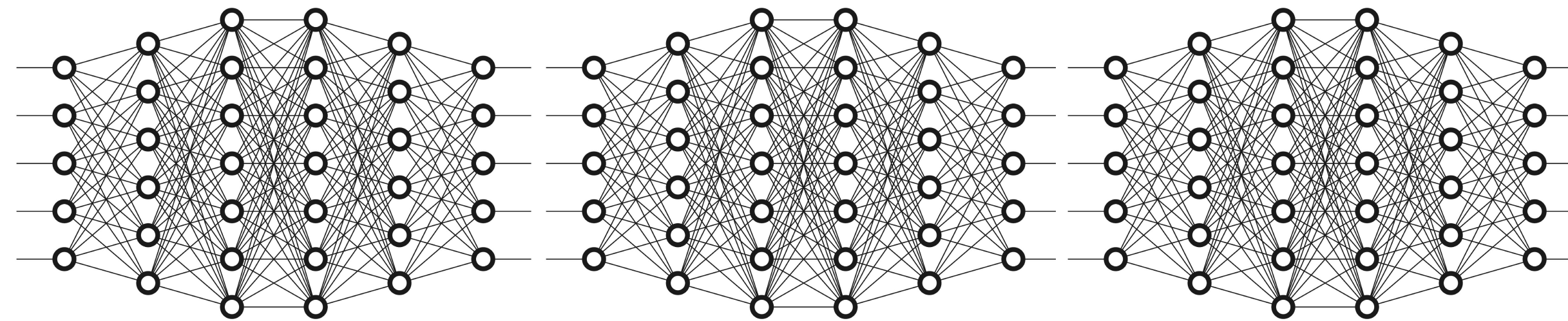




CPSC 425: Computer Vision



Lecture 20: Neural Networks Intro

Menu for Today

Topics:

- Introduction to neural networks

Readings:

- **Today's** Lecture: Forsyth & Ponce (2nd ed.) 16.1.3, 16.1.4, 16.1.9
- **Next** Lecture: Forsyth & Ponce (2nd ed.) 17.1–17.2

Reminders:

- **Assignment 2 & 3** graded, grades posted (let us know if there are issues)
- **Assignment 5** is due on **today**
- **Assignment 6** will be out **tonight** or **tomorrow**

Assignment 5

Computing the error for optical flow:

Assuming you are computing optical flow of Image 1 \rightarrow Image 2
(note, this is not the same as Image 2 \rightarrow Image 1)

1. Warp the Image 1 using estimated optical flow.
2. Subtract warped Image 1 from Image 2 pixel-by-pixel, then compute L2 norm of the difference per pixel. Result is a $W \times H$ image of L2 norms.
3. Average the L2 norms over all pixels.

We will **not** grade based on the error itself ...

Warning:

Our intro to **Neural Networks** will be light weight ...

... if you want to know more, take my **CPSC 532S** next year or **CPEN 455**

Recall: Linear Classifier

Defines a score function:

$$f(\mathbf{x}_i, \mathbf{W}, \mathbf{b}) = \mathbf{W}\mathbf{x}_i + \mathbf{b}$$

image features

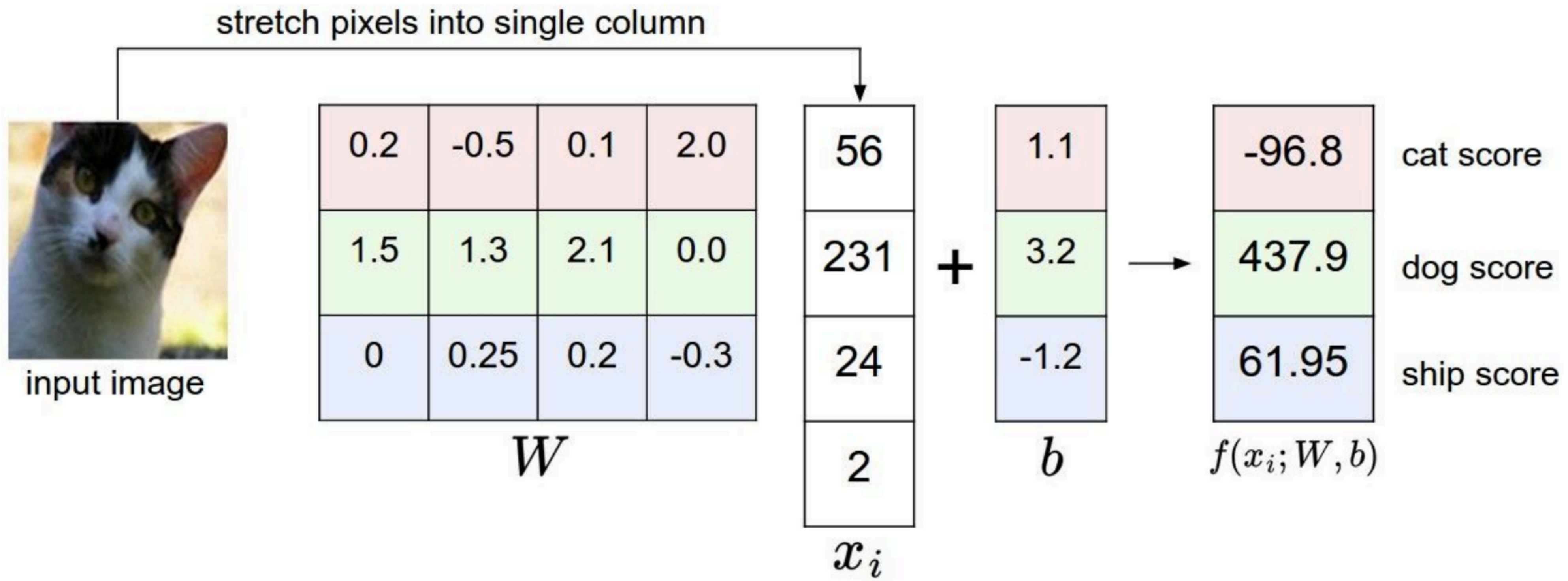
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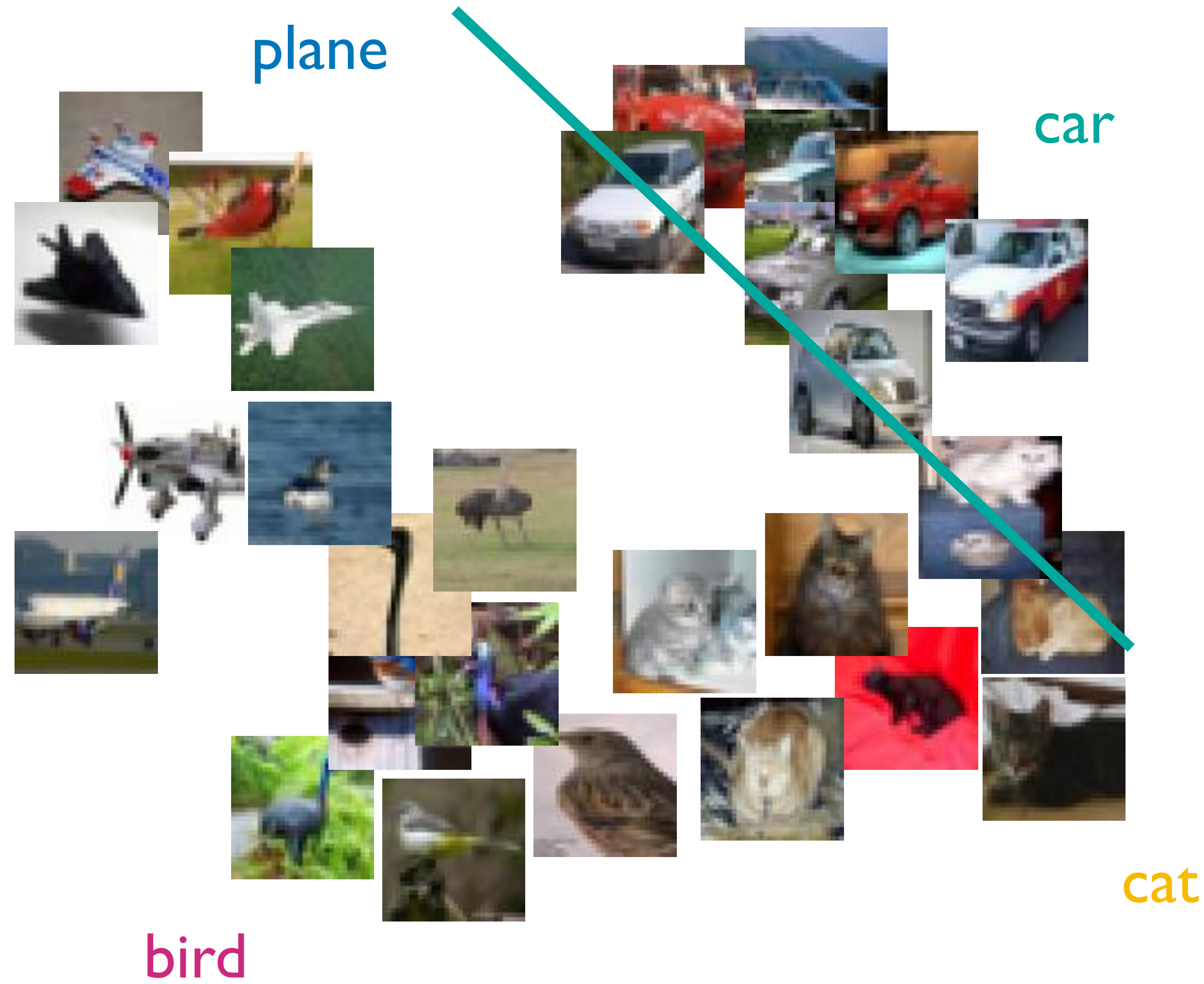
Example with an image with 4 pixels, and 3 classes (cat/dog/ship)



