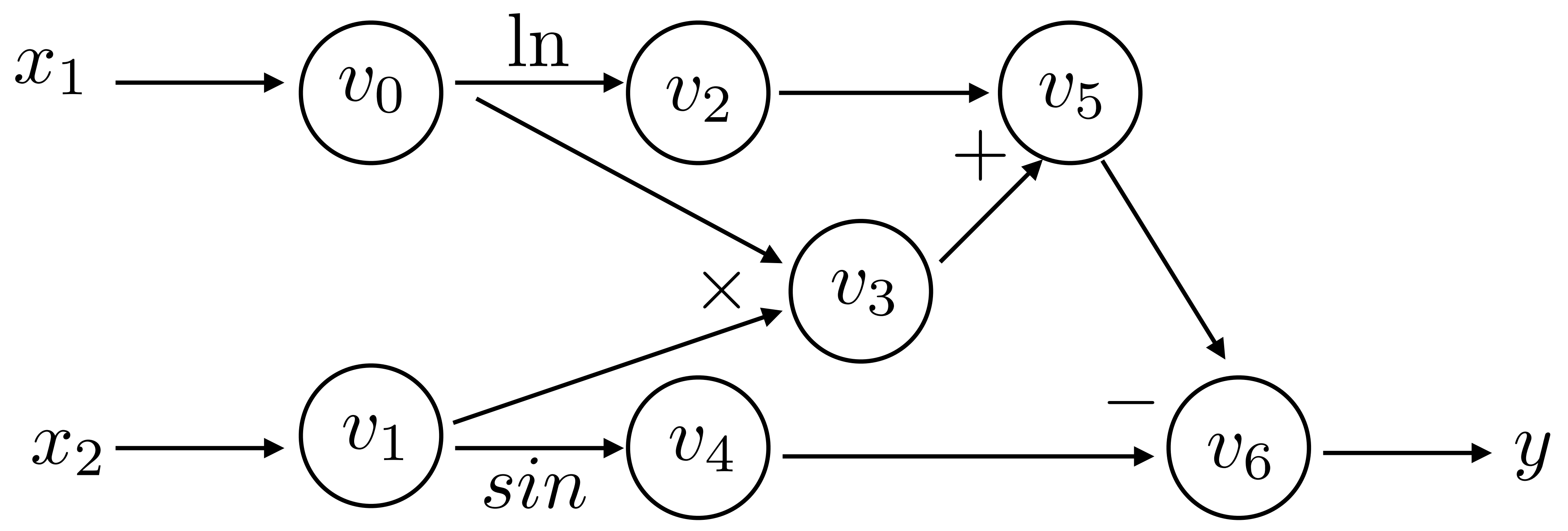
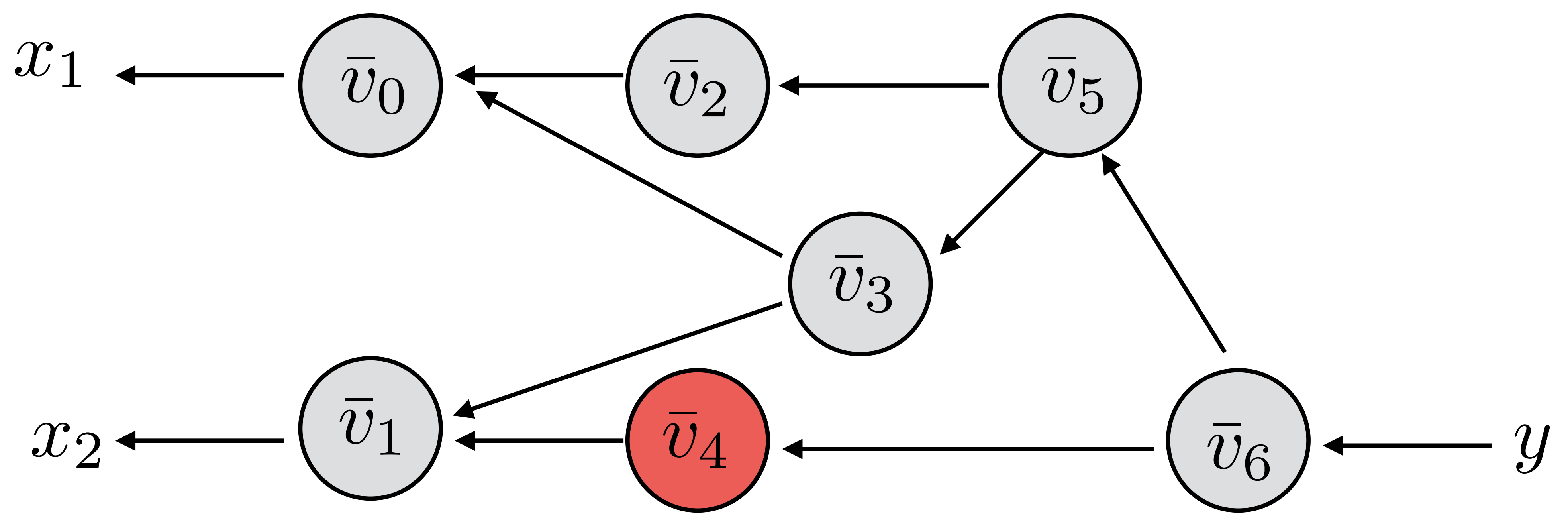
AutoDiff - **Reverse Mode**





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$\bar{v}_5 = \bar{v}_6 \dfrac{\partial v_6}{\partial v_5} = \bar{v}_6 \cdot 1$	1x1 = 1
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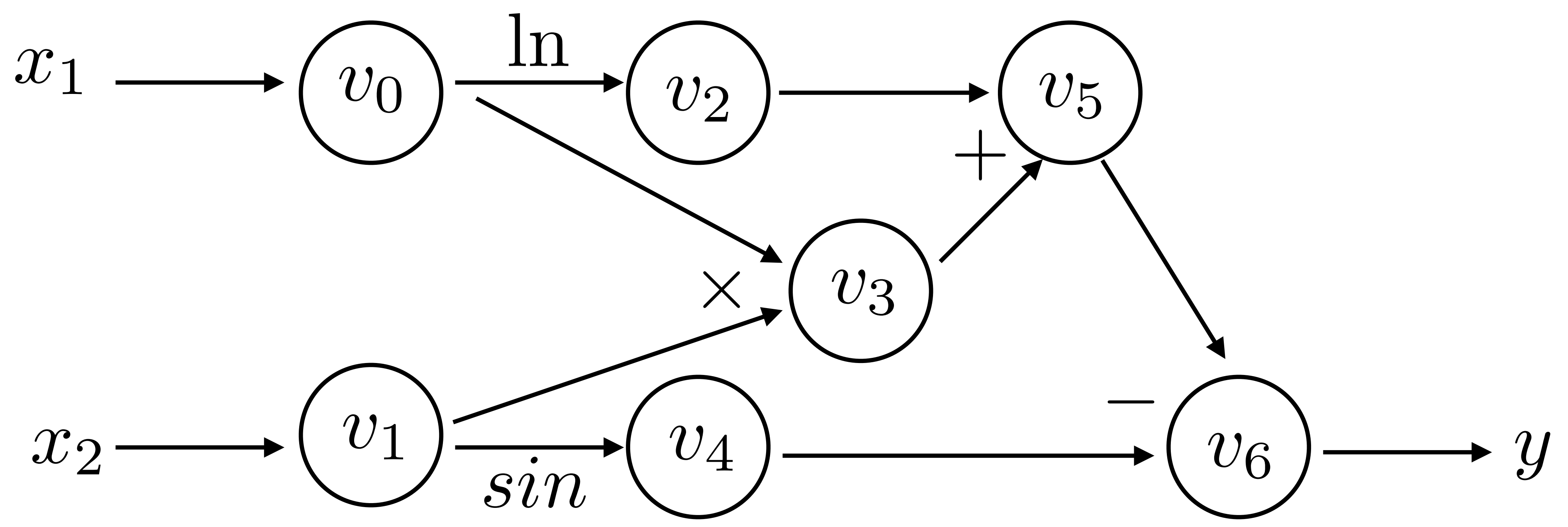
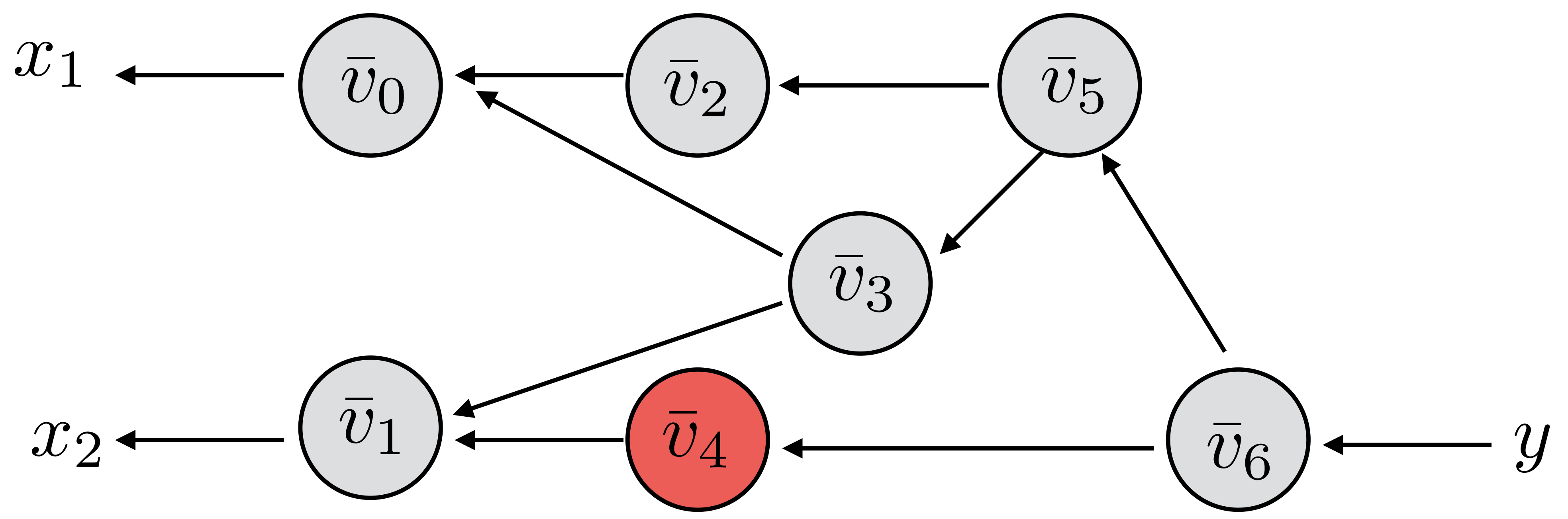
AutoDiff - **Reverse Mode**





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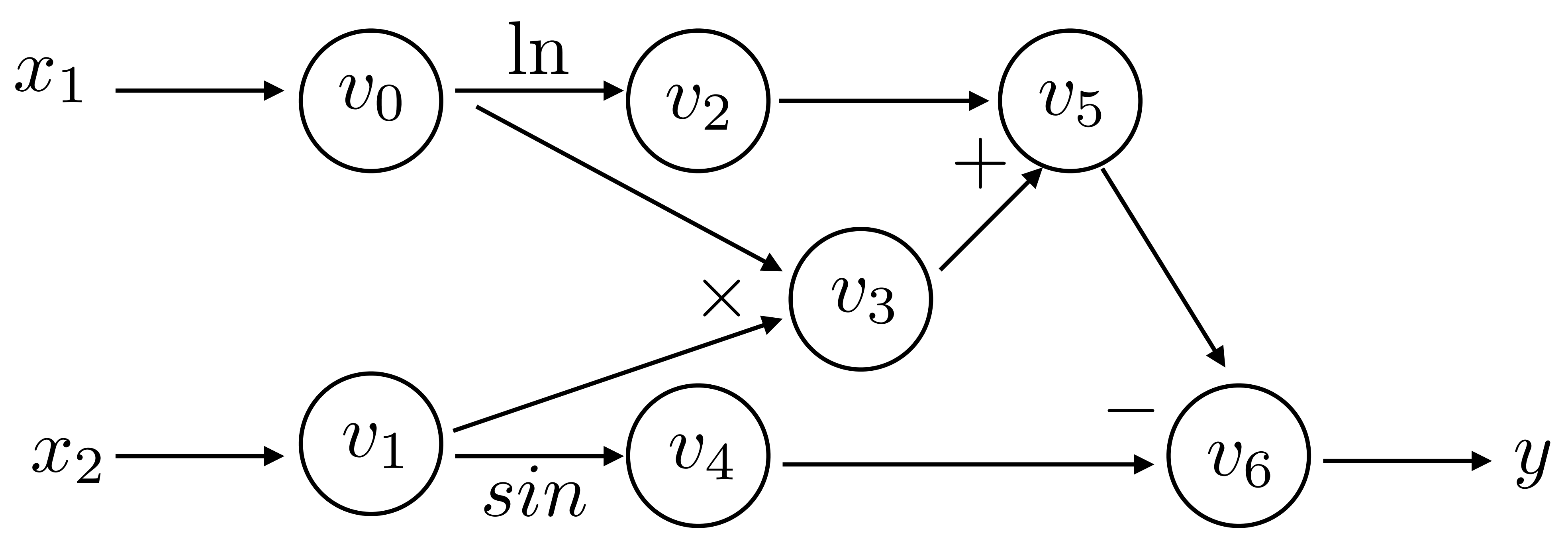
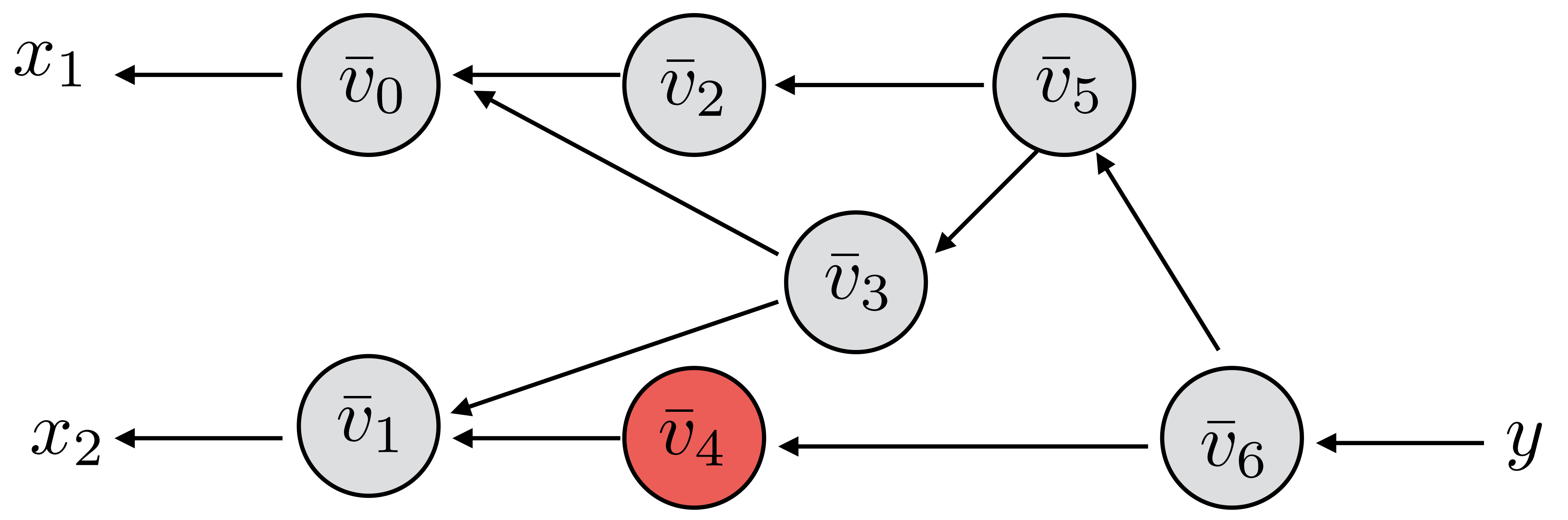
Backwards Derivative Trace:

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

AutoDiff - **Reverse Mode**





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$y = v_6$	11.652

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
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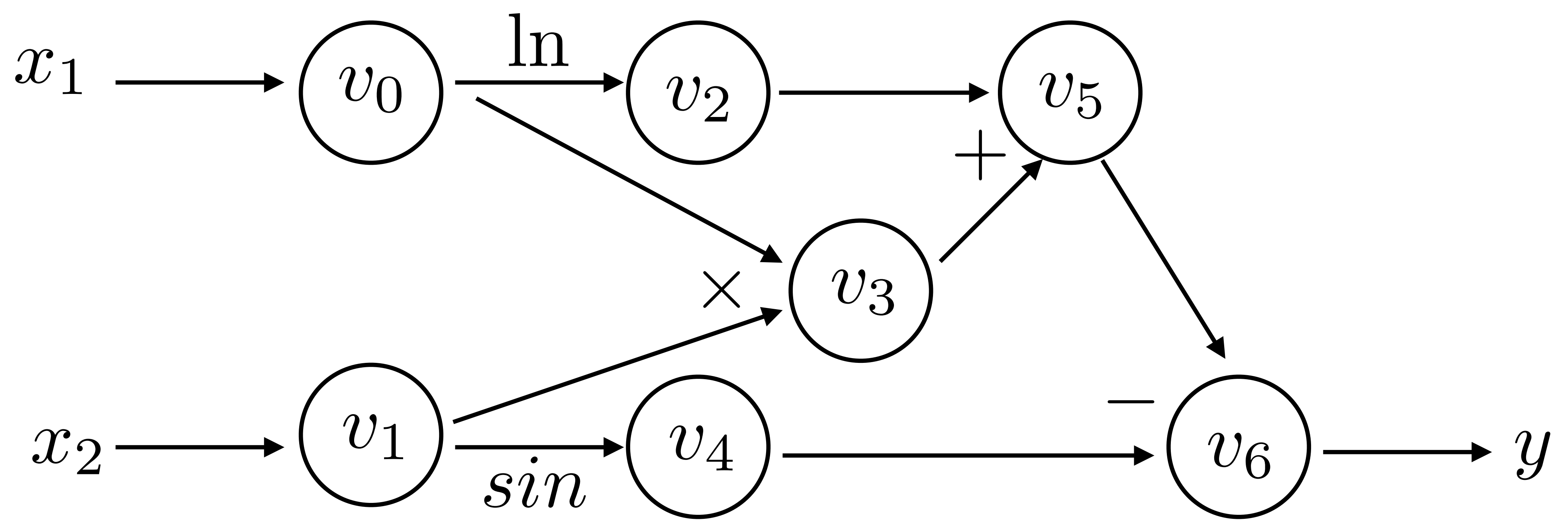
AutoDiff - **Reverse Mode**



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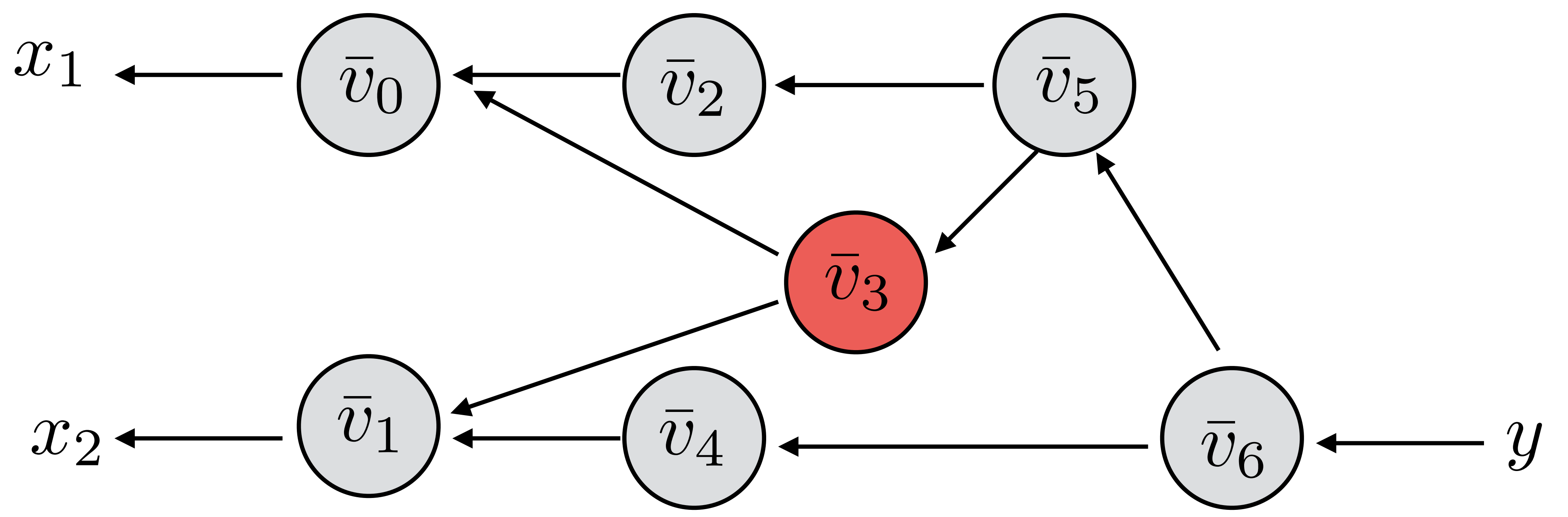

Backwards Derivative Trace:

$\bar{v}_3 = \bar{v}_5 \dfrac{\partial v_5}{\partial v_3}$	
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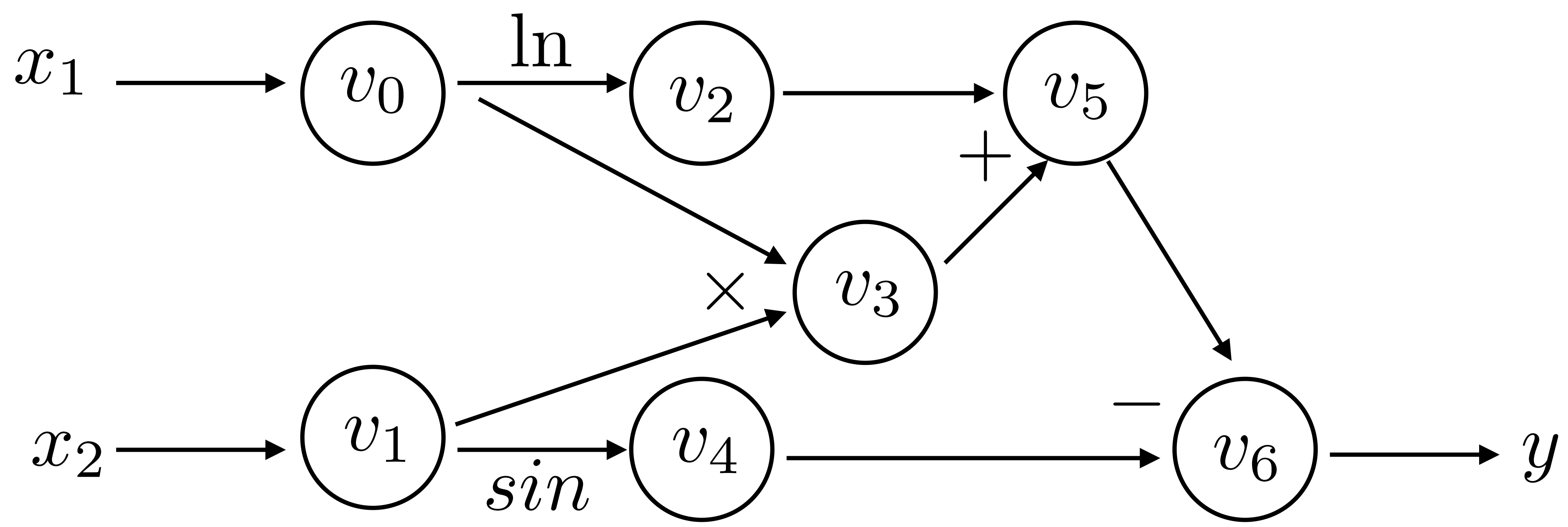
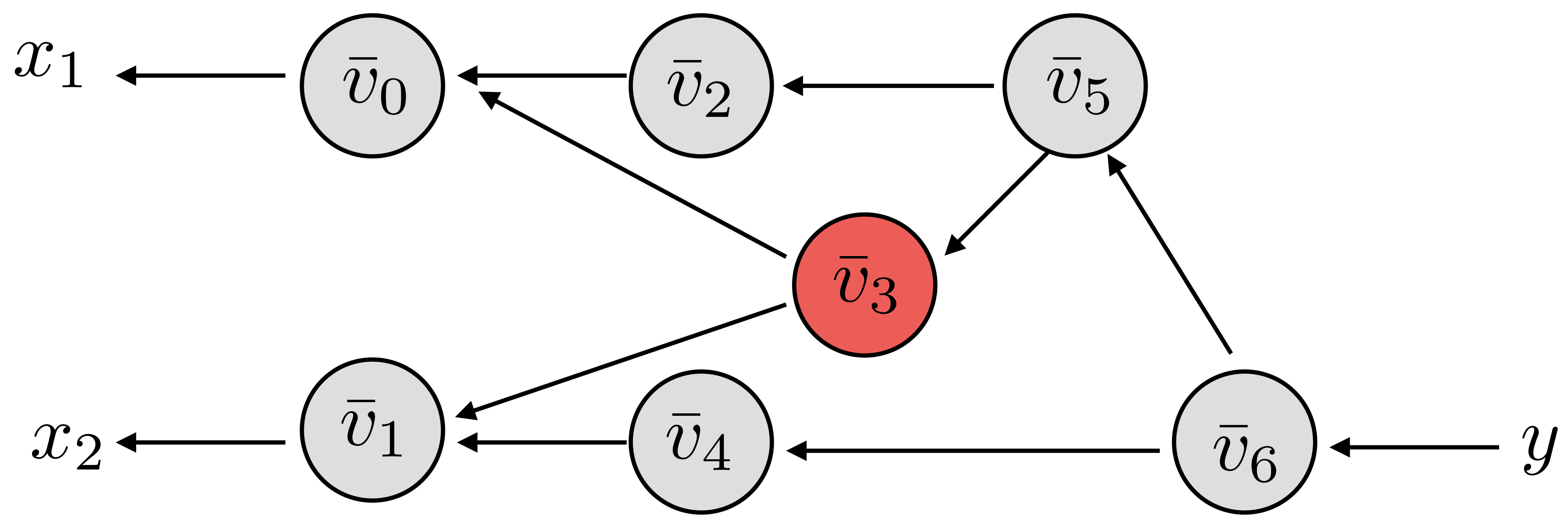
$\bar{v}_6 = \dfrac{\partial y}{\partial v_6}$	1

AutoDiff - **Reverse Mode**





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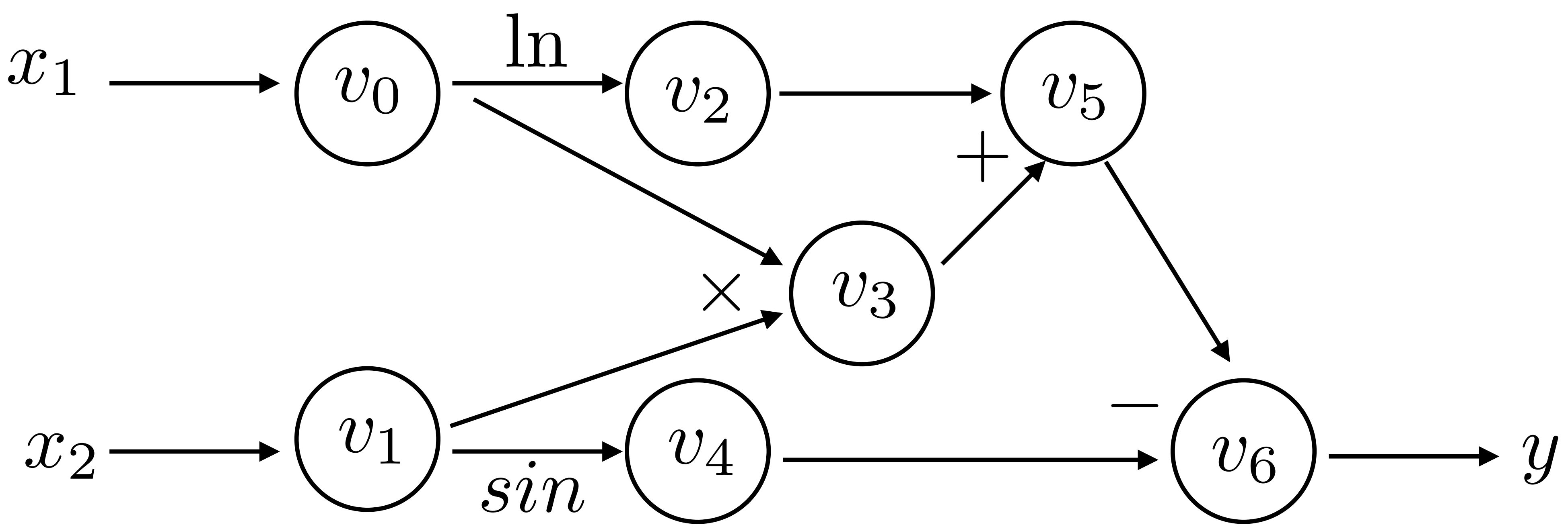
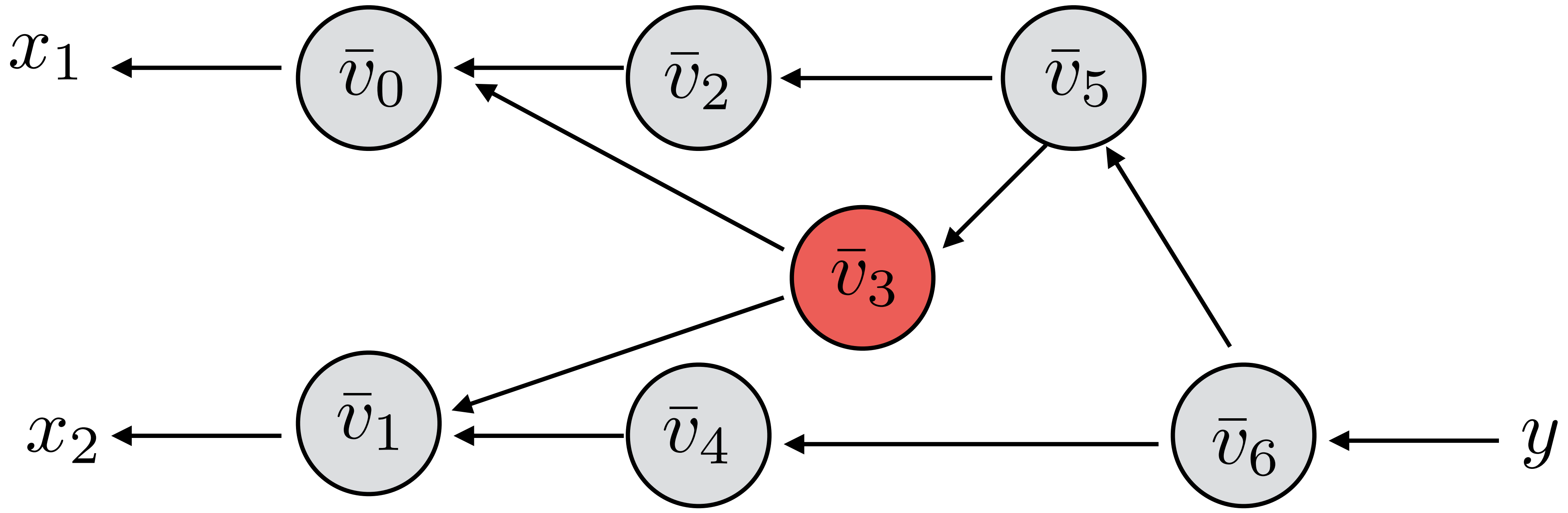
AutoDiff - **Reverse Mode**