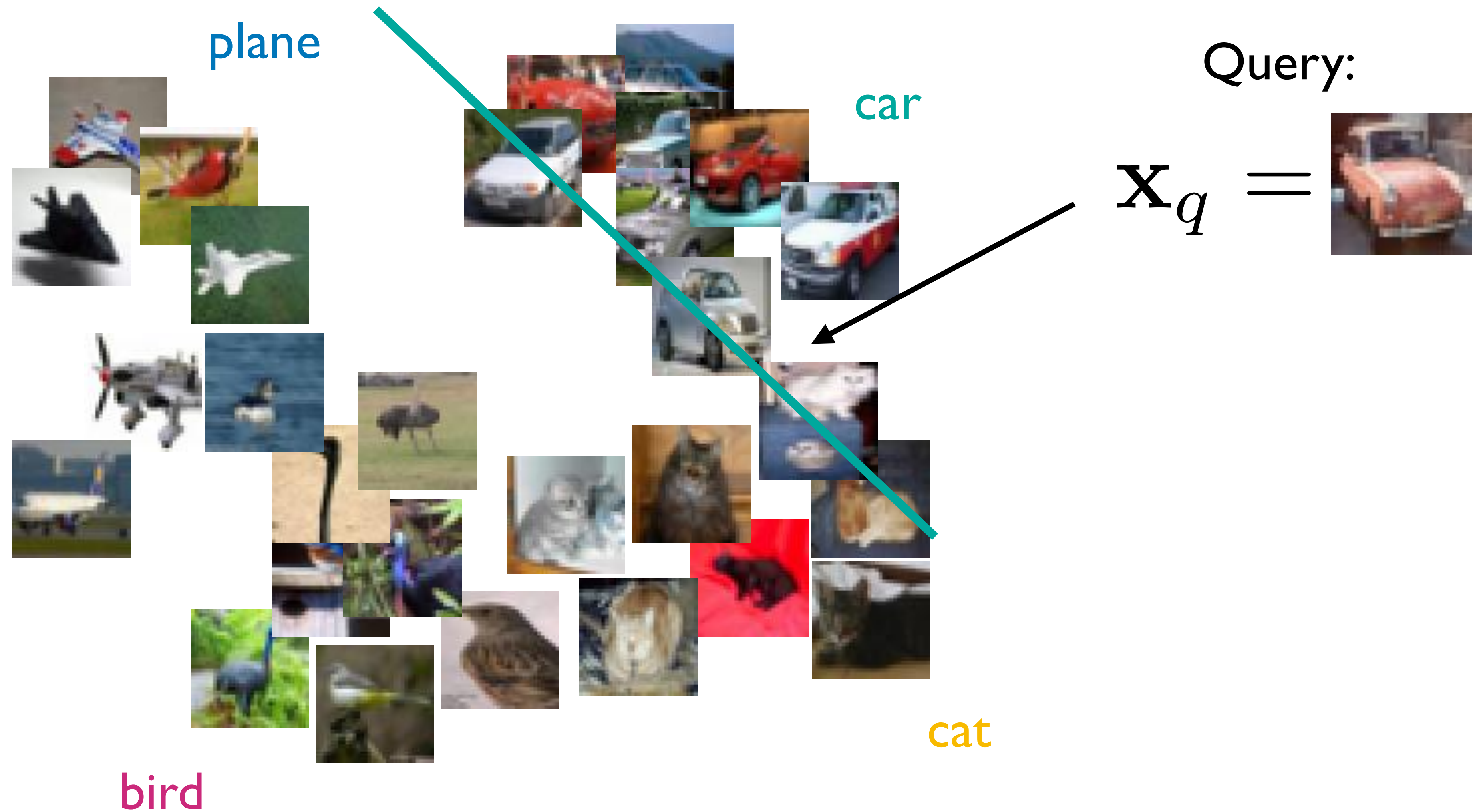
1-vs-All Linear SVM



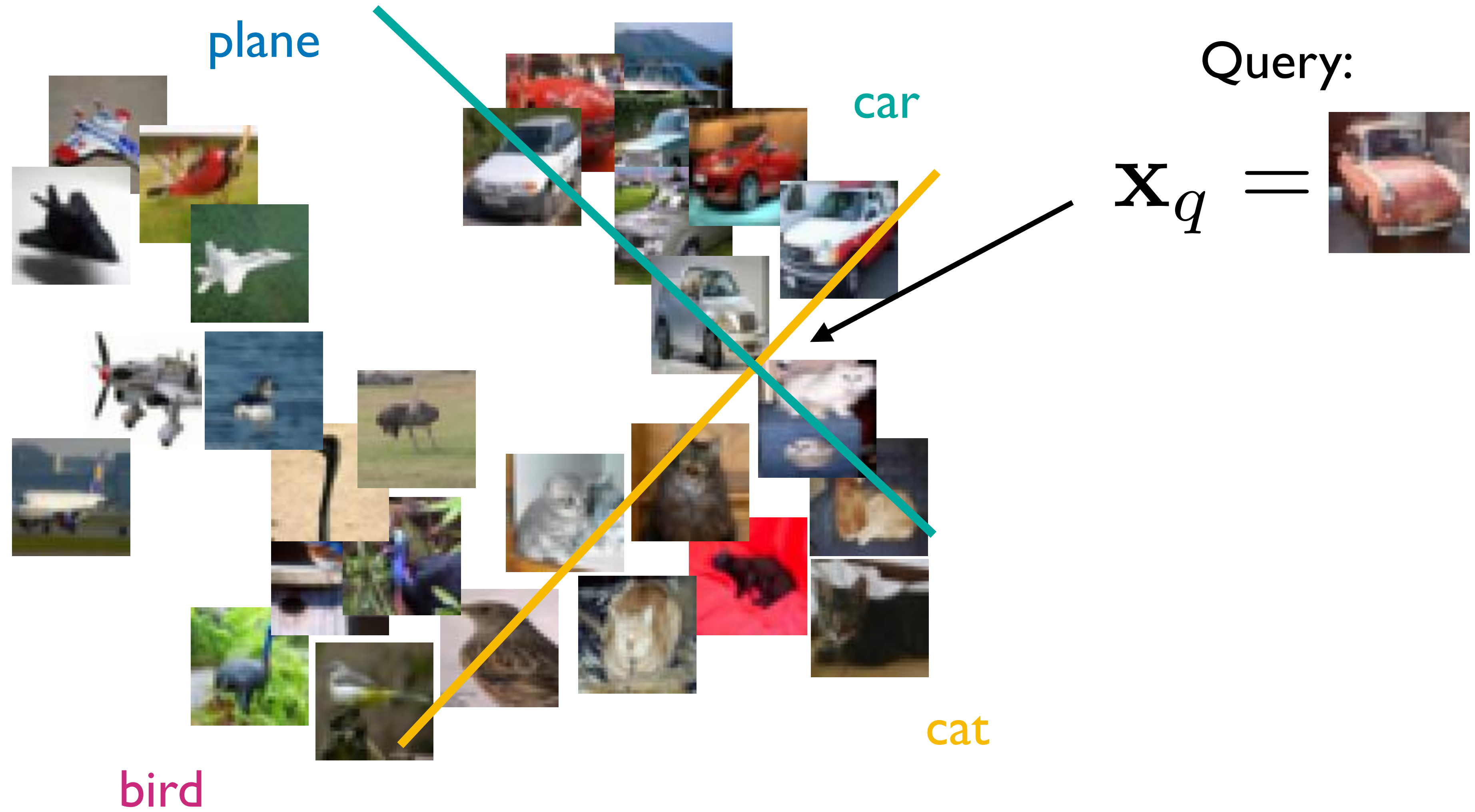
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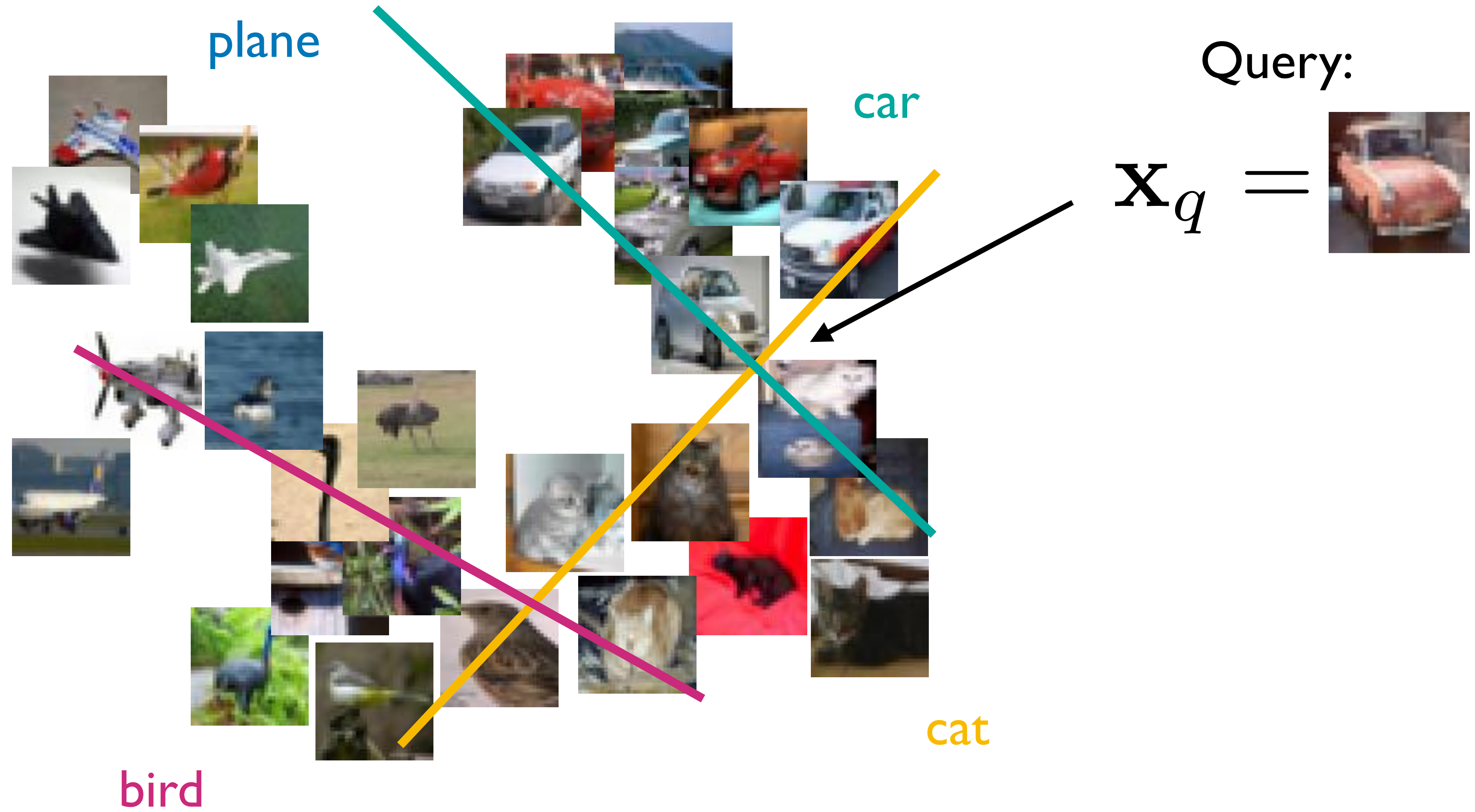
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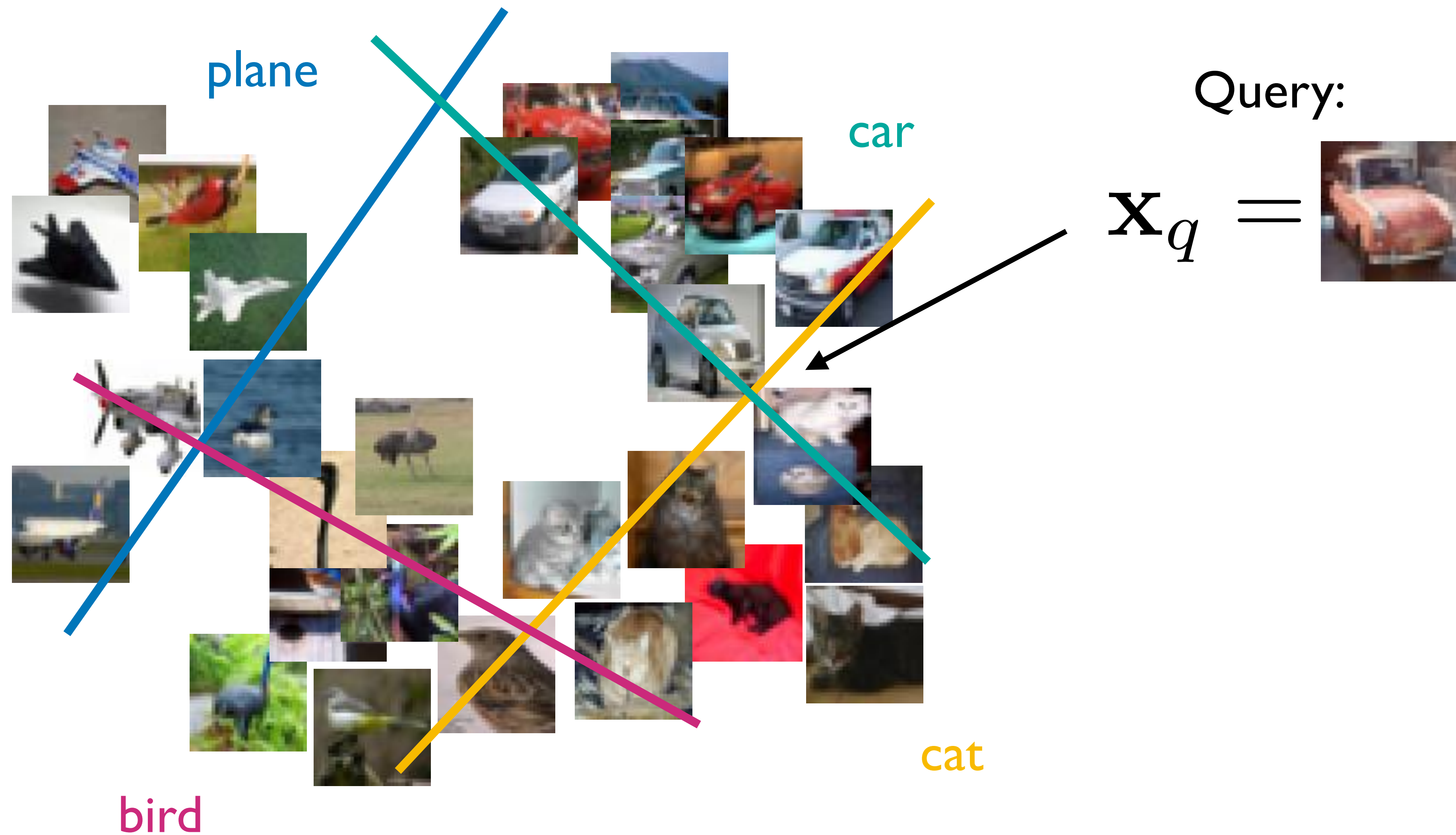
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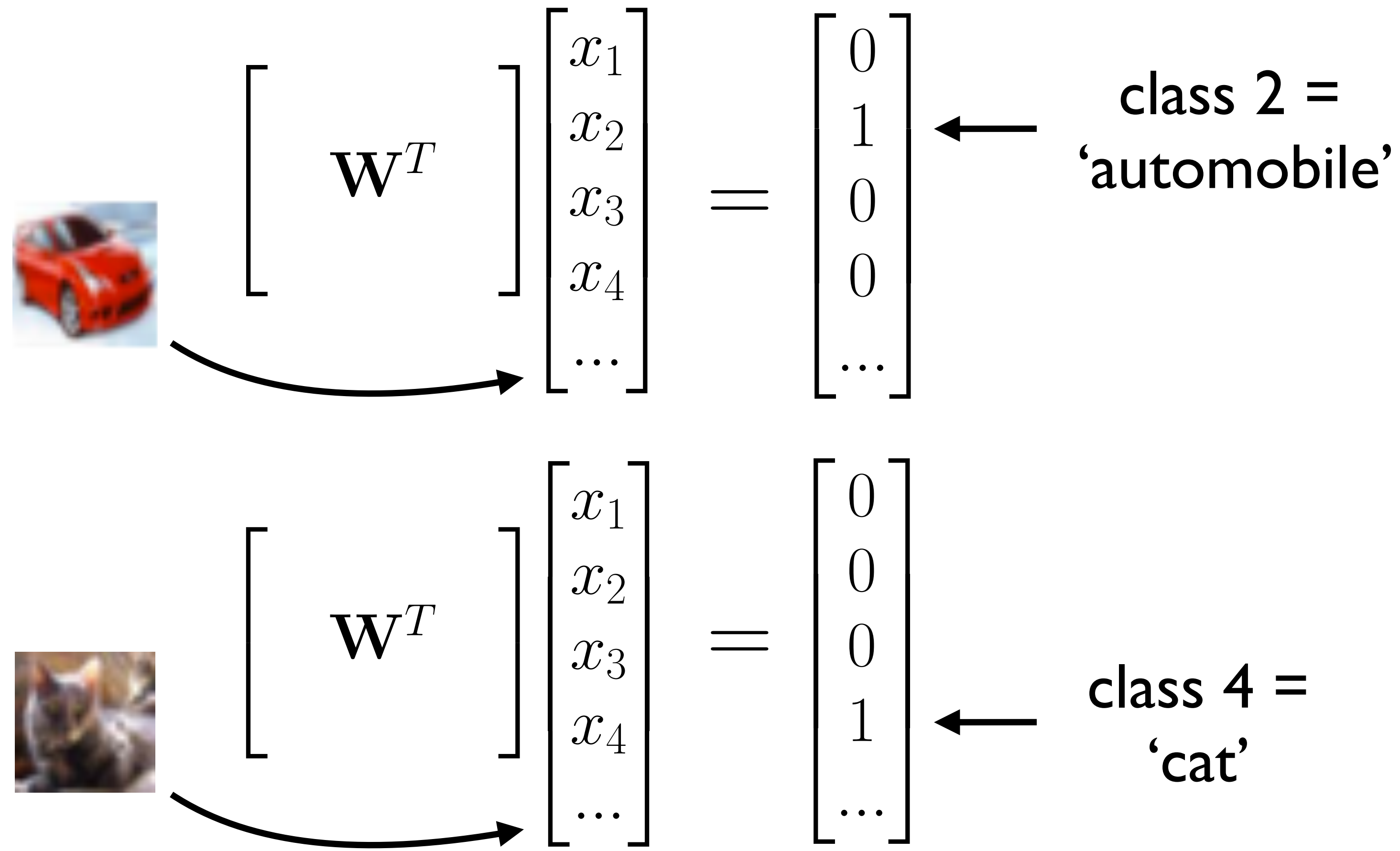


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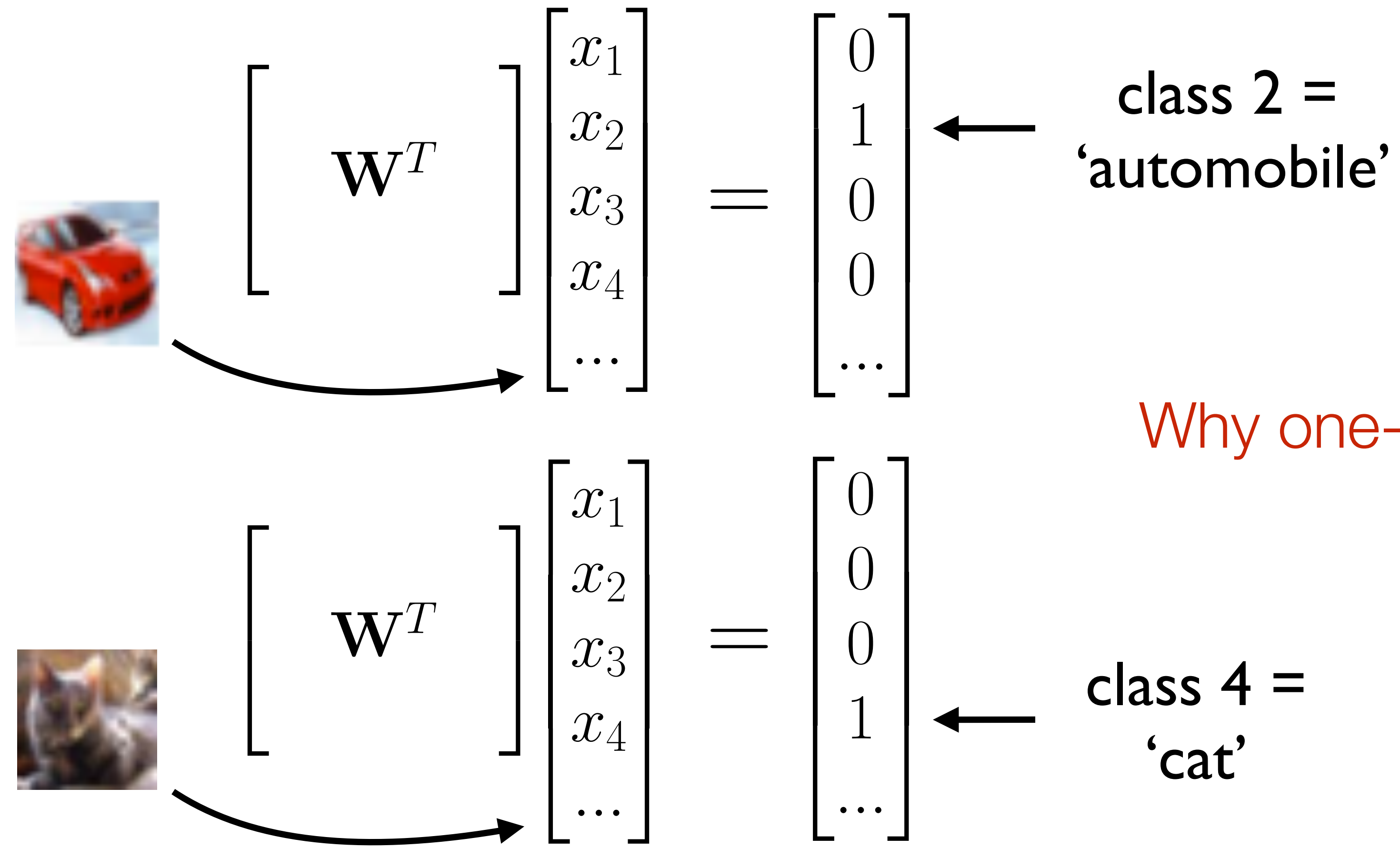
One-hot Regression

An alternative solution is to regress to one-hot targets = 1 vs all classifiers



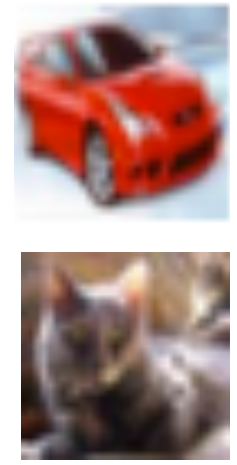
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One-hot Regression

Transpose




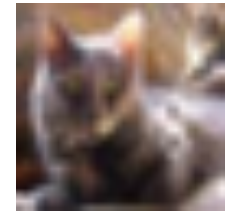
$$\begin{bmatrix} x_{11} & x_{12} & x_{13} & \dots \\ x_{21} & x_{22} & x_{23} & \dots \\ x_{31} & x_{32} & x_{33} & \dots \\ \dots & & & \end{bmatrix}$$

$$\begin{bmatrix} \mathbf{W} \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 & 0 & \dots \\ 0 & 0 & 0 & 1 & \dots \\ \dots & \dots & & & \end{bmatrix} \begin{matrix} \text{auto} \\ \text{cat} \end{matrix}$$

$$\mathbf{XW} = \mathbf{T}$$

One-hot Regression

Transpose

$\left\{ \begin{array}{c} \text{# training images} \\ \updownarrow \end{array} \right.$  

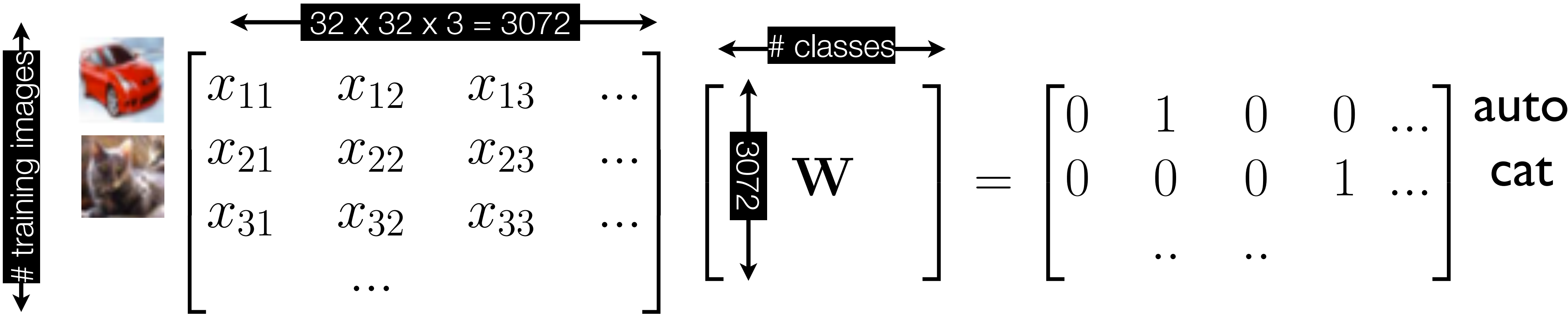
$\leftarrow 32 \times 32 \times 3 = 3072 \rightarrow$

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Solve regression problem by Least Squares

$$\mathcal{L} = |\mathbf{XW} - \mathbf{T}|^2$$

One-hot Regression

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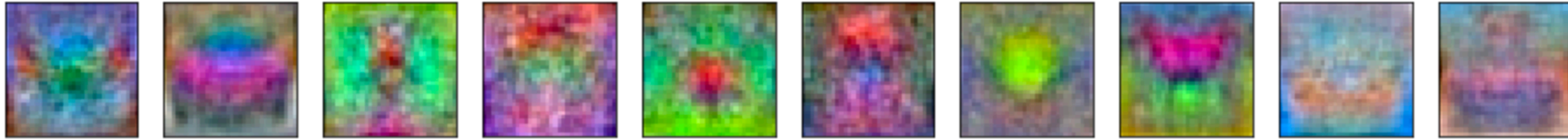
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Why this maybe sub-optimal?

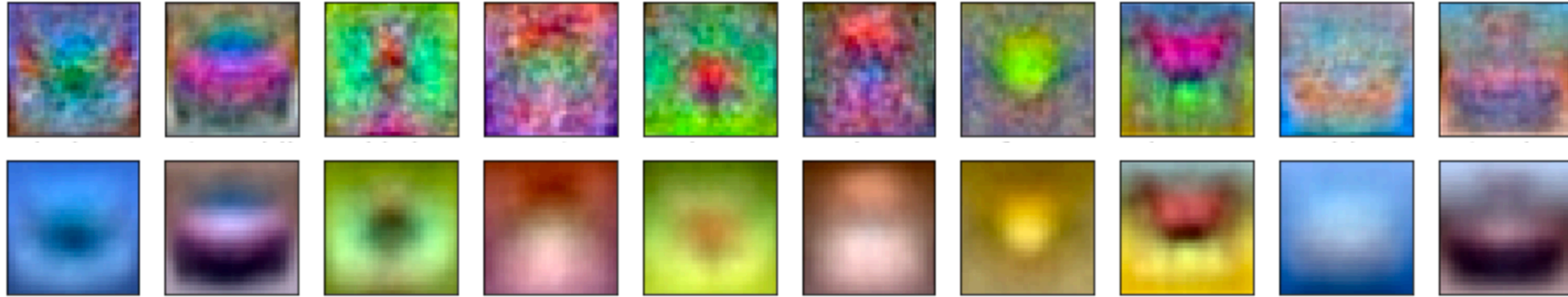
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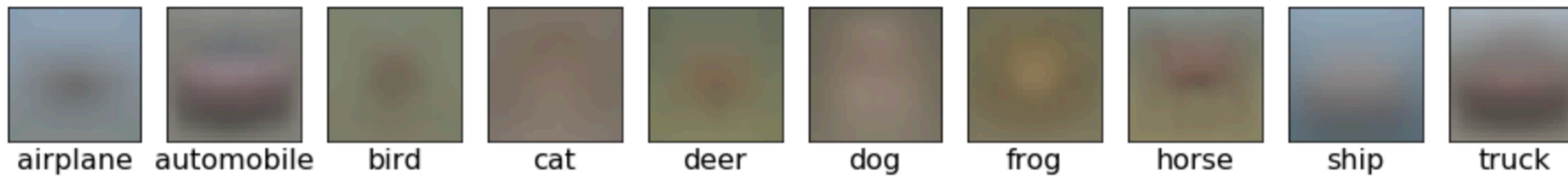
$$\mathcal{L} = \|\mathbf{X}\mathbf{W} - \mathbf{T}\|^2 + \lambda\|\mathbf{W}\|^2$$

Recall: **Nearest Mean** Classifier

Find the nearest mean and assign class:

$$c_q = \arg \min_i |\mathbf{x}_q - \mathbf{m}_i|^2$$

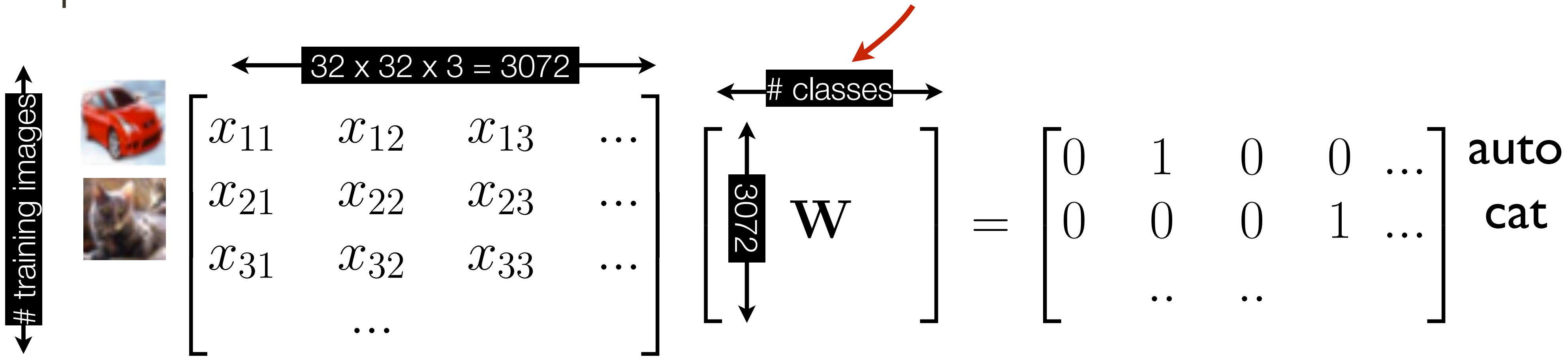
CIFAR10 class means:



One-hot Regression

10 Neurons with simple-linear (identity) activation function

Transpose

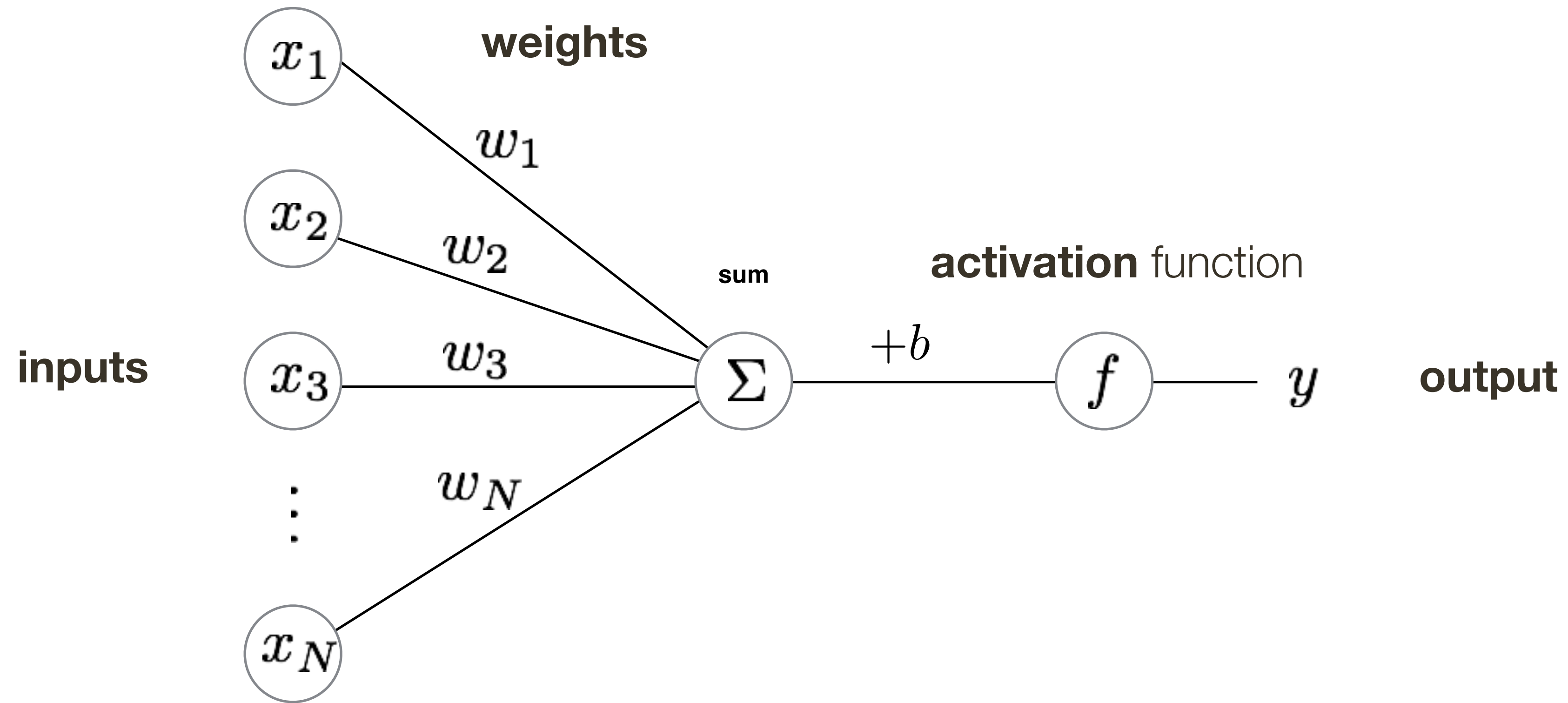


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Solve regression problem by Least Squares