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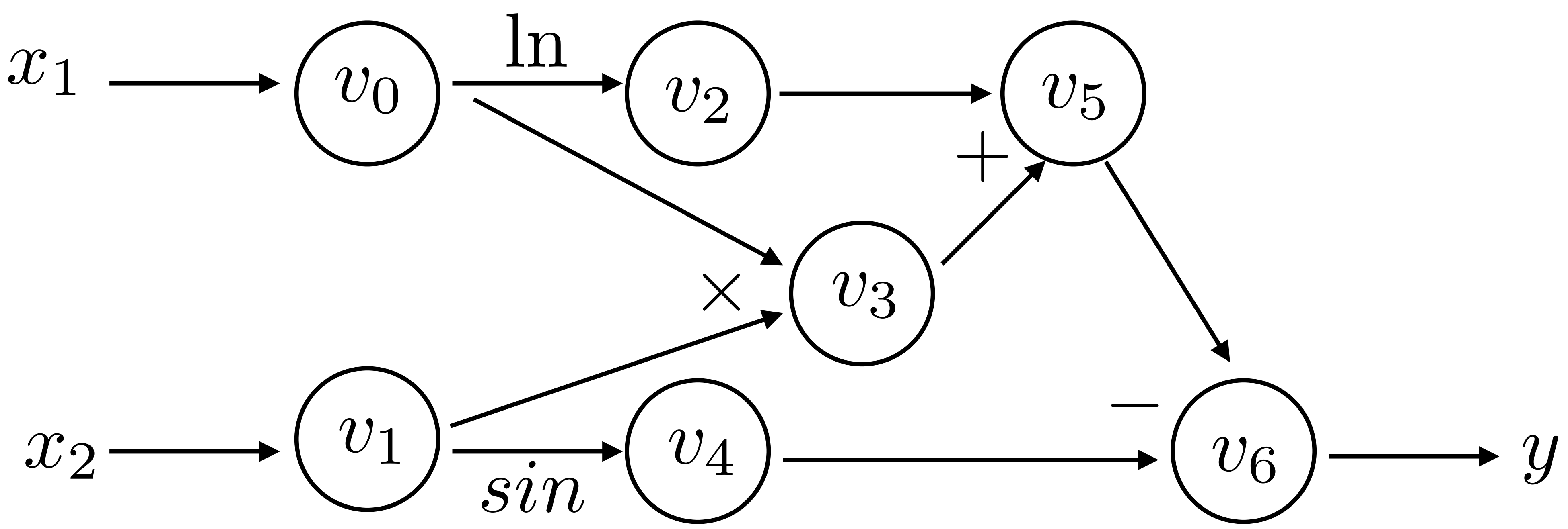
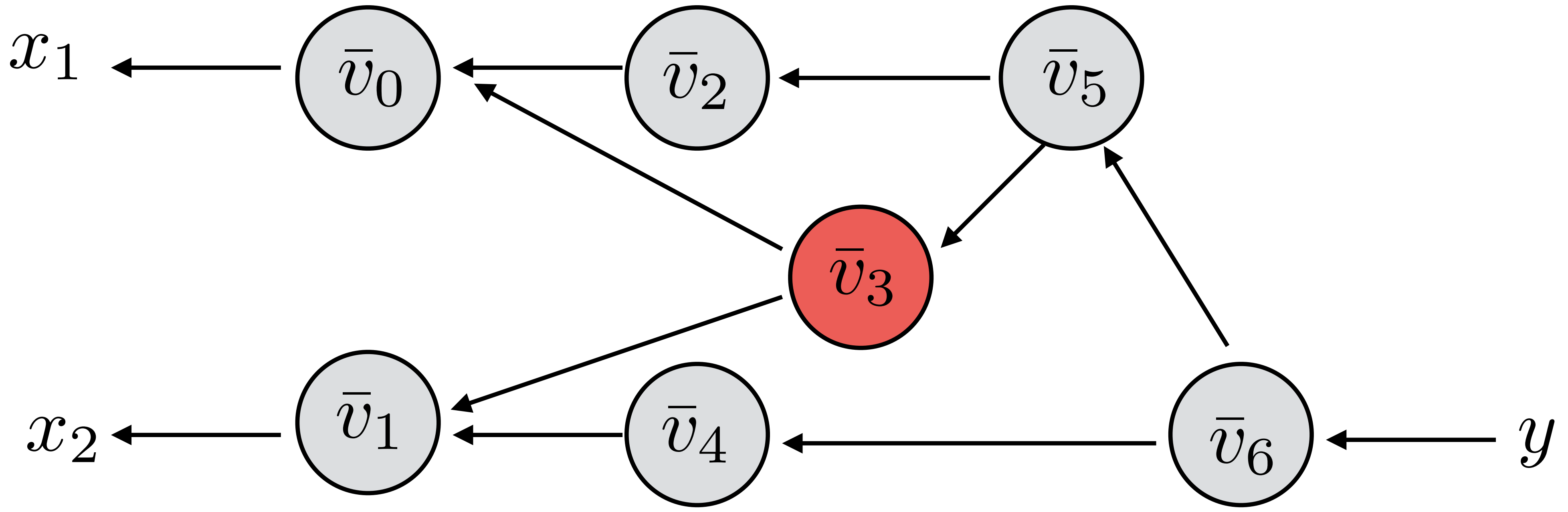
AutoDiff - **Reverse Mode**





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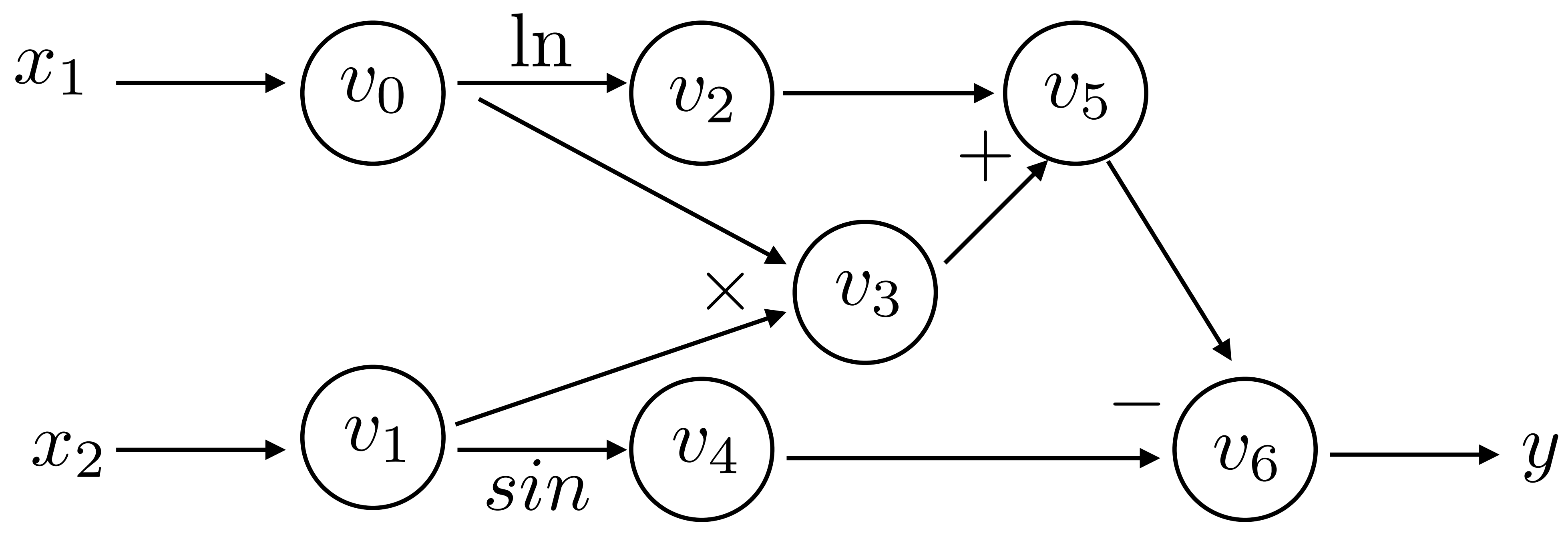
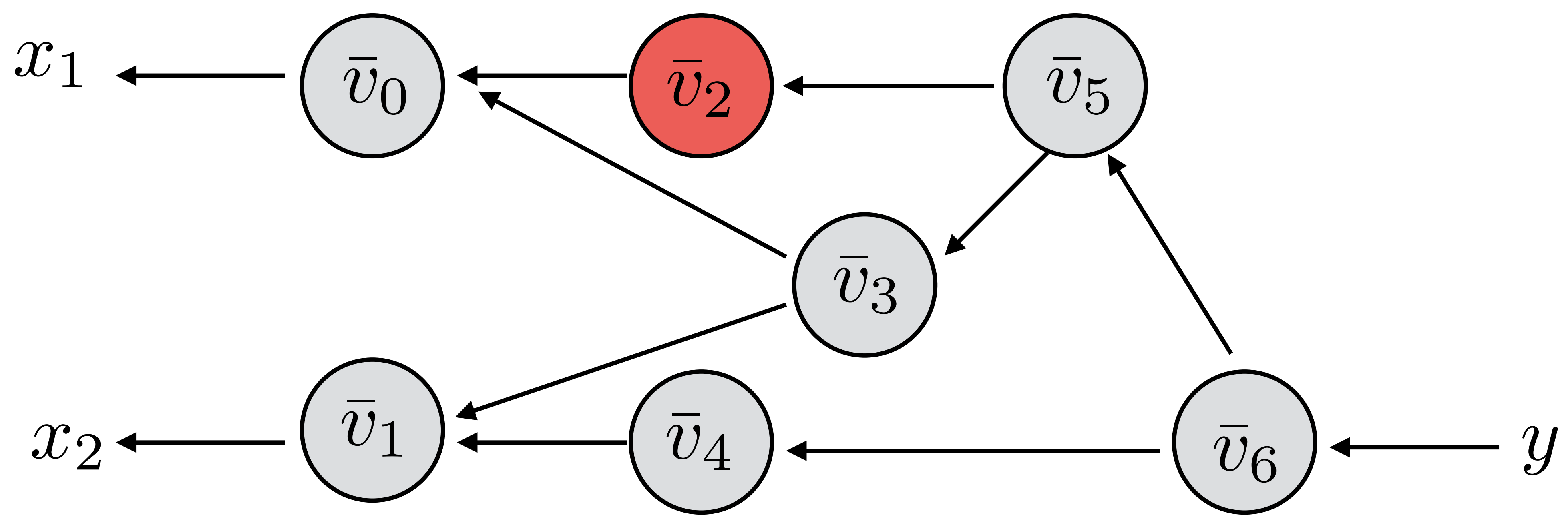
AutoDiff - **Reverse Mode**





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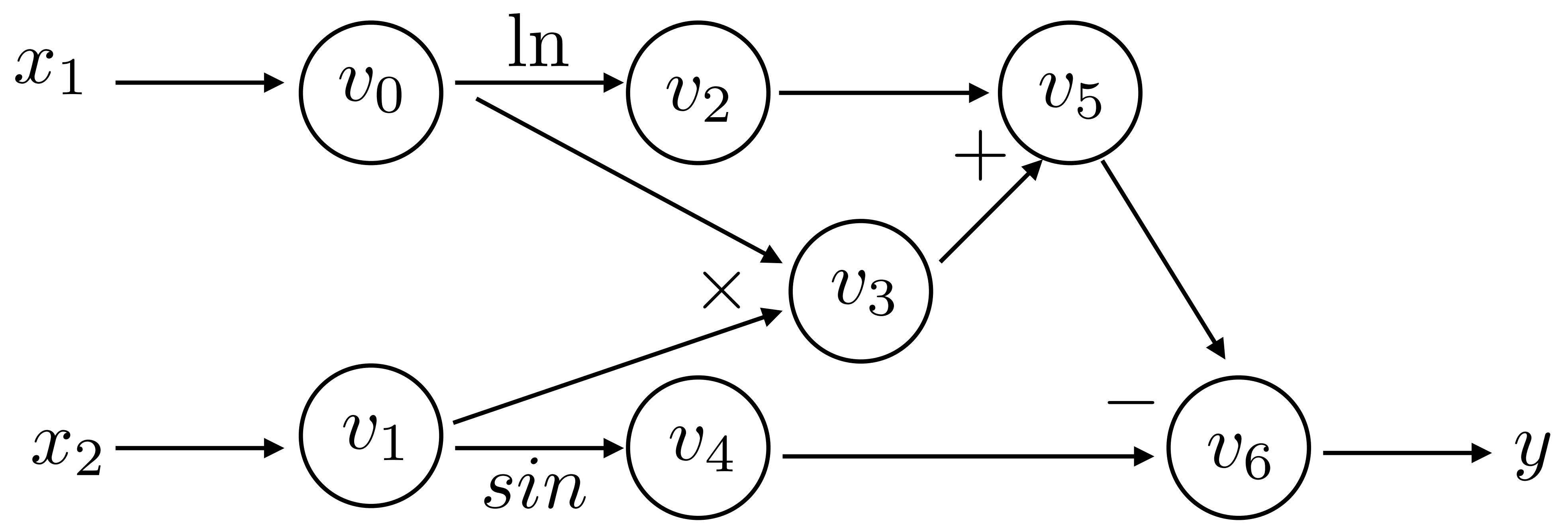
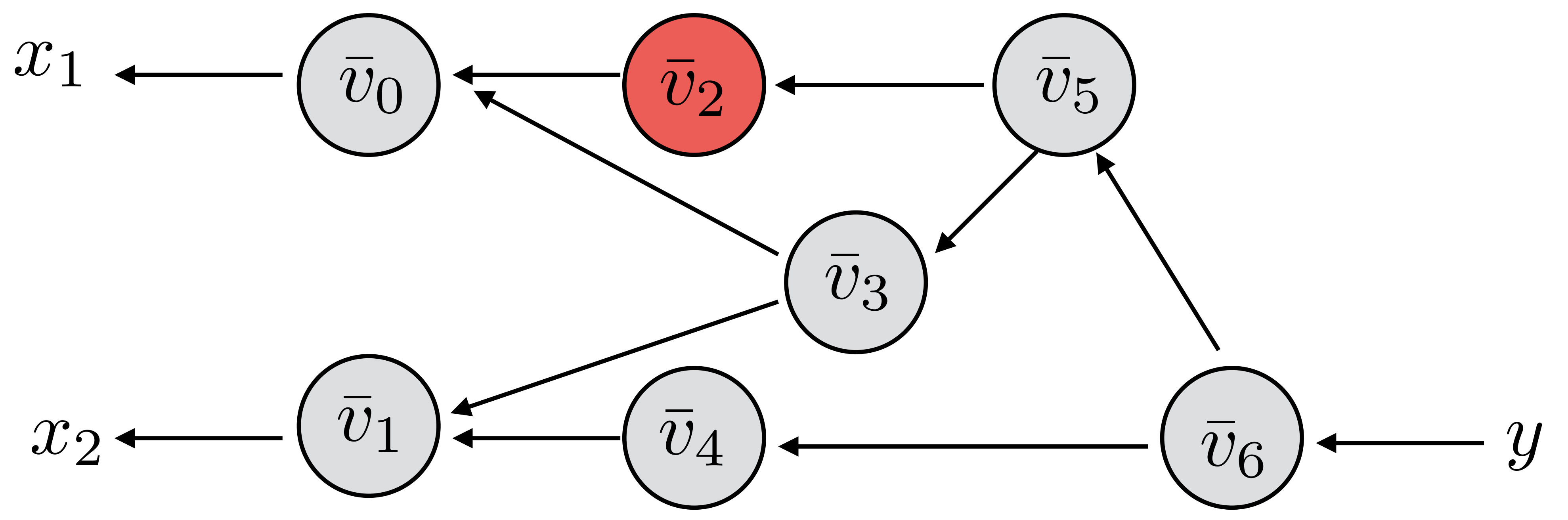
Backwards Derivative Trace:

$\bar{v}_2 = \bar{v}_5 \frac{\partial v_5}{\partial v_2}$	
$\bar{v}_3 = \bar{v}_5 \frac{\partial v_5}{\partial v_3} = \bar{v}_5 \cdot (1)$	1x1 = 1
$\bar{v}_4 = \bar{v}_6 \frac{\partial v_6}{\partial v_4} = \bar{v}_6 \cdot (-1)$	1x-1 = -1
$\bar{v}_5 = \bar{v}_6 \frac{\partial v_6}{\partial v_5} = \bar{v}_6 \cdot 1$	1x1 = 1
$\bar{v}_6 = \frac{\partial y}{\partial v_6}$	1

AutoDiff - **Reverse Mode**





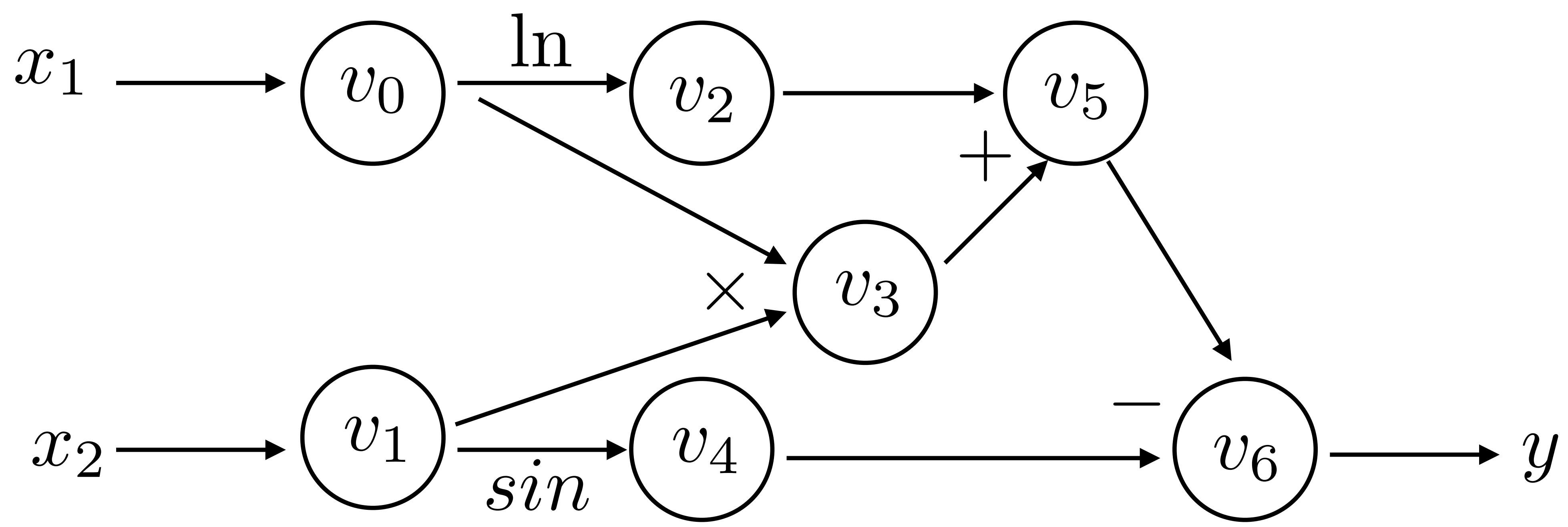
Forward Evaluation Trace:

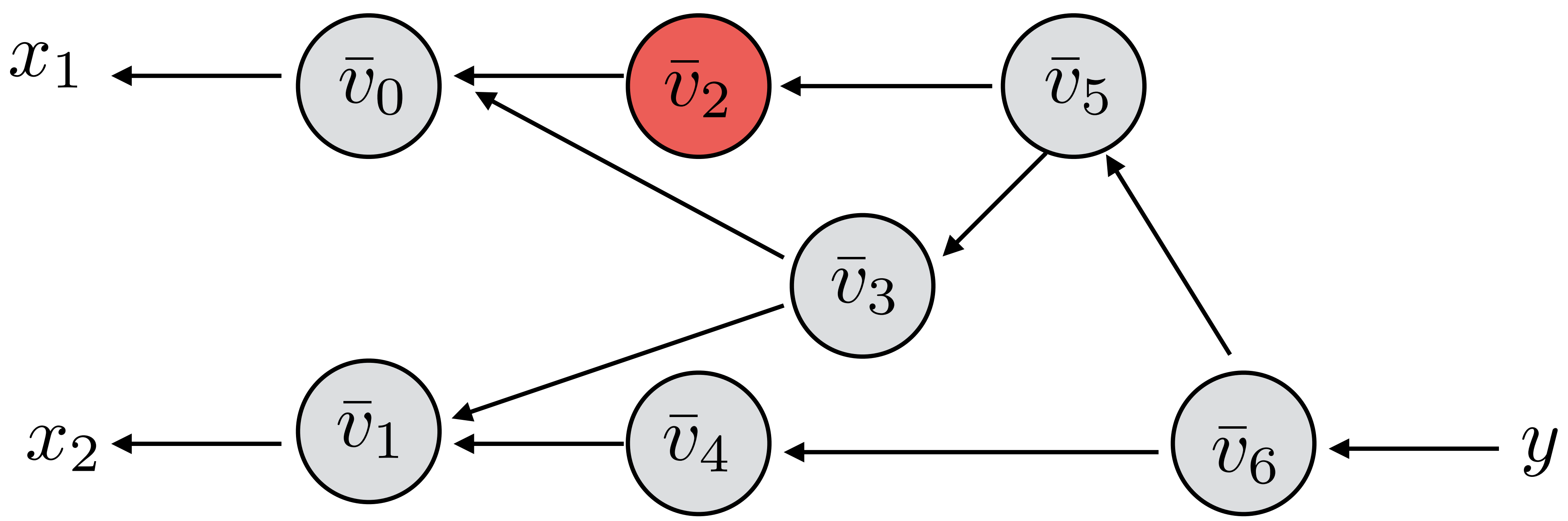
	$f(2,5)$
$v_0 = x_1$	2
$v_1 = x_2$	5
$v_2 = \ln(v_0)$	ln(2) = 0.693
$v_3 = v_0 \cdot v_1$	2 x 5 = 10
$v_4 = sin(v_1)$	sin(5) = 0.959
$\underline{v_5 = v_2 + v_3}$	0.693 + 10 = 10.693
$v_6 = v_5 - v_4$	10.693 + 0.959 = 11.652
$y = v_6$	11.652

Backwards Derivative Trace:

$\bar{v}_2 = \bar{v}_5 \dfrac{\partial v_5}{\partial v_2}$	
$\bar{v}_3 = \bar{v}_5 \dfrac{\partial v_5}{\partial v_3} = \bar{v}_5 \cdot (1)$	1x1 = 1
$\bar{v}_4 = \bar{v}_6 \dfrac{\partial v_6}{\partial v_4} = \bar{v}_6 \cdot (-1)$	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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Backwards Derivative Trace:

$\bar{v}_2 = \bar{v}_5 \dfrac{\partial v_5}{\partial v_2} = \bar{v}_5 \cdot (1)$	
$\bar{v}_3 = \bar{v}_5 \dfrac{\partial v_5}{\partial v_3} = \bar{v}_5 \cdot (1)$	1x1 = 1
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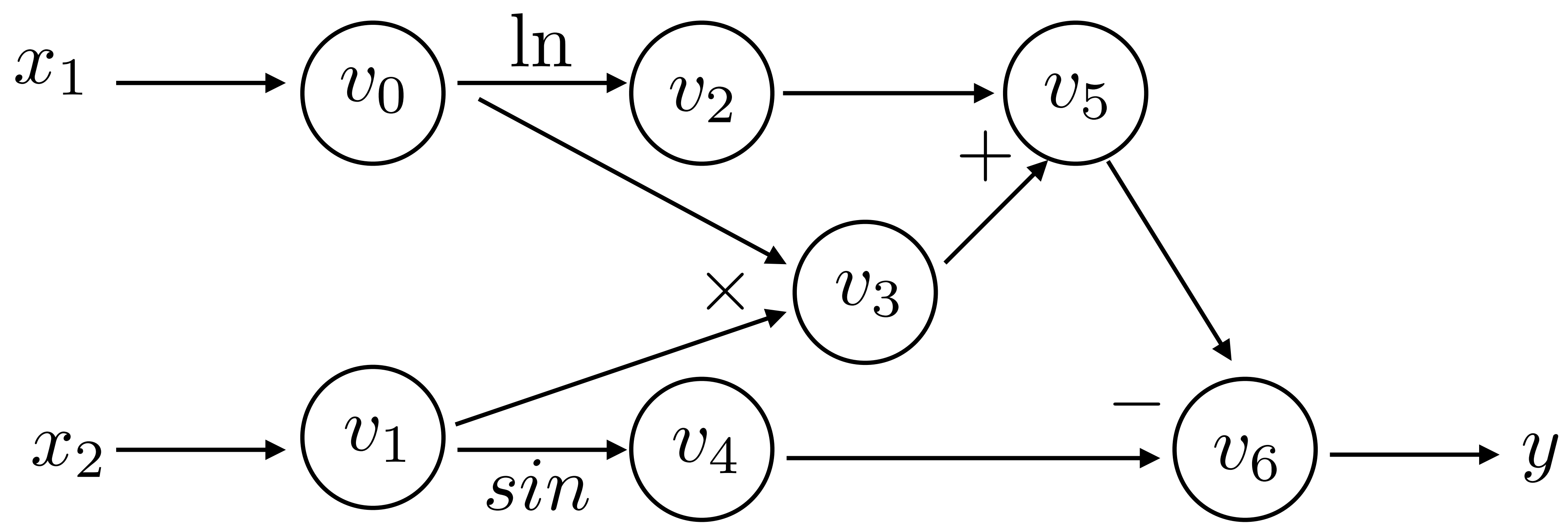
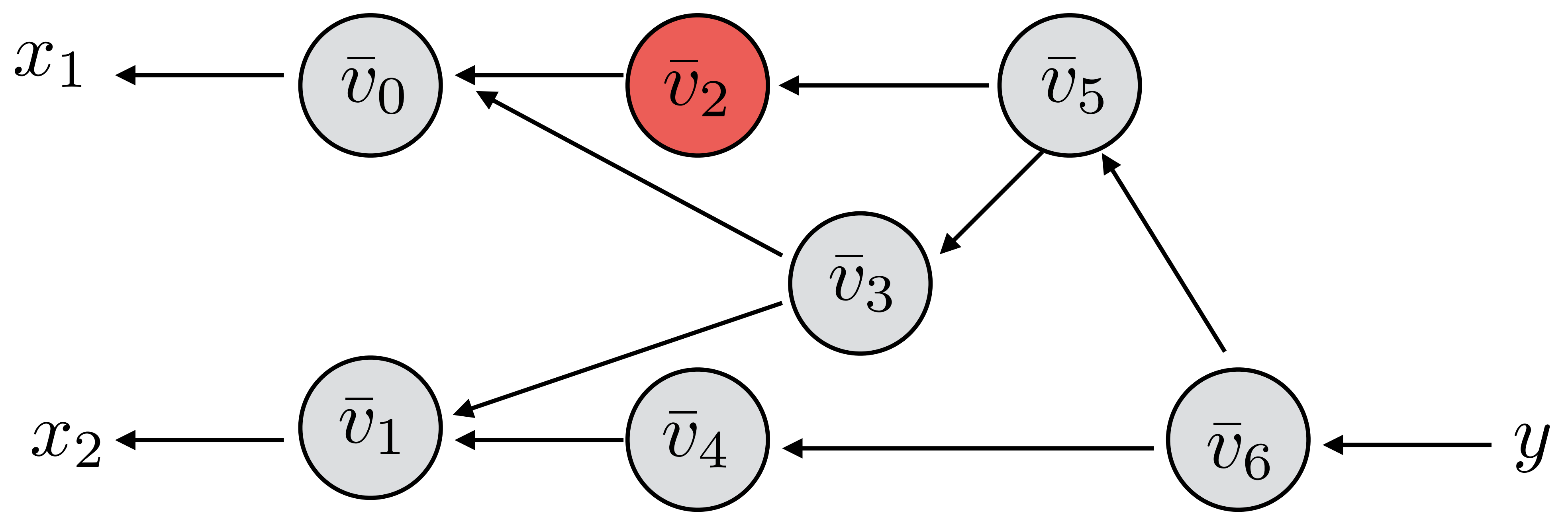
$\bar{v}_5 = \bar{v}_6 \dfrac{\partial v_6}{\partial v_5} = \bar{v}_6 \cdot 1$	1x1 = 1
$\bar{v}_6 = \dfrac{\partial y}{\partial v_6}$	1