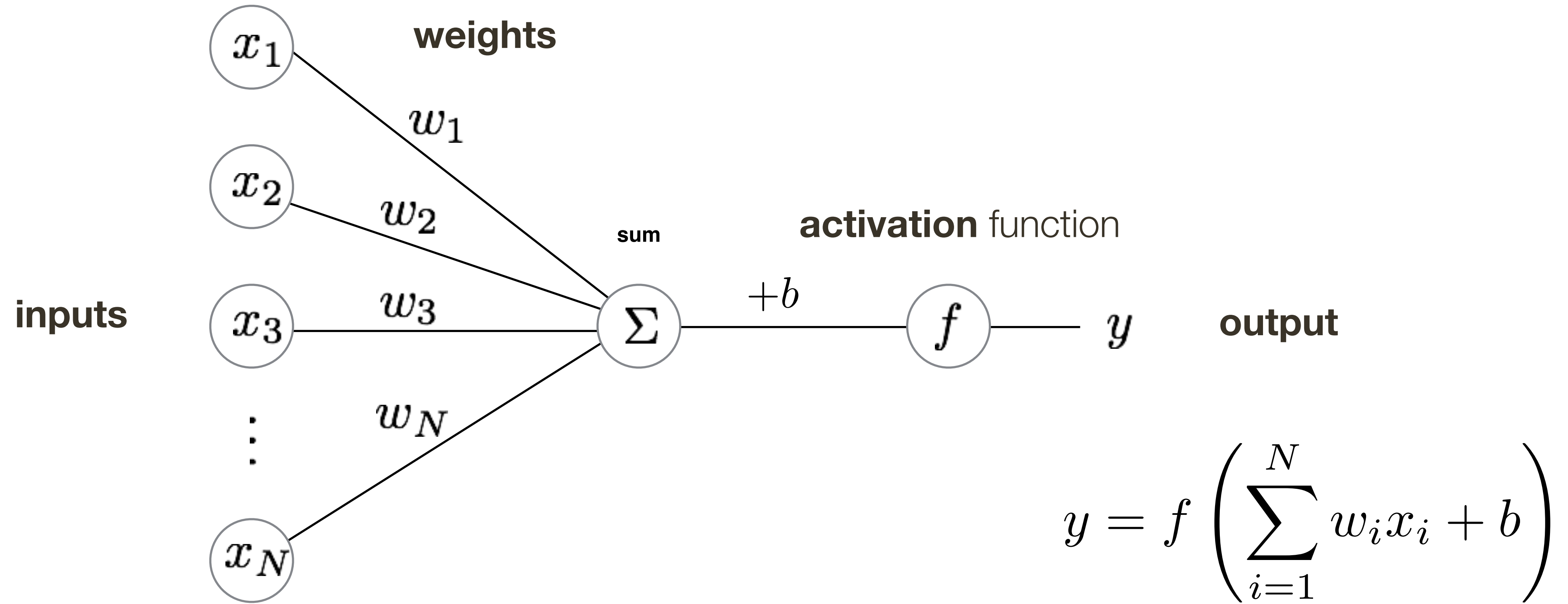
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A Neuron



- The basic unit of computation in a neural network is a neuron.
- A neuron accepts some number of input signals, computes their weighted sum, and applies an **activation function** (or **non-linearity**) to the sum.
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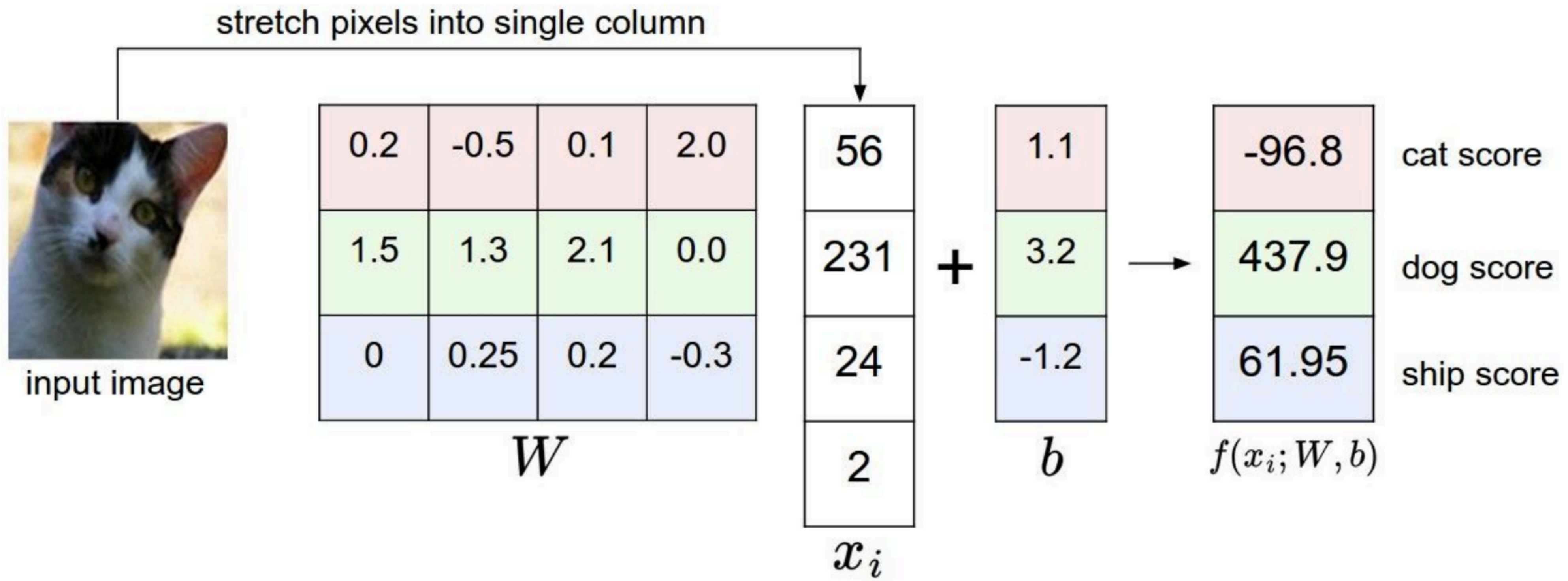
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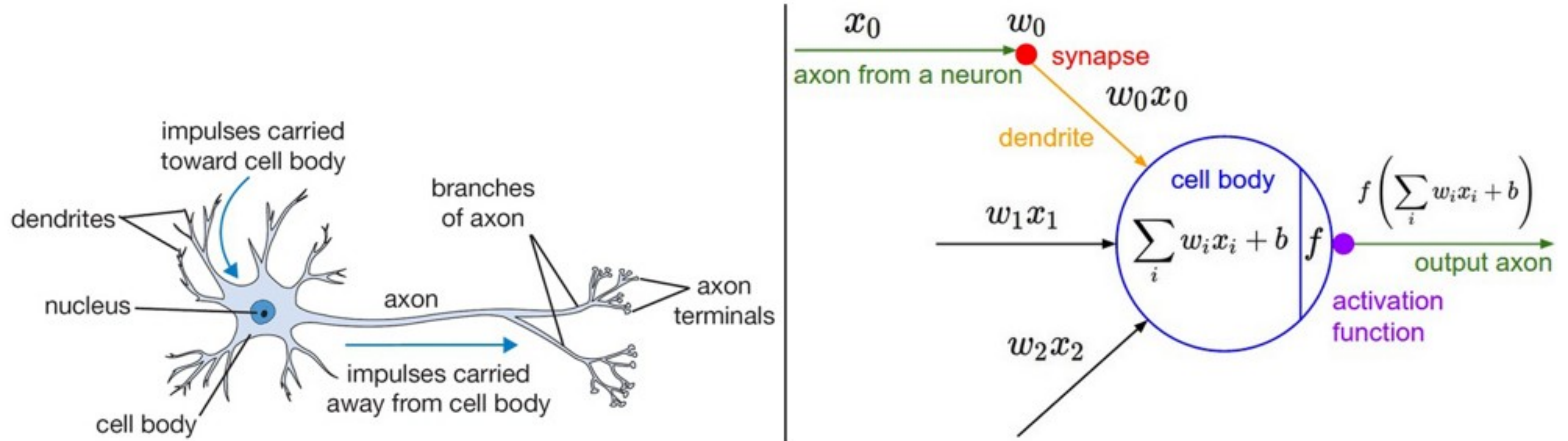
Recall: Linear Classifier

Example with an image with 4 pixels, and 3 classes (cat/dog/ship)



Aside: Inspiration from Biology

Figure credit: Fei-Fei and Karpathy



A cartoon drawing of a biological neuron (left) and its mathematical model (right).

Neural nets/perceptrons are loosely inspired by biology.

But they certainly are not a model of how the brain works, or even how neurons work.

Activation Function: **Sigmoid**

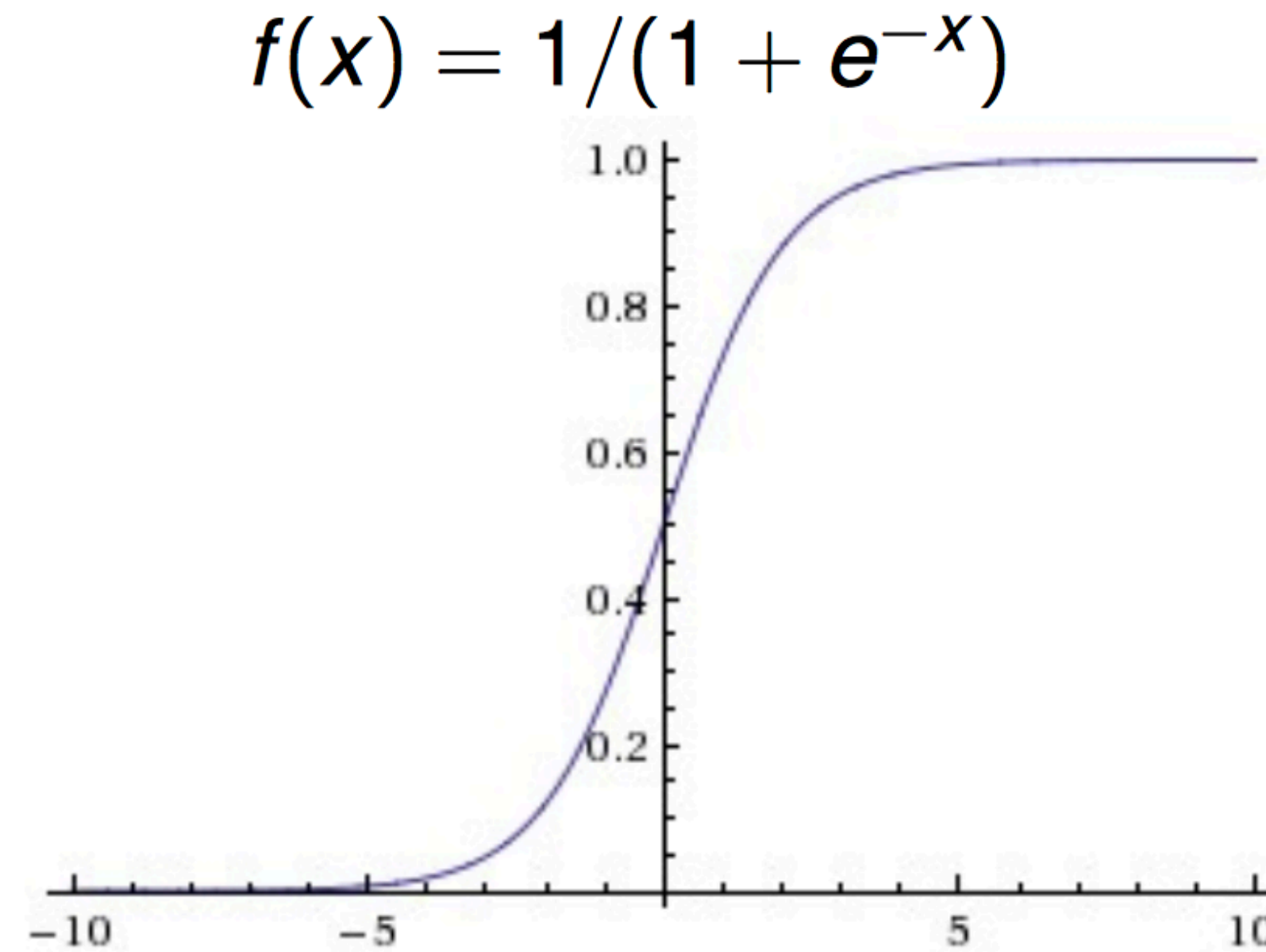


Figure credit: Fei-Fei and Karpathy

Common in many early neural networks

Biological analogy to saturated firing rate of neurons

Maps the input to the range [0, 1]

Activation Function: **ReLU** (Rectified Linear Unit)

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

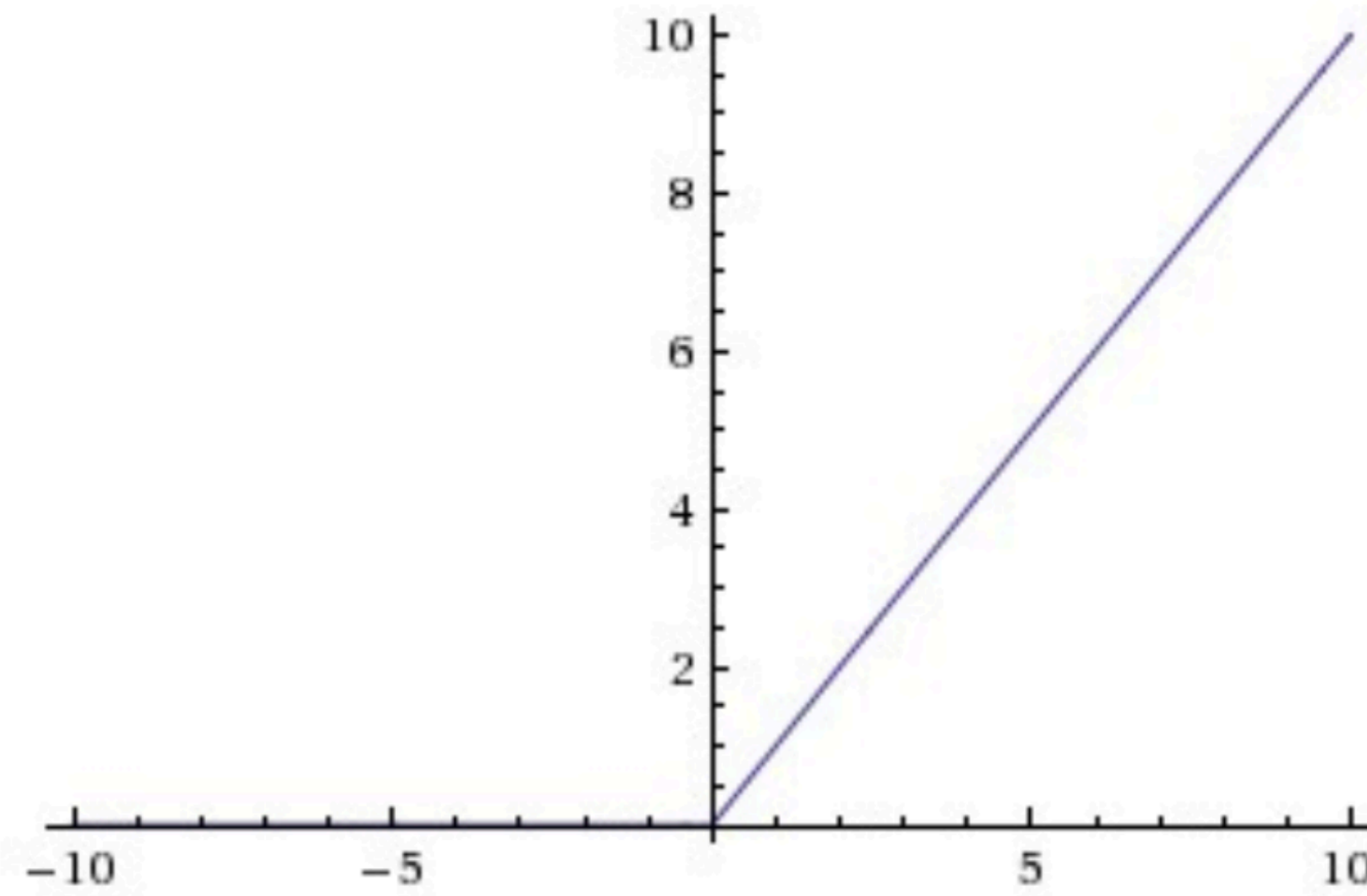
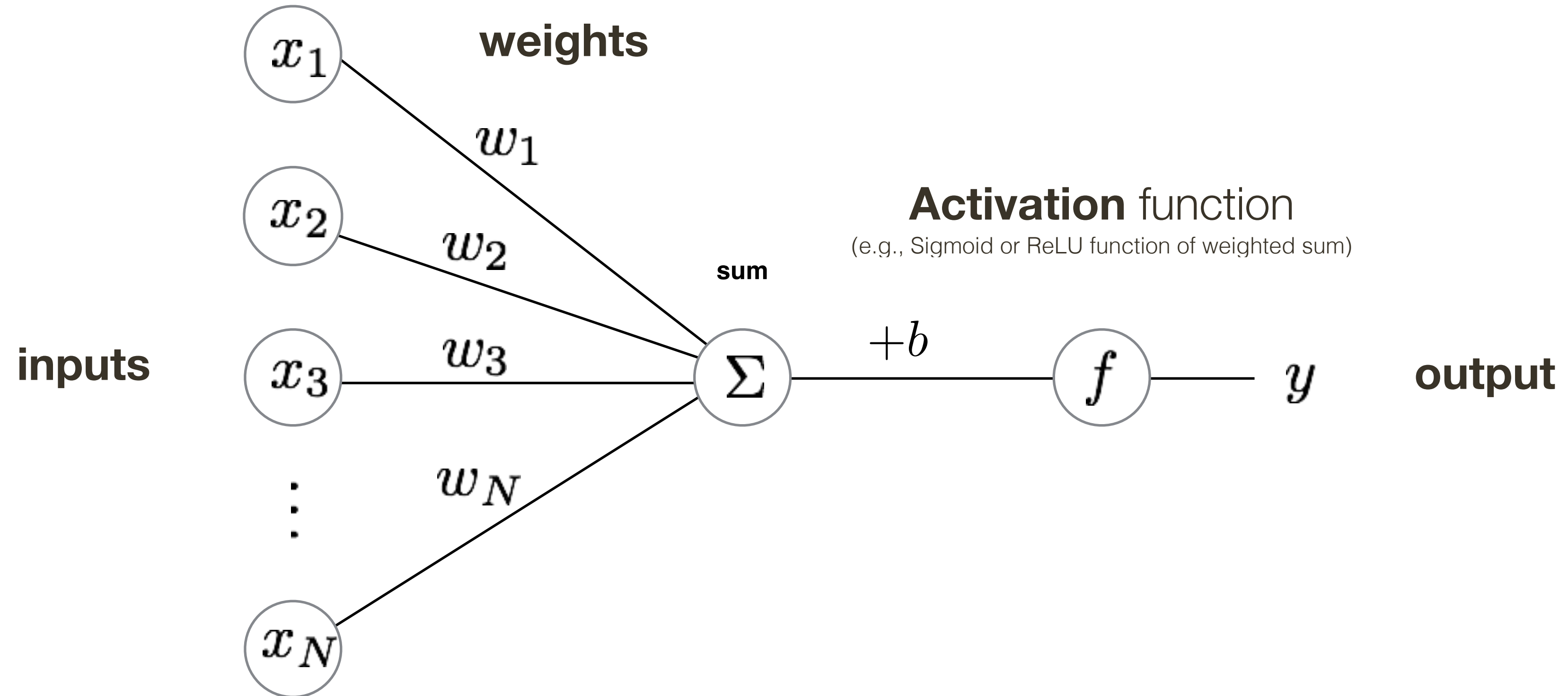


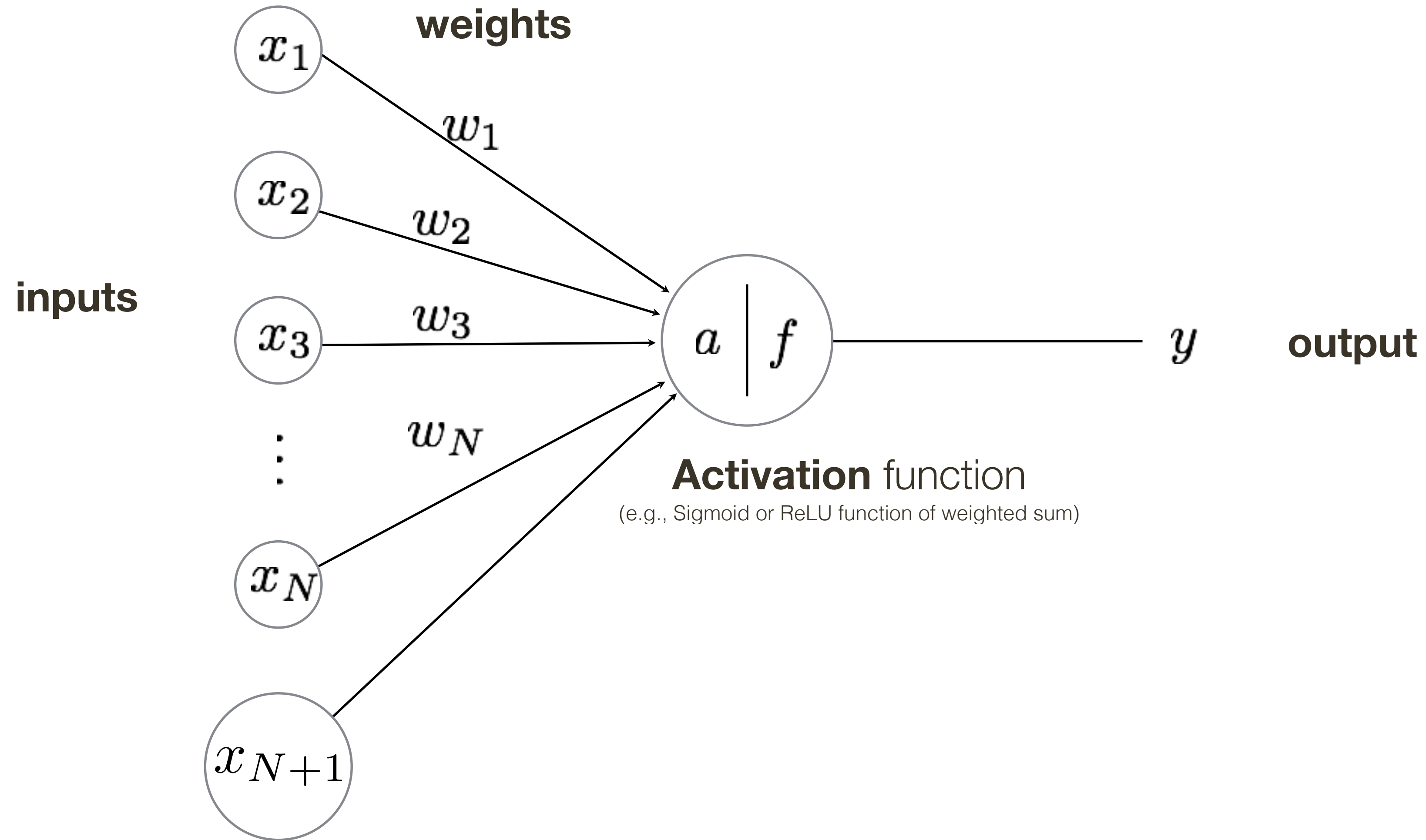
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Found to accelerate convergence during learning
Used in the most recent neural networks

A Neuron

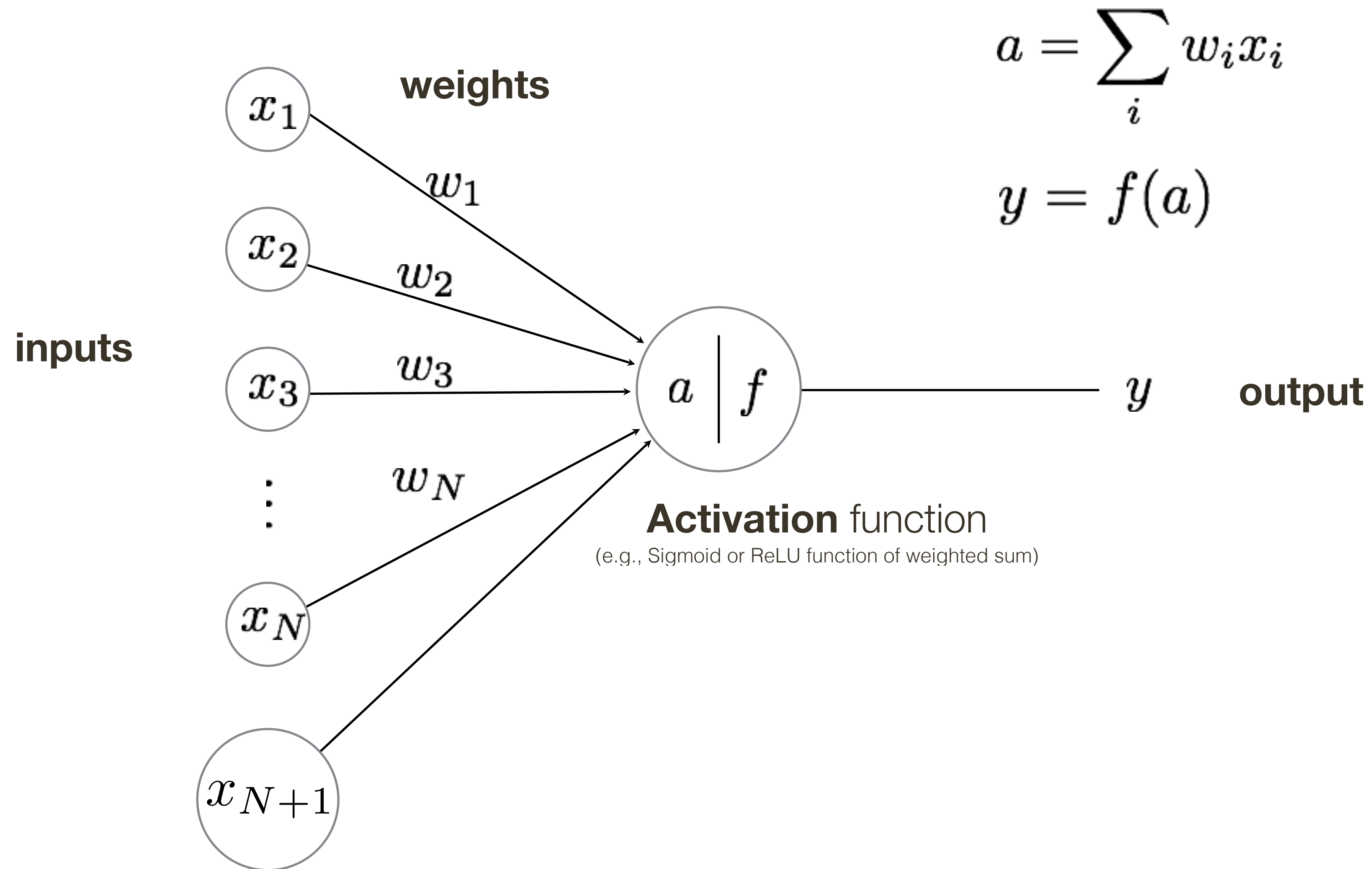


A Neuron ... another way to draw it ...