AutoDiff - **Reverse Mode**





Forward Evaluation Trace:

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Backwards Derivative Trace:

$\bar{v}_2 = \bar{v}_5 \dfrac{\partial v_5}{\partial v_2} = \bar{v}_5 \cdot (1)$	1x1 = 1
$\bar{v}_3 = \bar{v}_5 \dfrac{\partial v_5}{\partial v_3} = \bar{v}_5 \cdot (1)$	1x1 = 1
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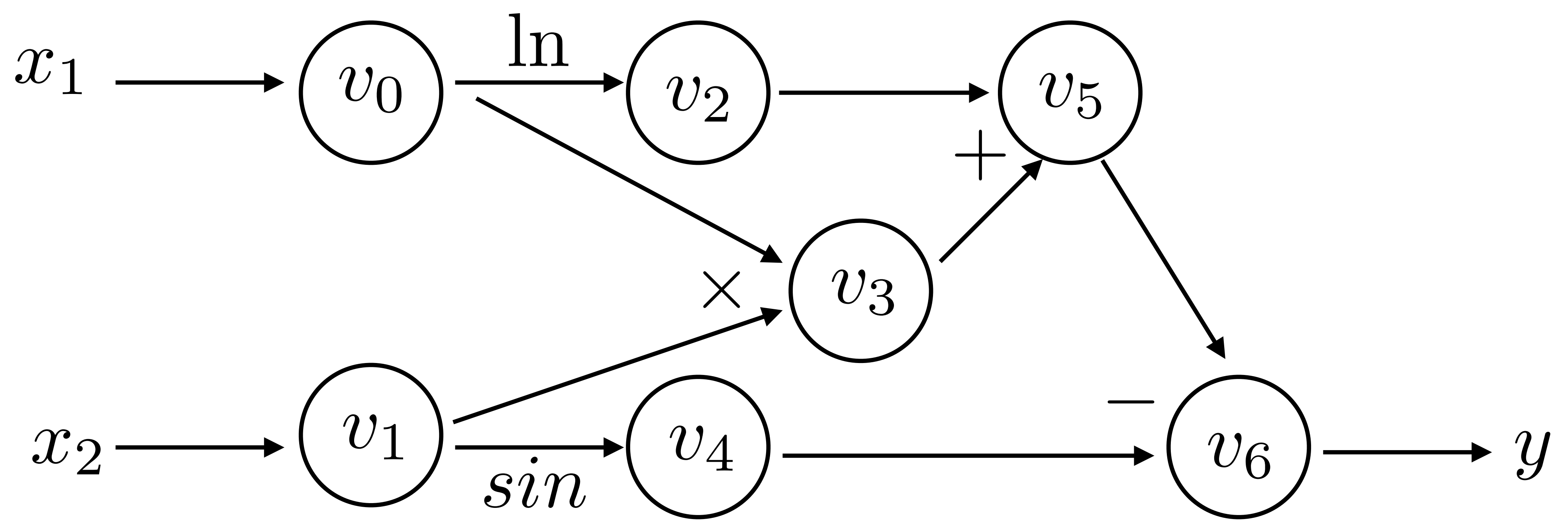
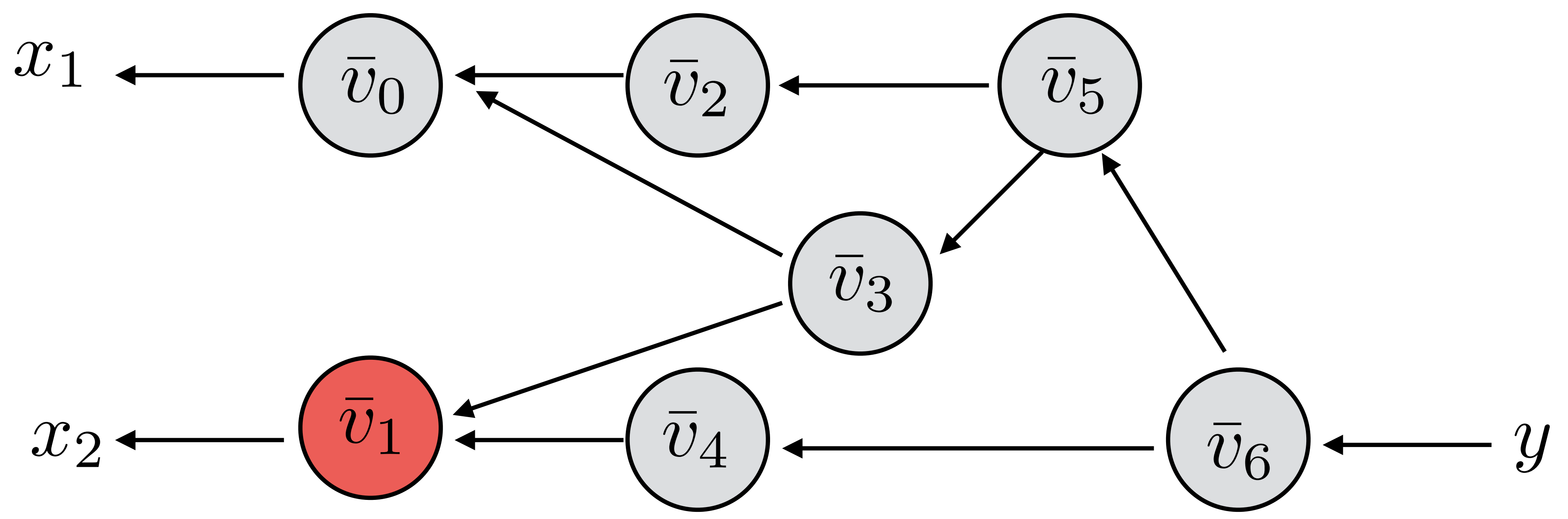
$\bar{v}_5 = \bar{v}_6 \dfrac{\partial v_6}{\partial v_5} = \bar{v}_6 \cdot 1$	1x1 = 1
$\bar{v}_6 = \dfrac{\partial y}{\partial v_6}$	1

AutoDiff - **Reverse Mode**





Backwards Derivative Trace:

$\bar{v}_1$	
$\bar{v}_2 = \bar{v}_5 \frac{\partial v_5}{\partial v_2} = \bar{v}_5 \cdot (1)$	1x1 = 1
$\bar{v}_3 = \bar{v}_5 \frac{\partial v_5}{\partial v_3} = \bar{v}_5 \cdot (1)$	1x1 = 1
$\bar{v}_4 = \bar{v}_6 \frac{\partial v_6}{\partial v_4} = \bar{v}_6 \cdot (-1)$	1x-1 = -1
$\bar{v}_5 = \bar{v}_6 \frac{\partial v_6}{\partial v_5} = \bar{v}_6 \cdot 1$	1x1 = 1
$\bar{v}_6 = \frac{\partial y}{\partial v_6}$	1

Forward Evaluation Trace:

	$f(2,5)$
$v_0 = x_1$	2
$v_1 = x_2$	5
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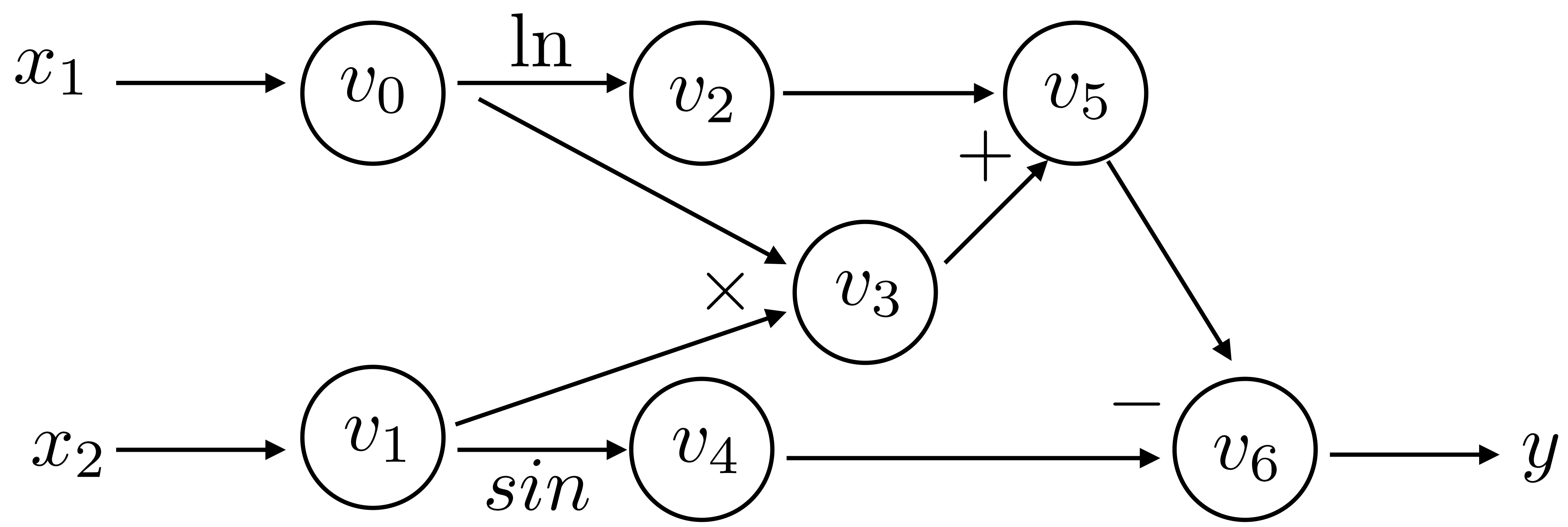
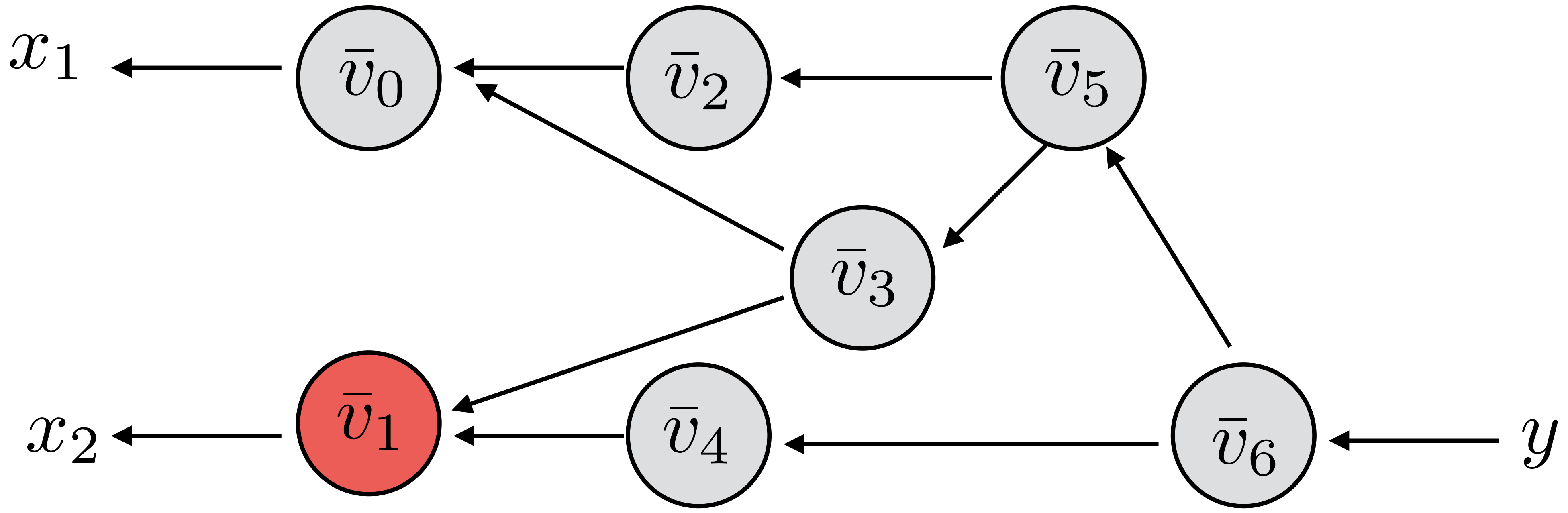
AutoDiff - **Reverse Mode**





Forward Evaluation Trace:

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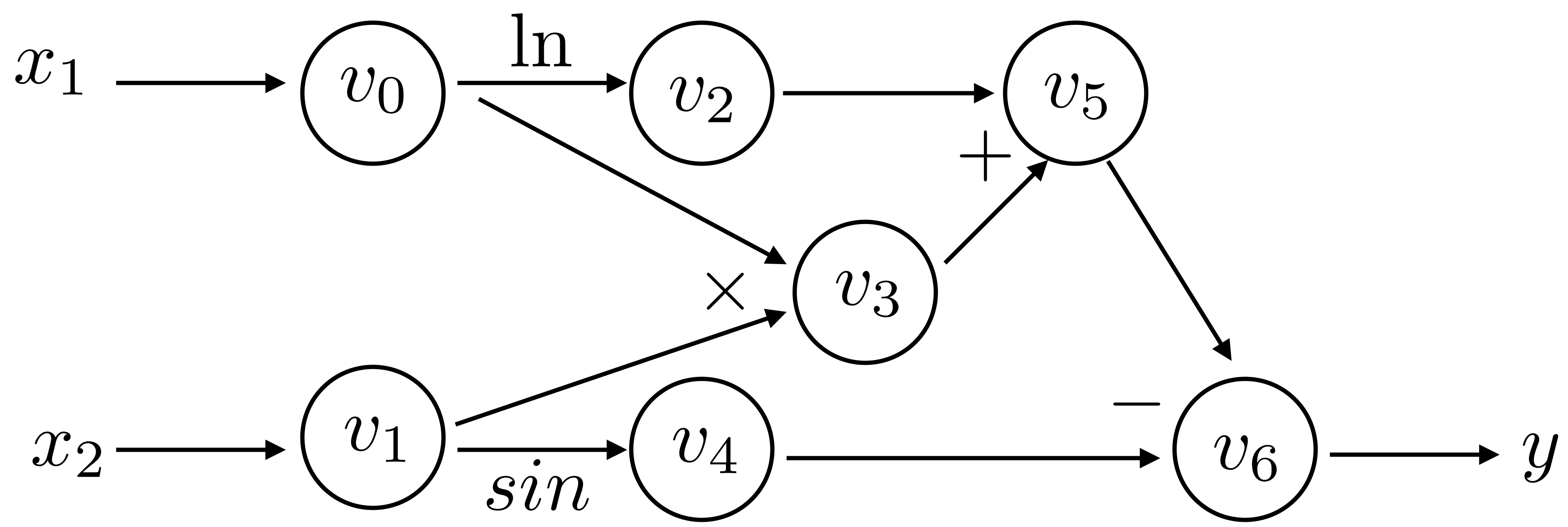
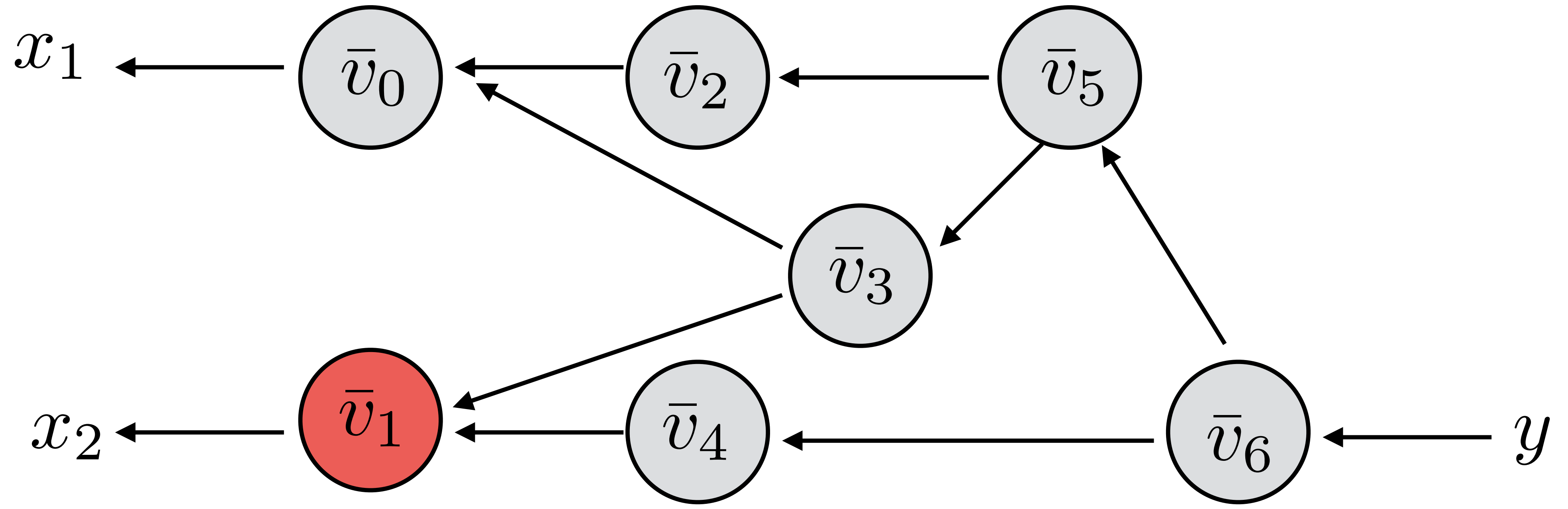
$v_5 = v_2 + v_3$	0.693 + 10 = 10.693
$v_6 = v_5 - v_4$	10.693 + 0.959 = 11.652
$y = v_6$	11.652