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(1) Combine the sum and activation function

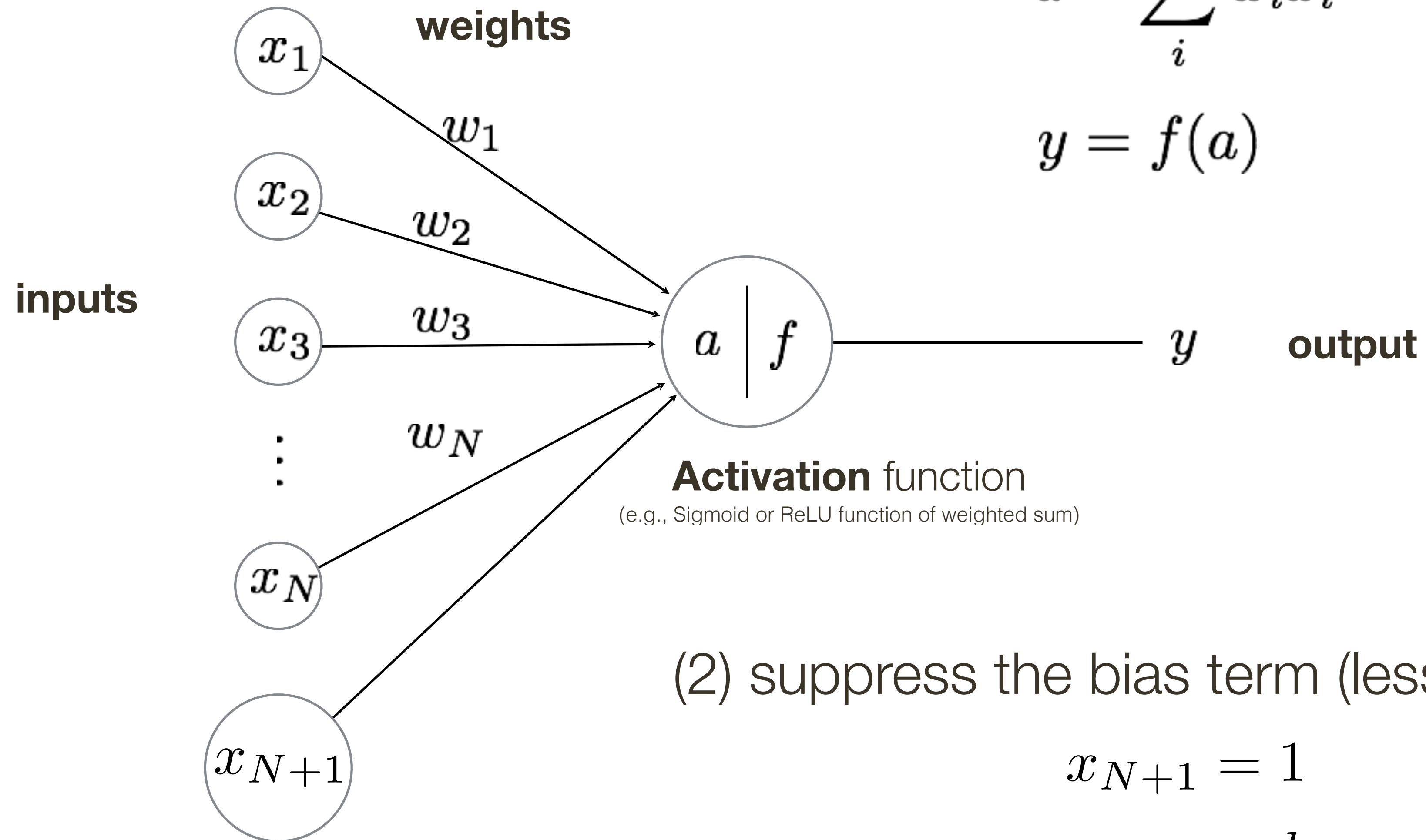


A Neuron ... another way to draw it ...

(1) Combine the sum and activation function

$$a = \sum_i w_i x_i$$

$$y = f(a)$$



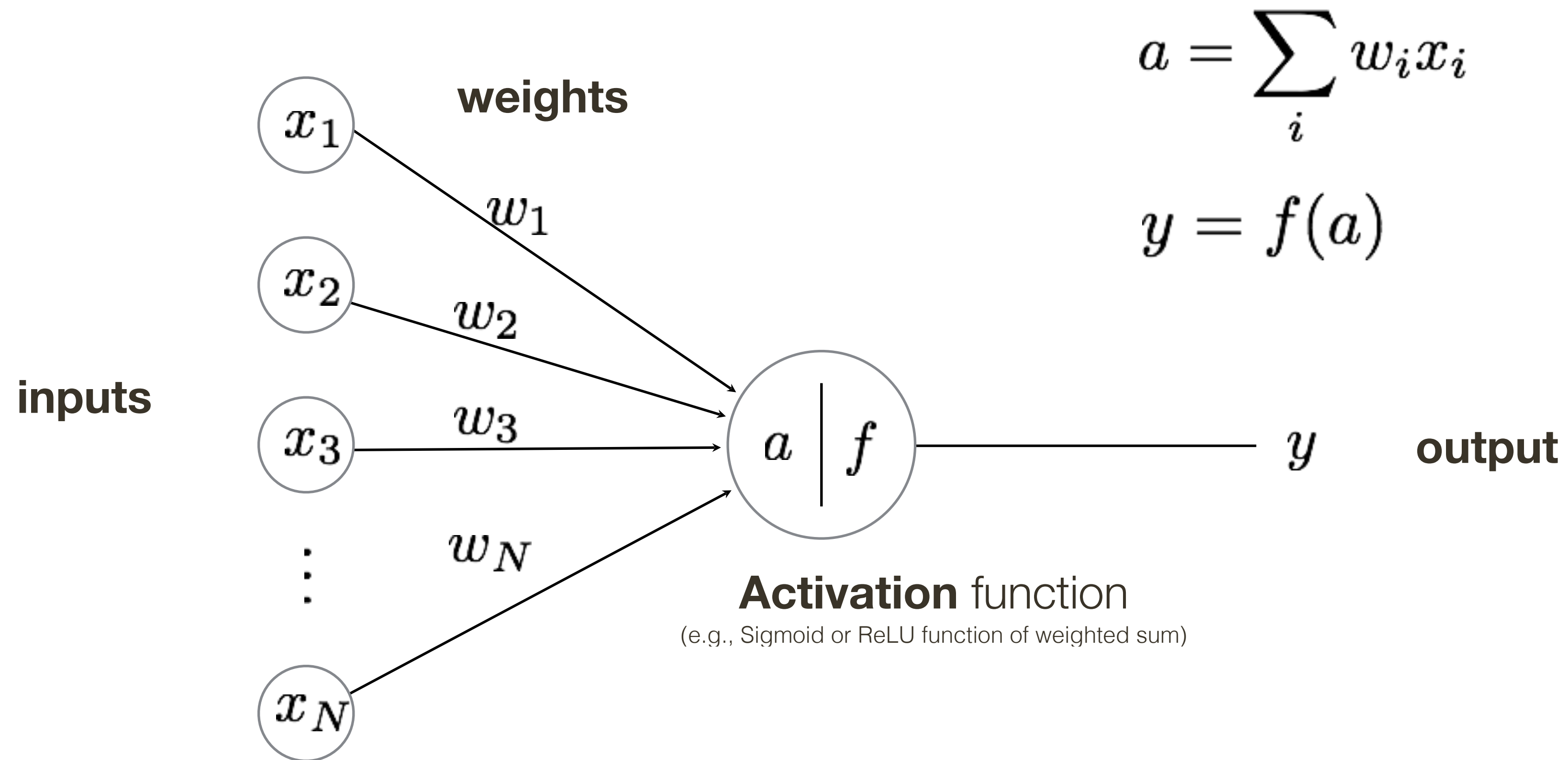
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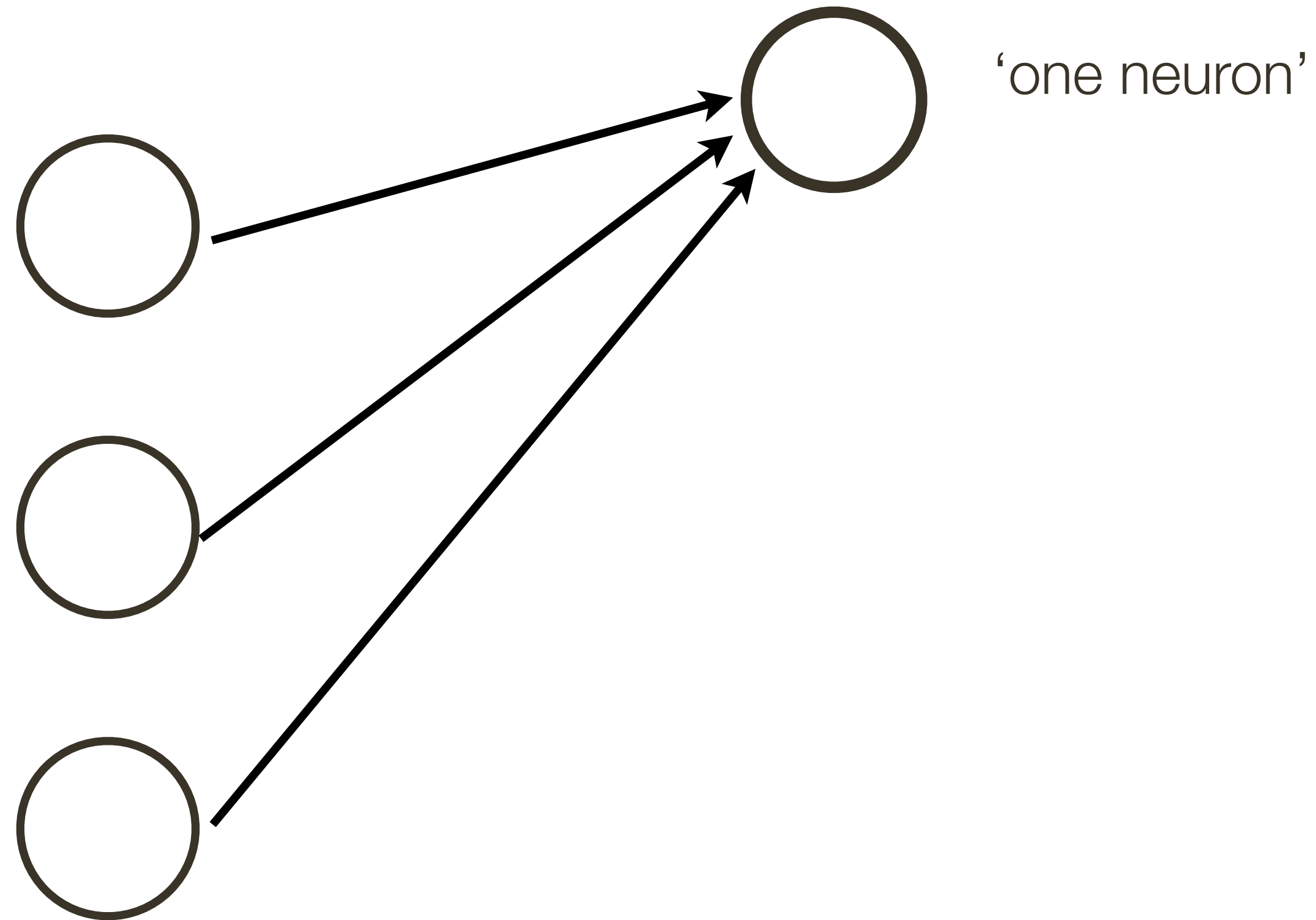


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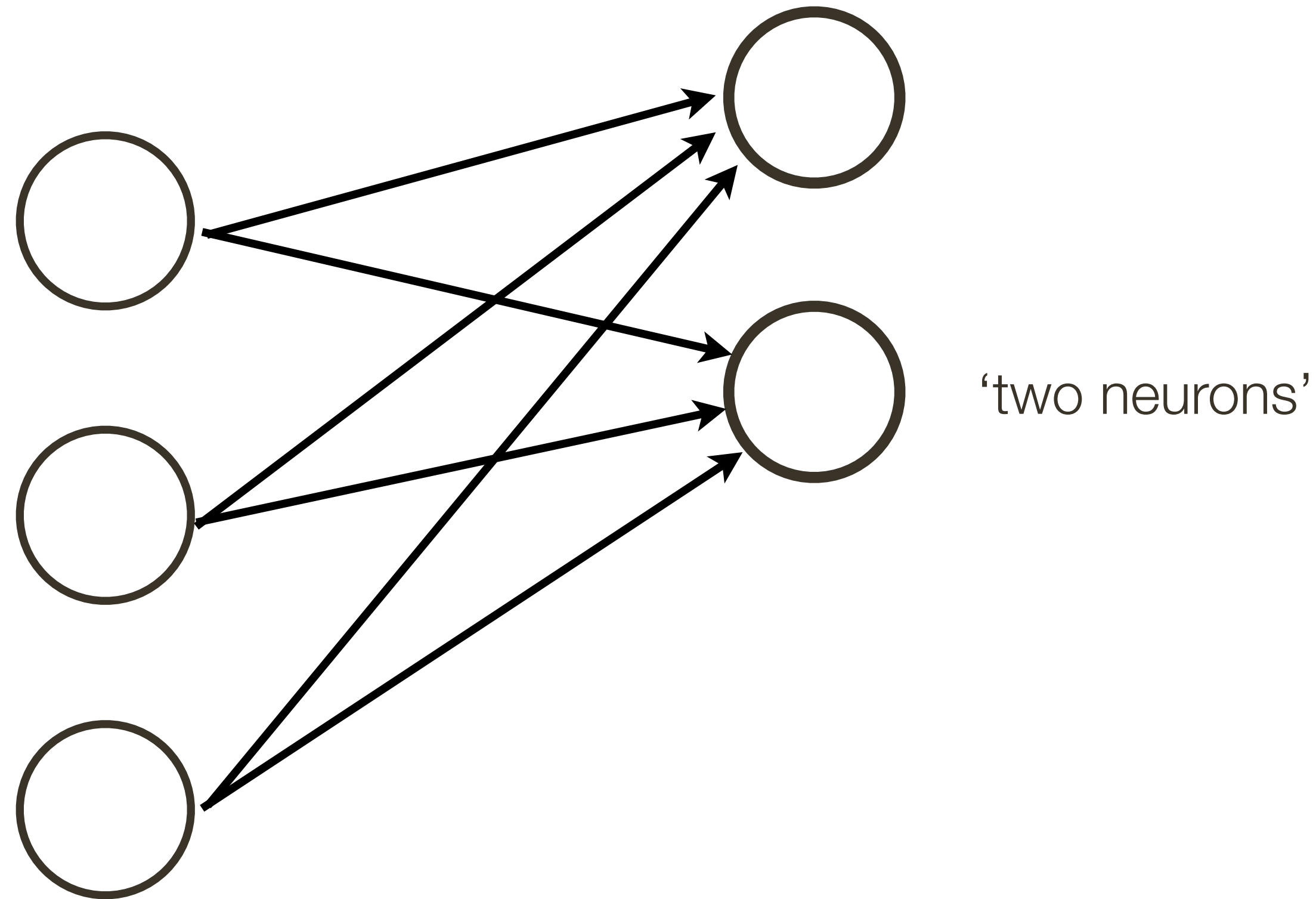
Neural Network

Connect a bunch of neurons together — a collection of connected neurons



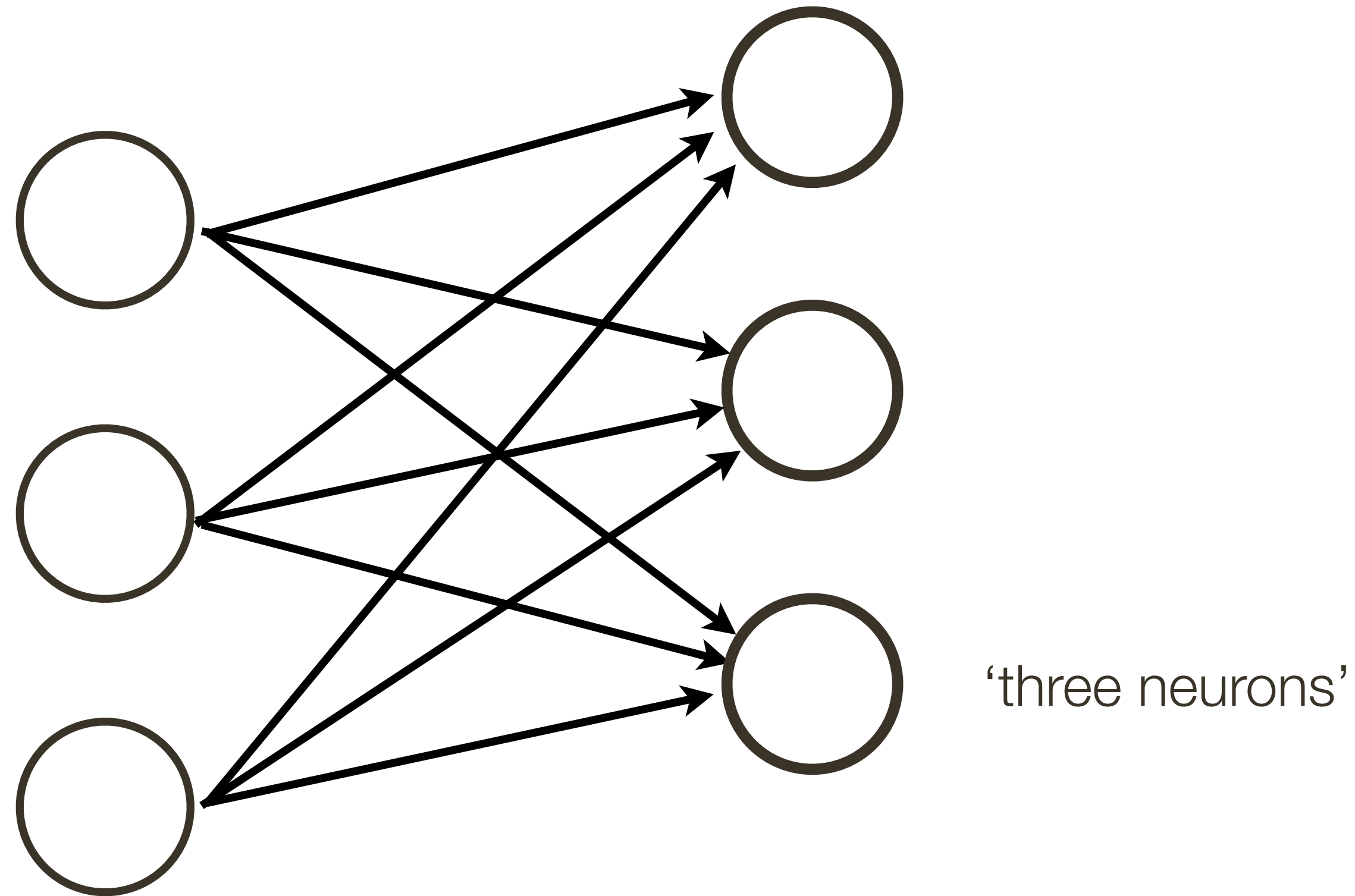
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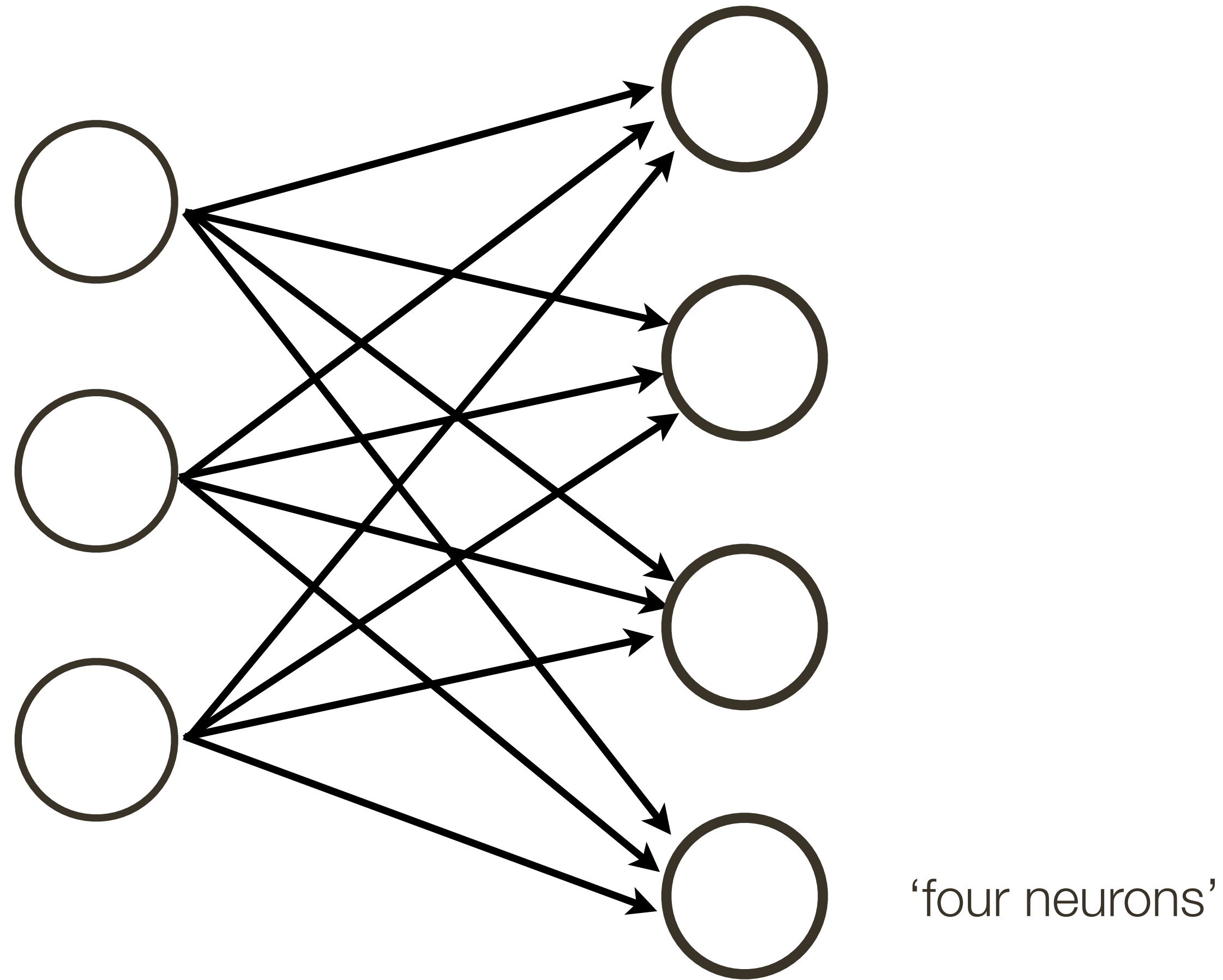
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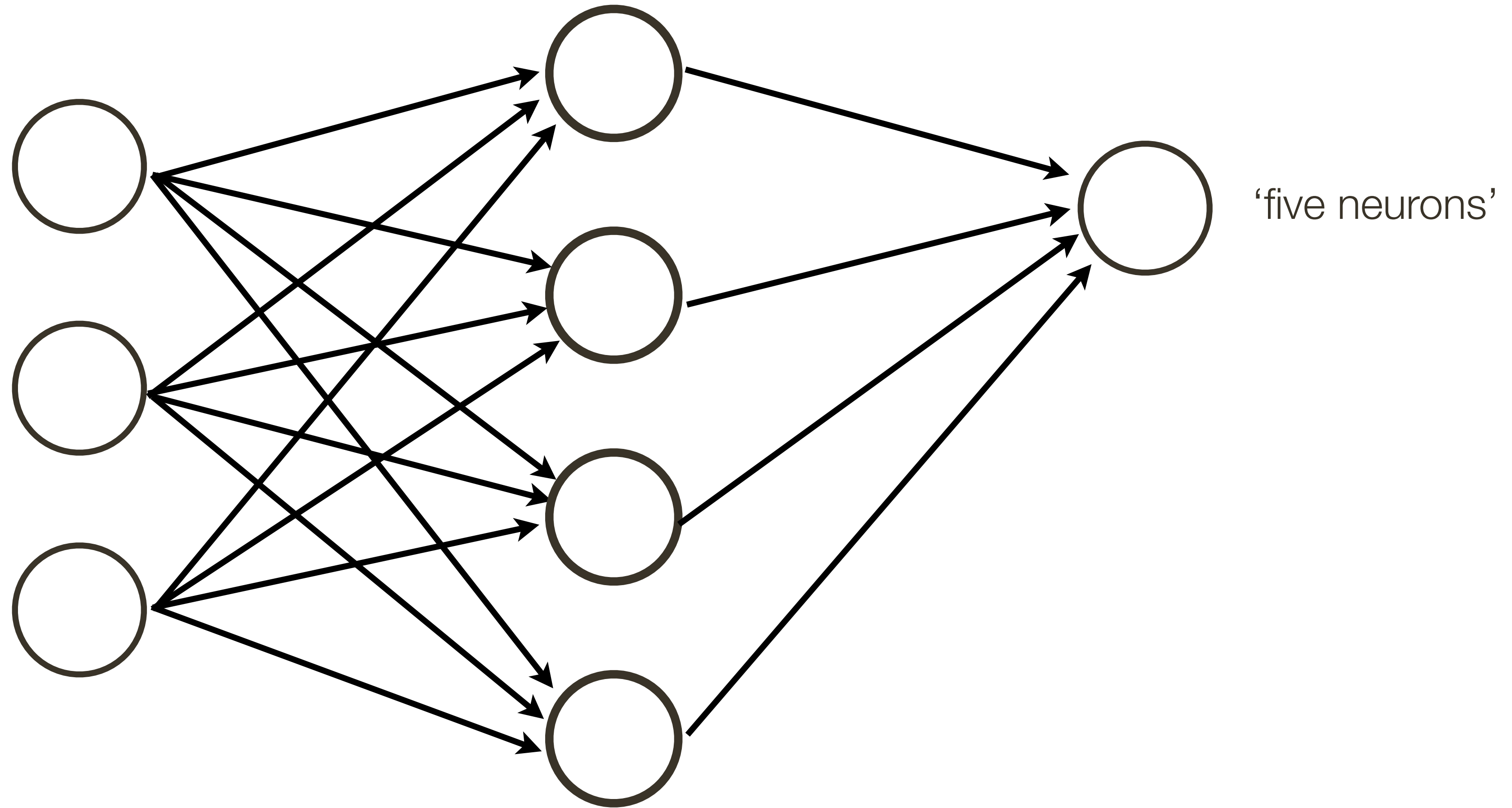
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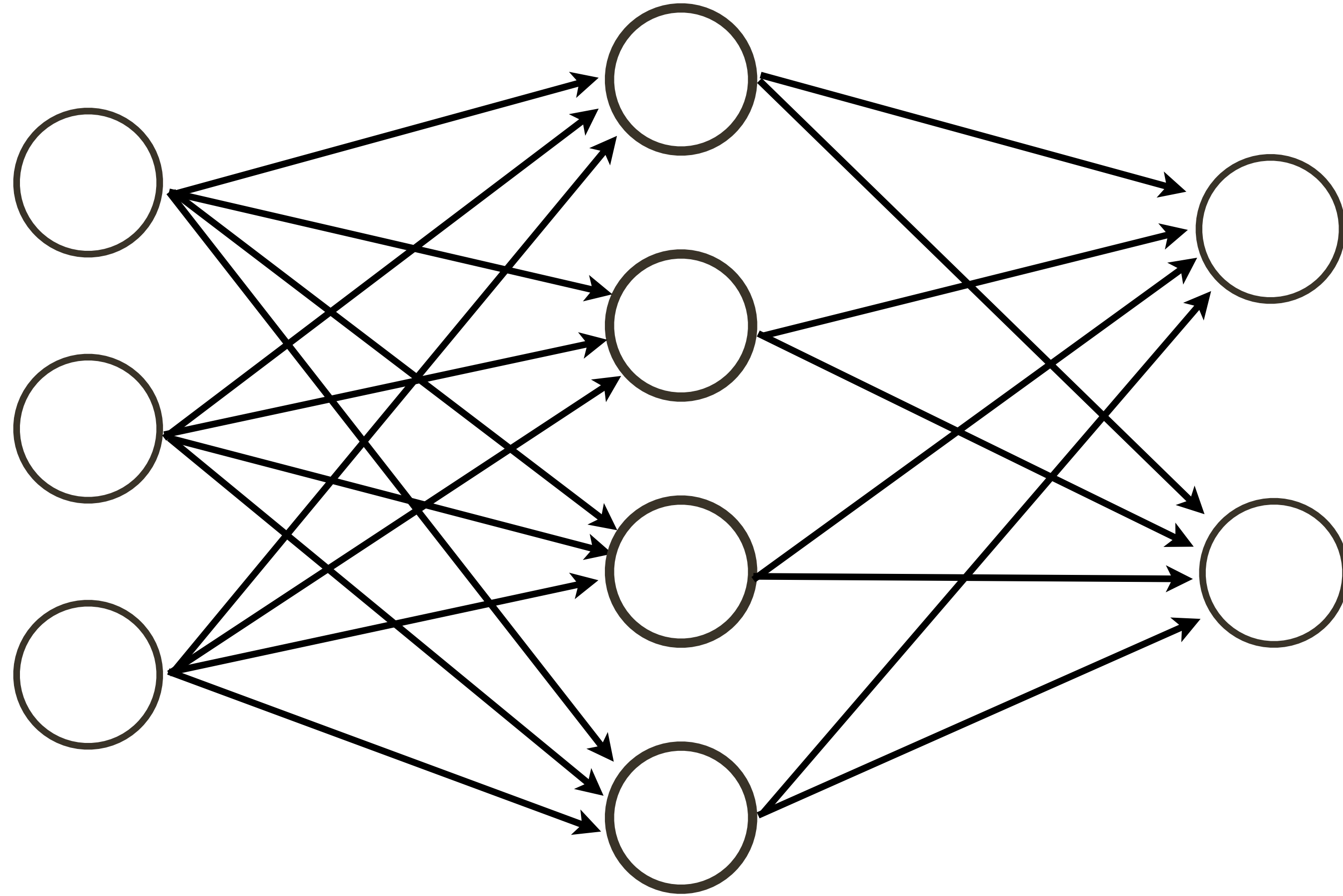
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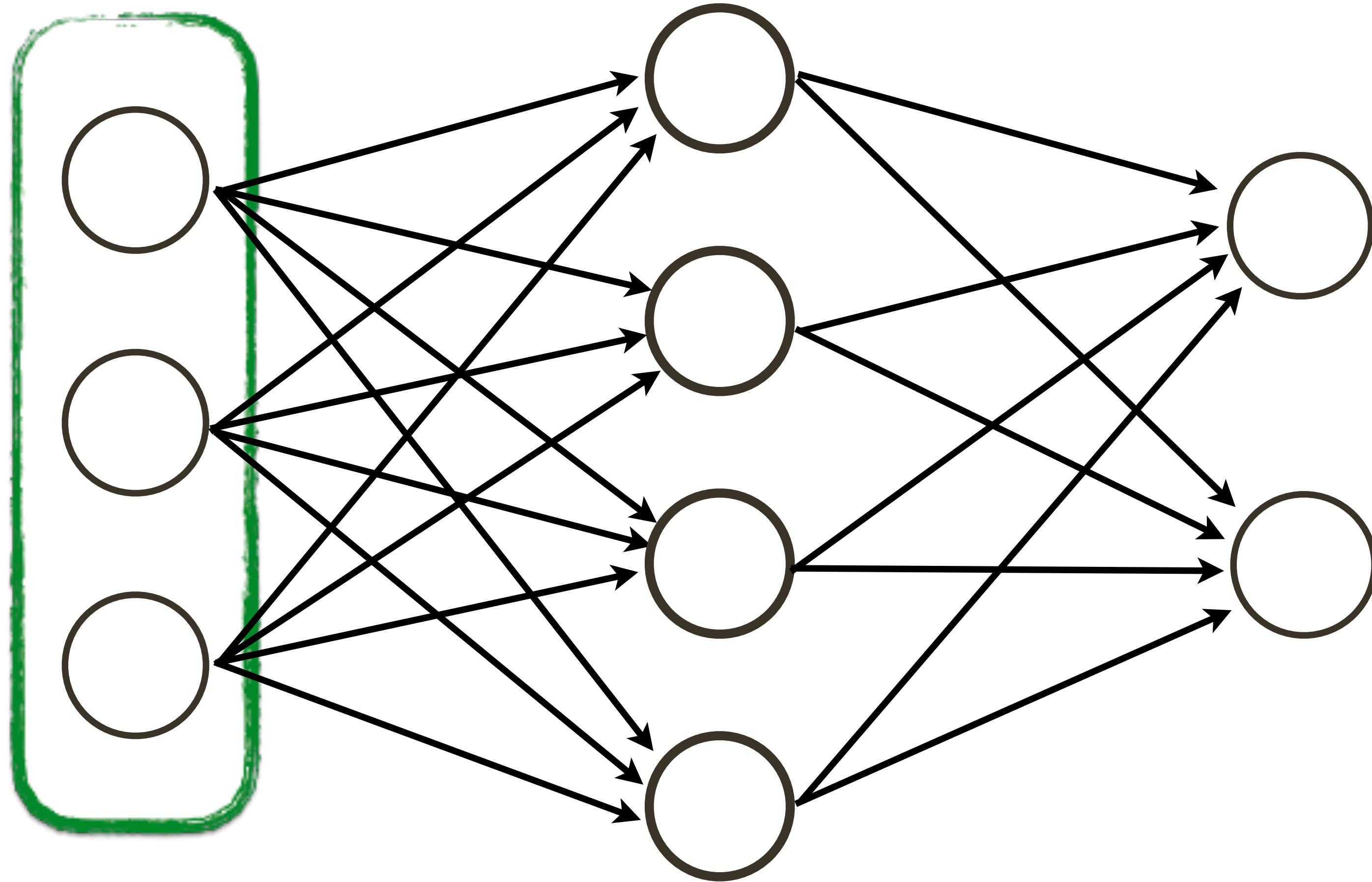
Neural Network