Backwards Derivative Trace:

$\bar{v}_1 = \bar{v}_3 \dfrac{\partial v_3}{\partial v_1} + \bar{v}_4 \dfrac{\partial v_4}{\partial v_1}$	
$\bar{v}_2 = \bar{v}_5 \dfrac{\partial v_5}{\partial v_2} = \bar{v}_5 \cdot (1)$	1x1 = 1
$\bar{v}_3 = \bar{v}_5 \dfrac{\partial v_5}{\partial v_3} = \bar{v}_5 \cdot (1)$	1x1 = 1
$\bar{v}_4 = \bar{v}_6 \dfrac{\partial v_6}{\partial v_4} = \bar{v}_6 \cdot (-1)$	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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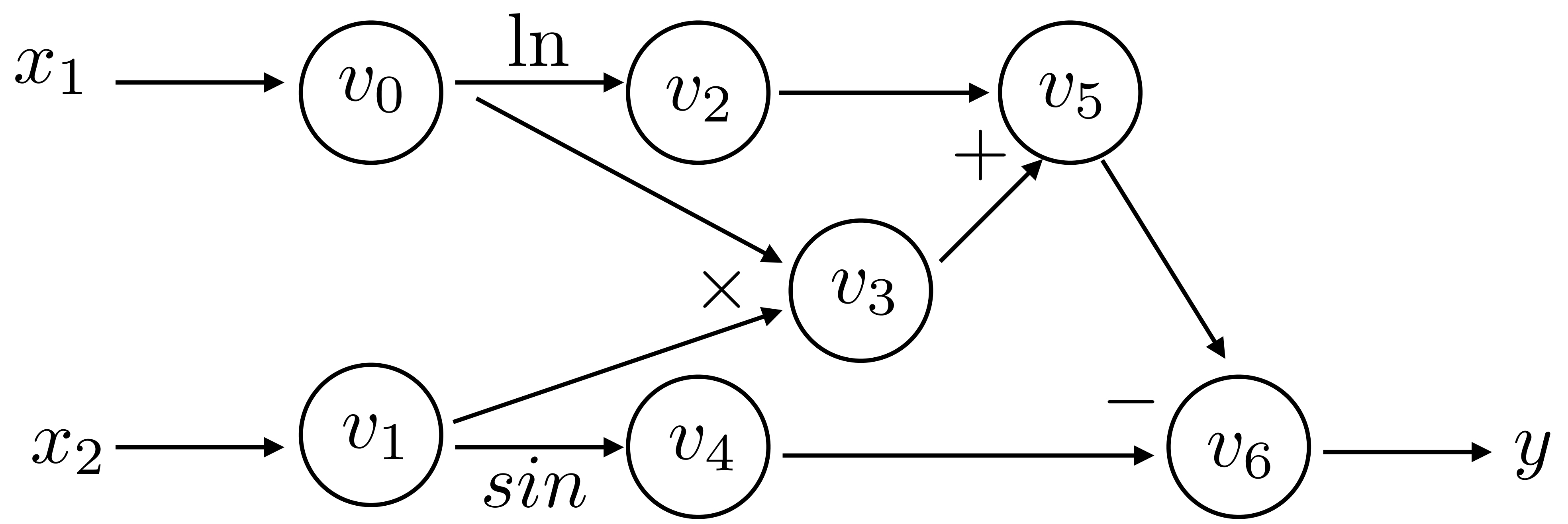
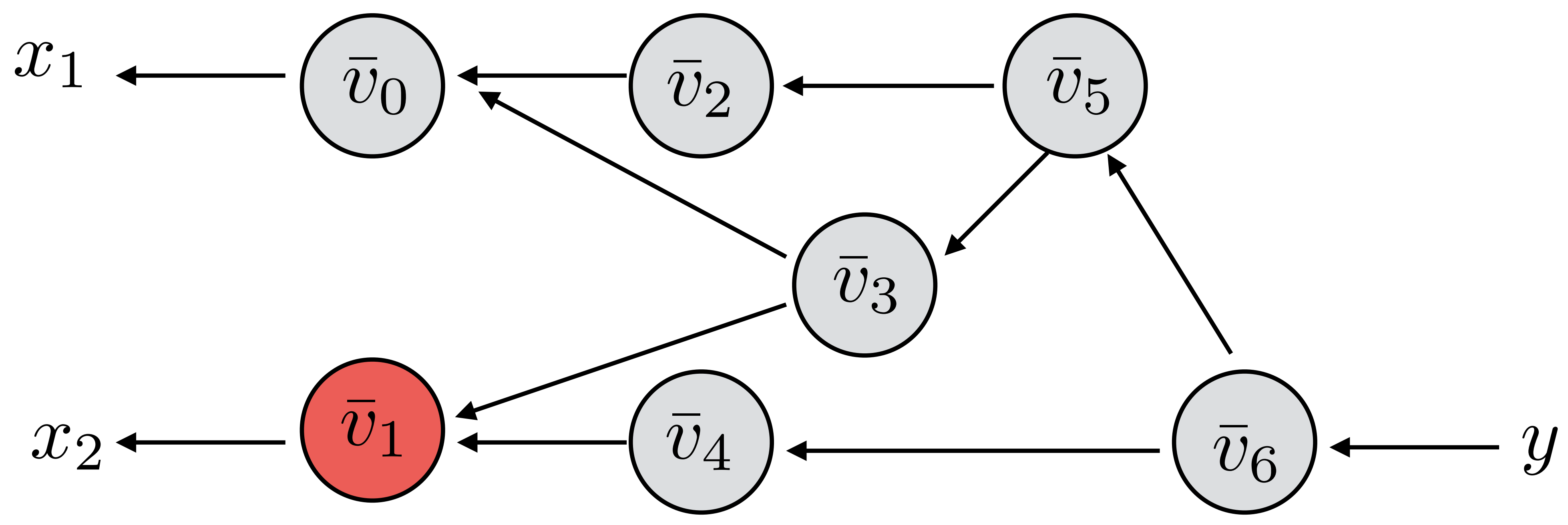
$v_6 = v_5 - v_4$	10.693 + 0.959 = 11.652
$y = v_6$	11.652

Backwards Derivative Trace:

$\bar{v}_1 = \bar{v}_3 \dfrac{\partial v_3}{\partial v_1} + \bar{v}_4 \dfrac{\partial v_4}{\partial v_1}$	
$\bar{v}_2 = \bar{v}_5 \dfrac{\partial v_5}{\partial v_2} = \bar{v}_5 \cdot (1)$	1x1 = 1
$\bar{v}_3 = \bar{v}_5 \dfrac{\partial v_5}{\partial v_3} = \bar{v}_5 \cdot (1)$	1x1 = 1
$\bar{v}_4 = \bar{v}_6 \dfrac{\partial v_6}{\partial v_4} = \bar{v}_6 \cdot (-1)$	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**





Backwards Derivative Trace:

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$\bar{v}_2 = \bar{v}_5 \frac{\partial v_5}{\partial v_2} = \bar{v}_5 \cdot (1)$	1x1 = 1
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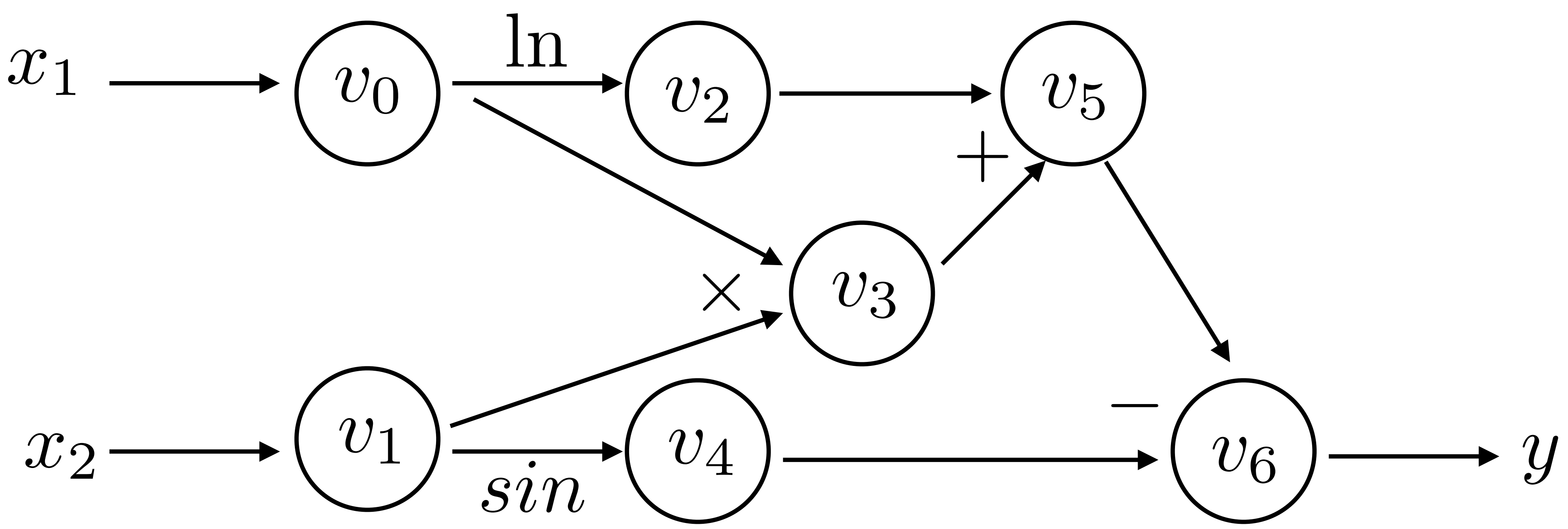
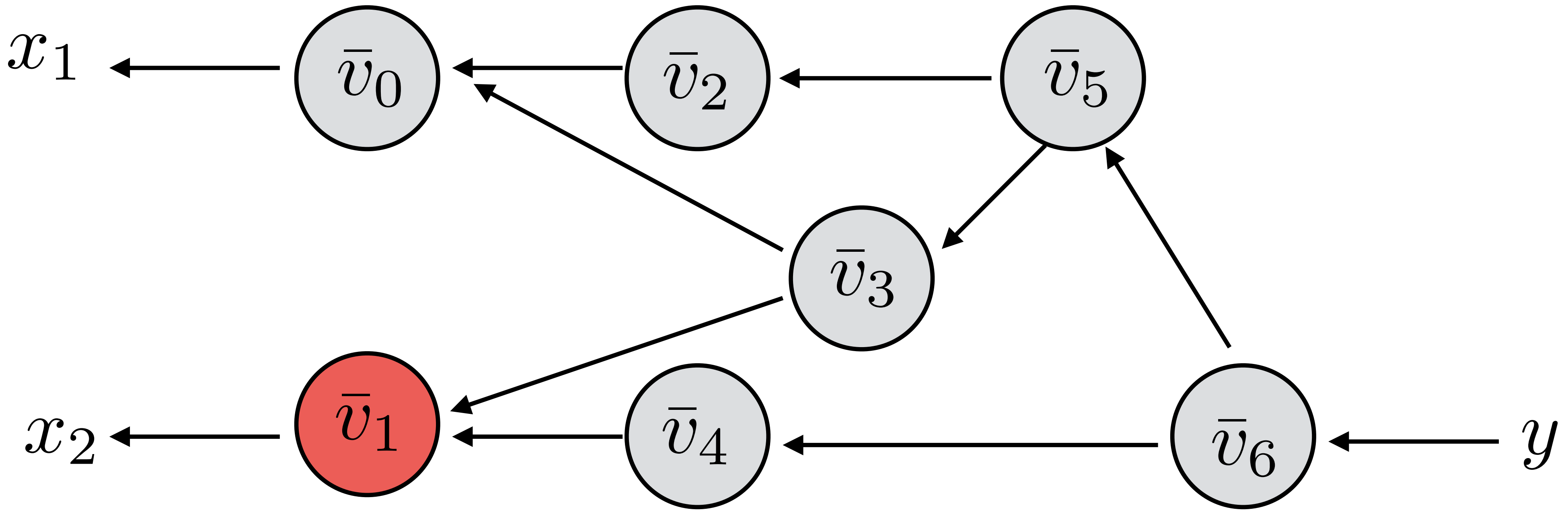
$\bar{v}_5 = \bar{v}_6 \frac{\partial v_6}{\partial v_5} = \bar{v}_6 \cdot 1$	1x1 = 1
$\bar{v}_6 = \frac{\partial y}{\partial v_6}$	1

AutoDiff - **Reverse Mode**





Forward Evaluation Trace:

	$f(2,5)$
$v_0 = x_1$	2
$v_1 = x_2$	5
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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
$\bar{v}_2 = \bar{v}_5 \frac{\partial v_5}{\partial v_2} = \bar{v}_5 \cdot (1)$	1x1 = 1
$\bar{v}_3 = \bar{v}_5 \frac{\partial v_5}{\partial v_3} = \bar{v}_5 \cdot (1)$	1x1 = 1
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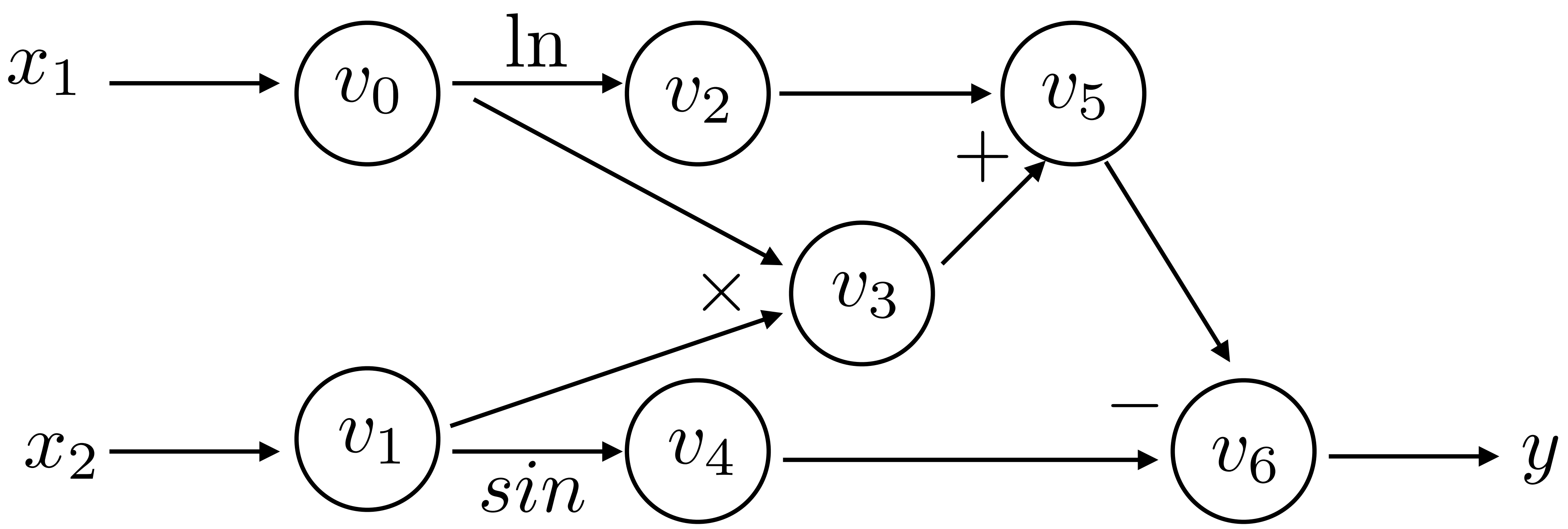
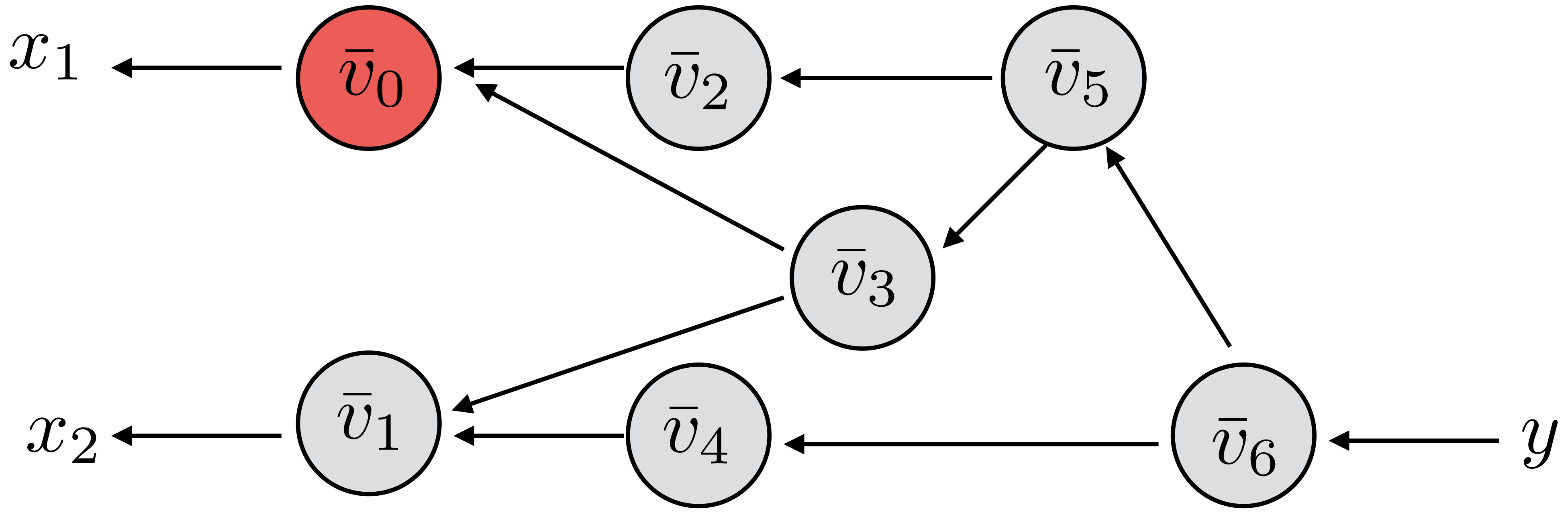
$\bar{v}_5 = \bar{v}_6 \frac{\partial v_6}{\partial v_5} = \bar{v}_6 \cdot 1$	1x1 = 1
$\bar{v}_6 = \frac{\partial y}{\partial v_6}$	1

AutoDiff - **Reverse Mode**





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	$f(2,5)$
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$y = v_6$	11.652

Backwards Derivative Trace:

$\bar{v}_0 = \bar{v}_3 \frac{\partial v_3}{\partial v_0} + \bar{v}_2 \frac{\partial v_2}{\partial v_0} = \bar{v}_3 v_1 + \bar{v}_2 \frac{1}{v_0}$	5.5
$\bar{v}_1 = \bar{v}_3 \frac{\partial v_3}{\partial v_1} + \bar{v}_4 \frac{\partial v_4}{\partial v_1} = \bar{v}_3 v_0 + \bar{v}_4 cos(v_1)$	1.716
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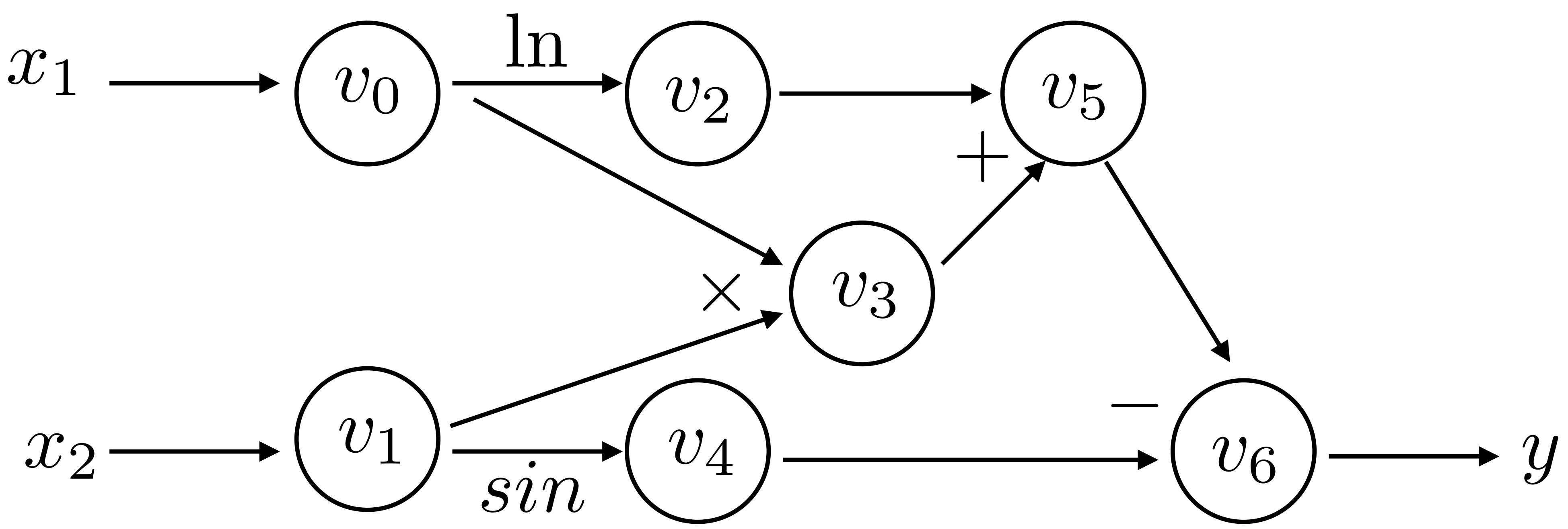
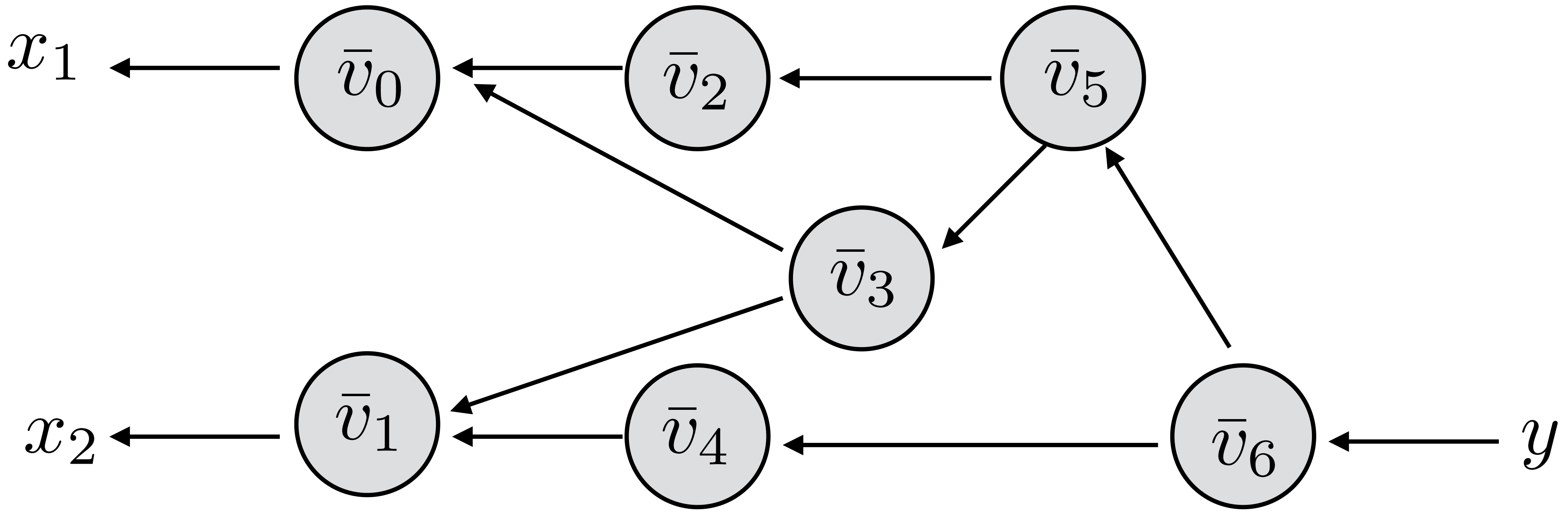
$\bar{v}_6 = \frac{\partial y}{\partial v_6}$	1

AutoDiff - **Reverse Mode**





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$\bar{v}_0 = \bar{v}_3 \frac{\partial v_3}{\partial v_0} + \bar{v}_2 \frac{\partial v_2}{\partial v_0} = \bar{v}_3 v_1 + \bar{v}_2 \frac{1}{v_0}$	**5.5**
$\bar{v}_1 = \bar{v}_3 \frac{\partial v_3}{\partial v_1} + \bar{v}_4 \frac{\partial v_4}{\partial v_1} = \bar{v}_3 v_0 + \bar{v}_4 cos(v_1)$	**1.716**
$\bar{v}_2 = \bar{v}_5 \frac{\partial v_5}{\partial v_2} = \bar{v}_5 \cdot (1)$	1x1 = 1
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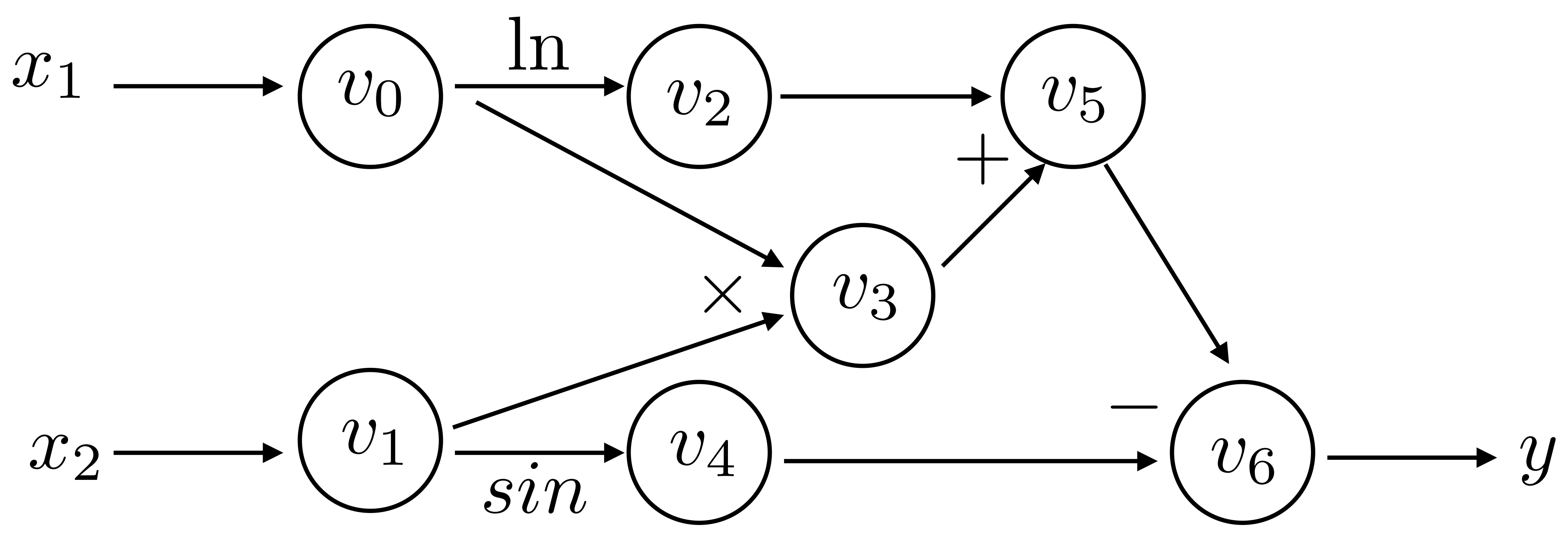
$\bar{v}_4 = \bar{v}_6 \frac{\partial v_6}{\partial v_4} = \bar{v}_6 \cdot (-1)$	1x-1 = -1
$\bar{v}_5 = \bar{v}_6 \frac{\partial v_6}{\partial v_5} = \bar{v}_6 \cdot 1$	1x1 = 1
$\bar{v}_6 = \frac{\partial y}{\partial v_6}$	1

Automatic Differentiation (AutoDiff)

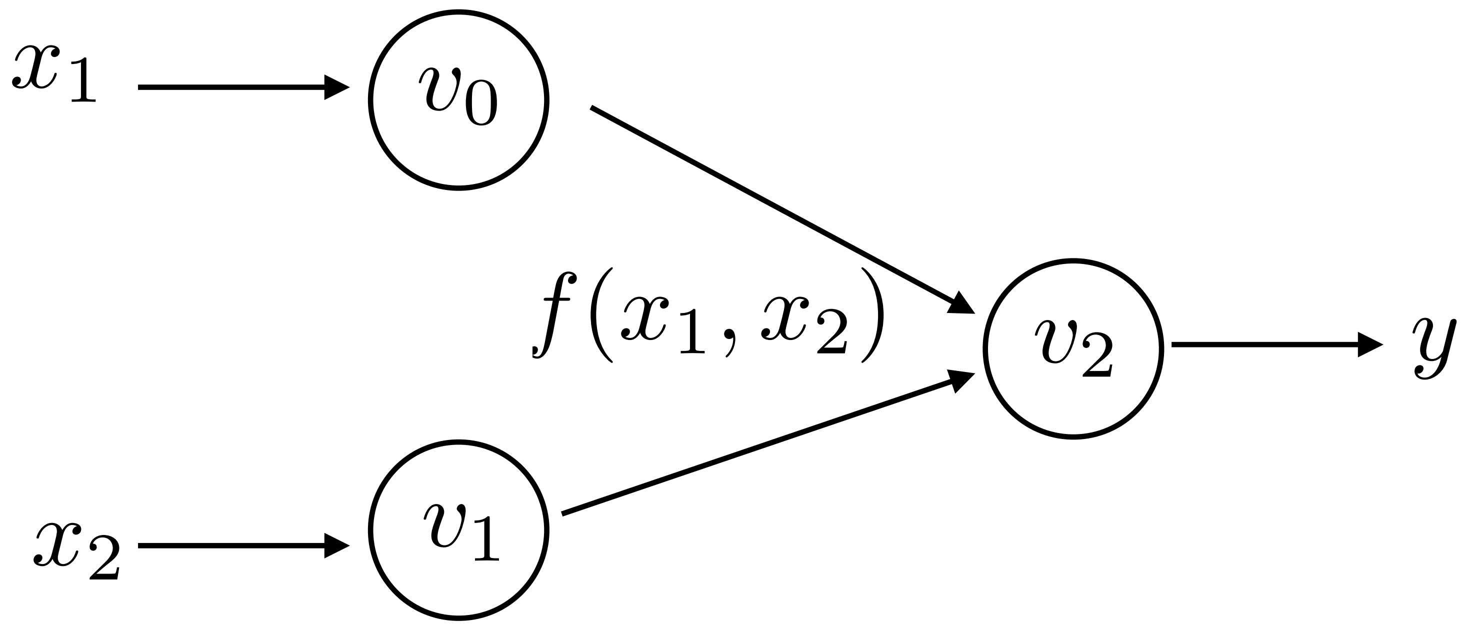
$$y = f(x_1, x_2) = \ln(x_1) + x_1 x_2 - sin(x_2)$$

AutoDiff can be done at various **granularities**

Elementary function granularity:

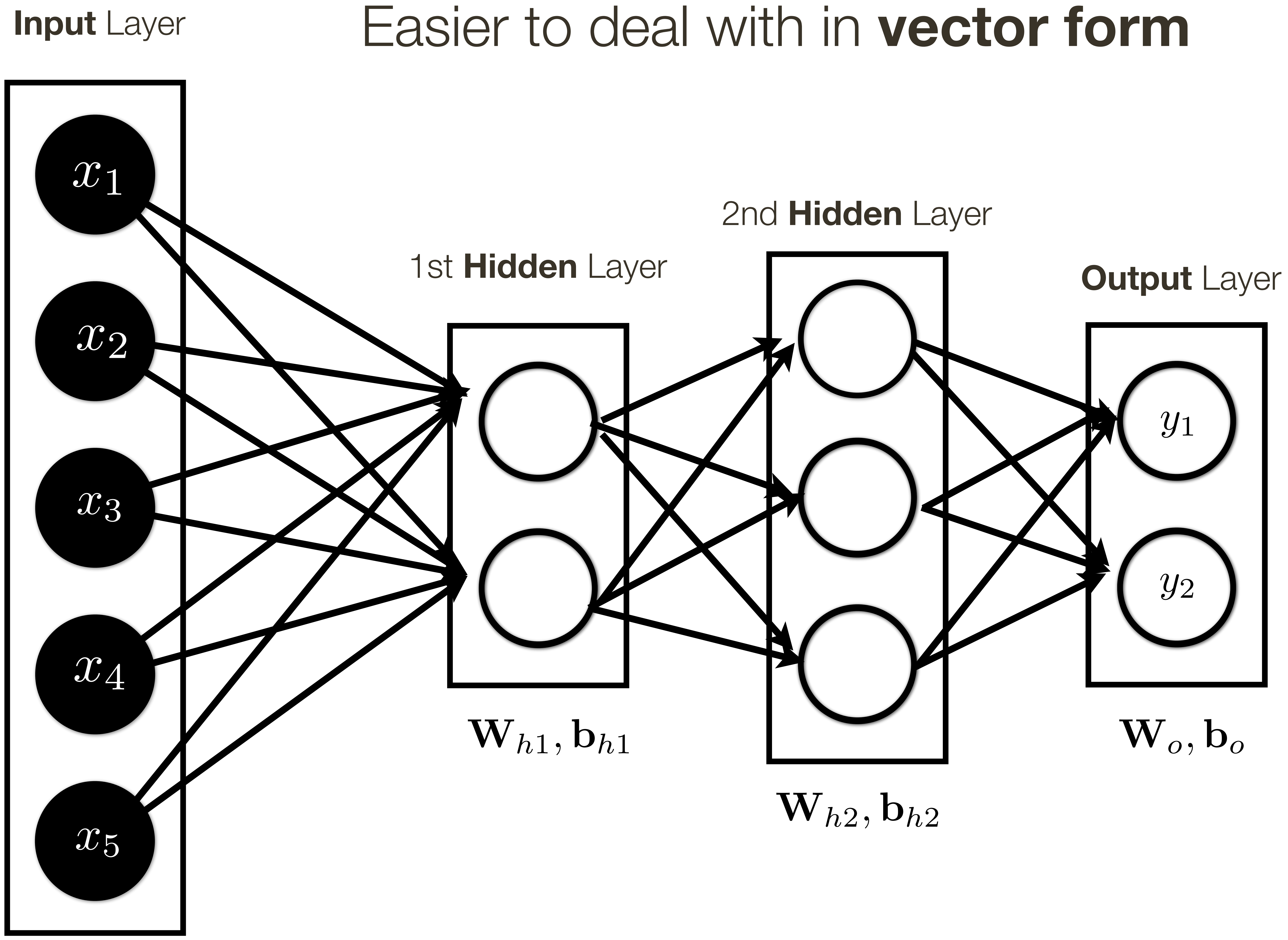


Complex function granularity:



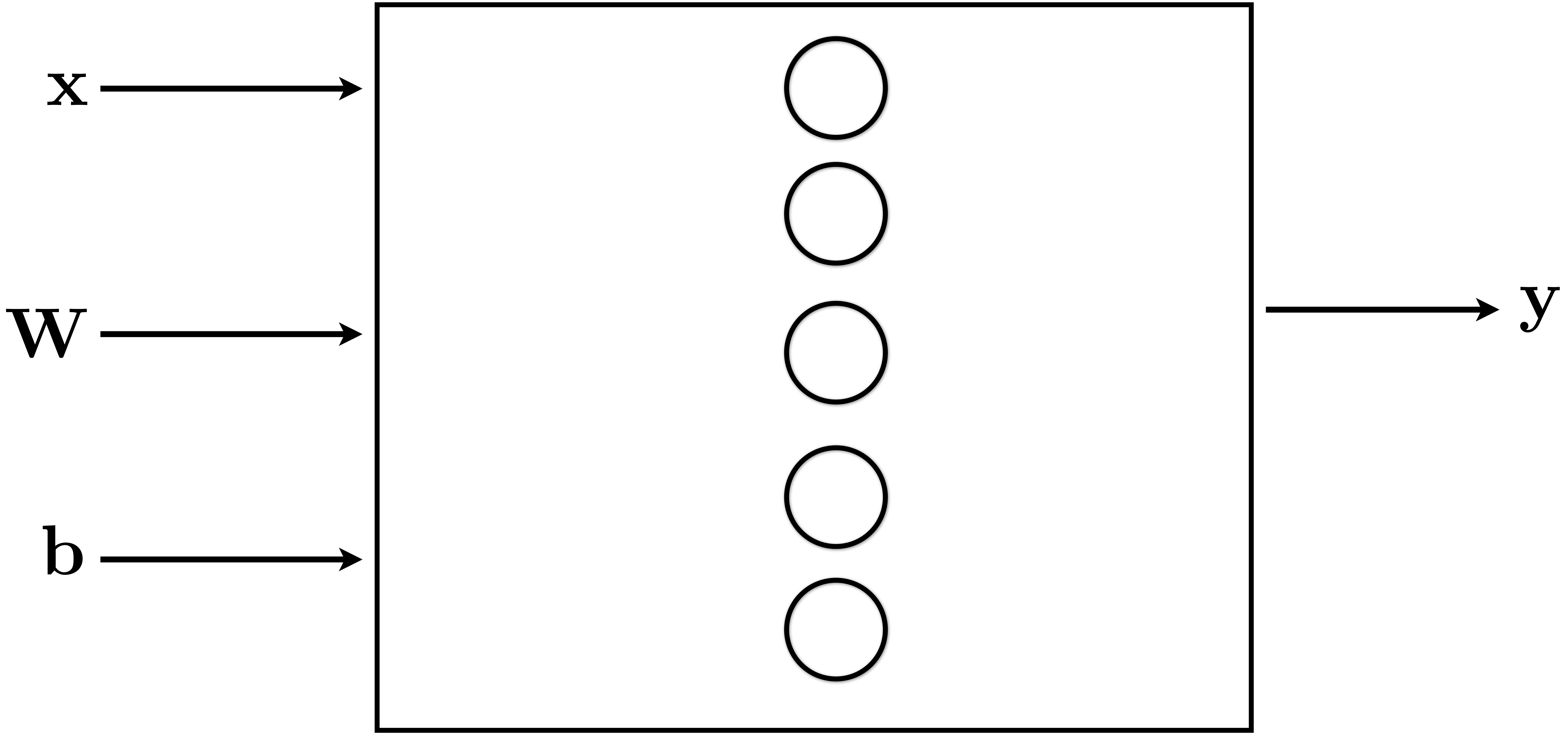
Backpropagation Practical Issues

Easier to deal with in **vector form**



Backpropagation Practical Issues

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

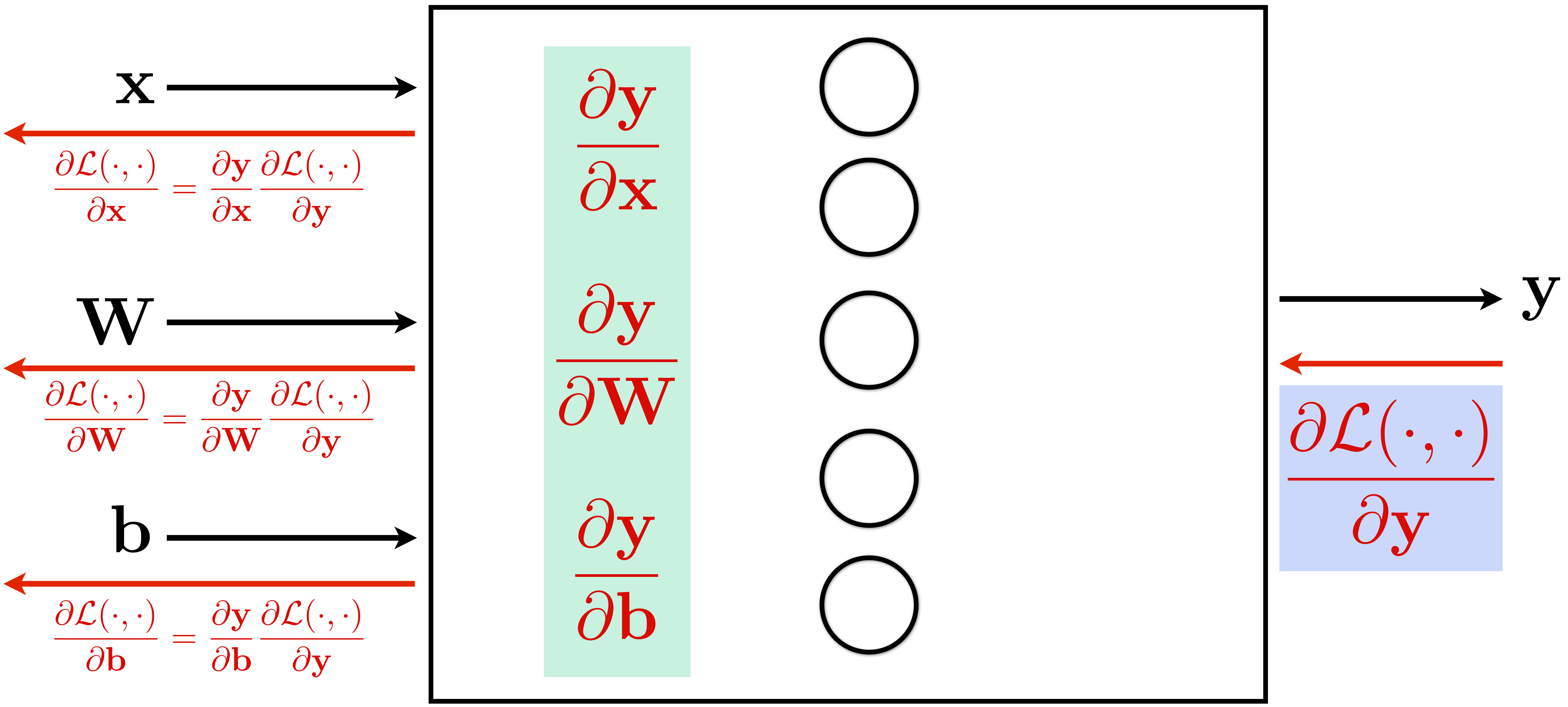


Backpropagation Practical Issues

"**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:

$$\mathbf{x} \longrightarrow \boxed{\textbf{sigmoid}} \longrightarrow \mathbf{y}$$

Jacobian of Sigmoid layer

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

Element-wise sigmoid layer:

$$\mathbf{x} \longrightarrow \boxed{\textbf{sigmoid}} \longrightarrow \mathbf{y}$$

What is the dimension of **Jacobian**?

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?

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