This network is also called a **Multi-layer Perceptron** (MLP)

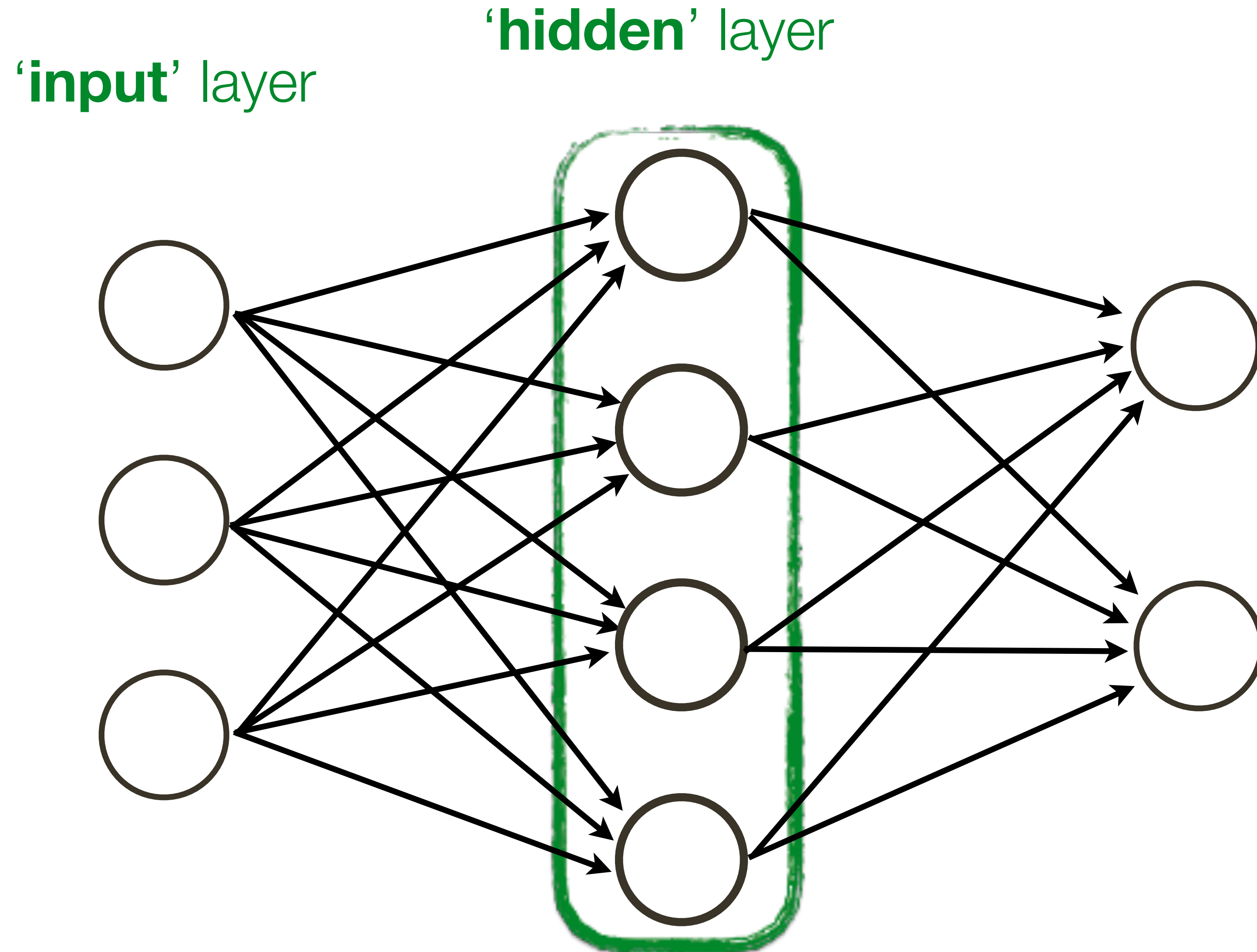


Neural Network: **Terminology**

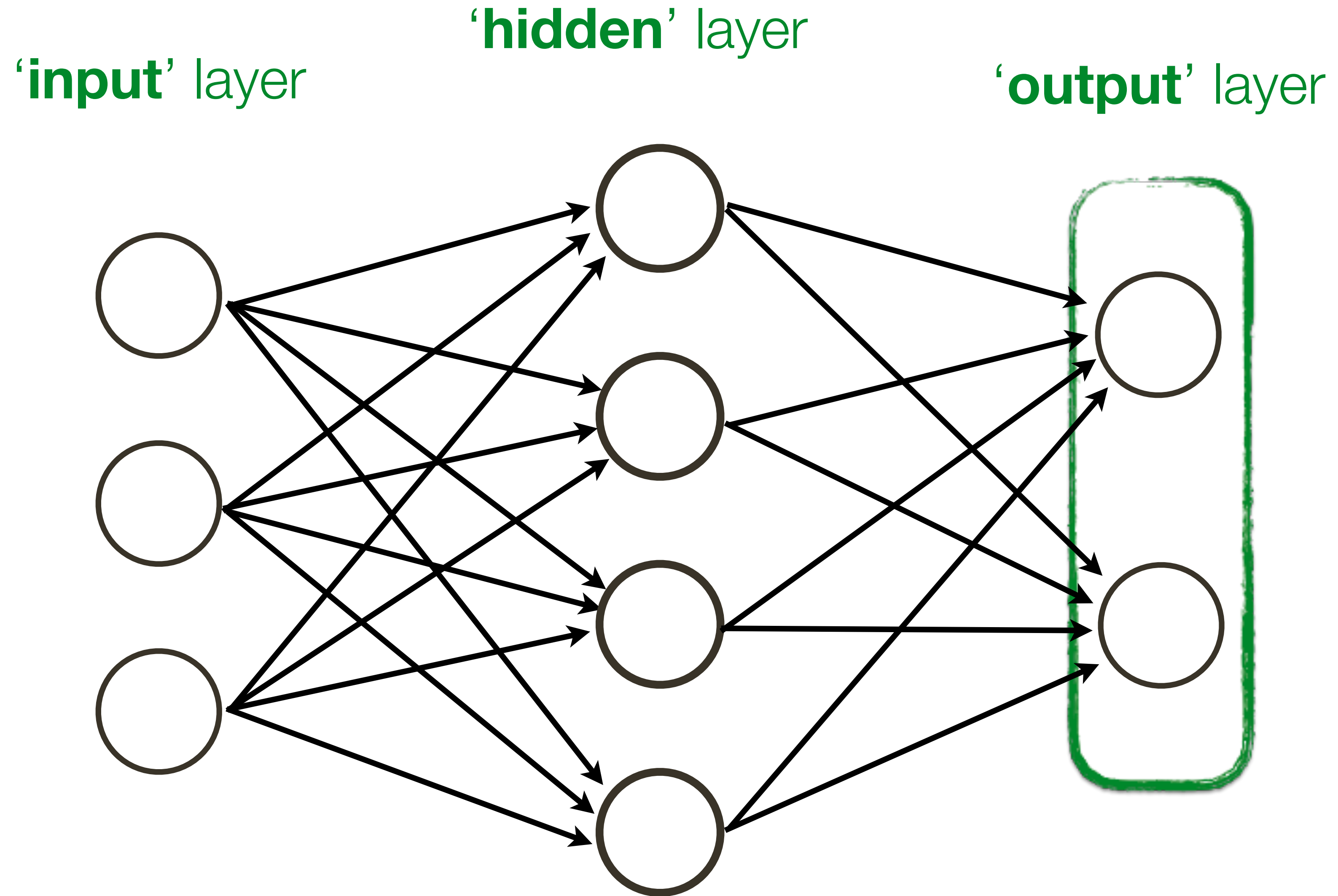
'input' layer



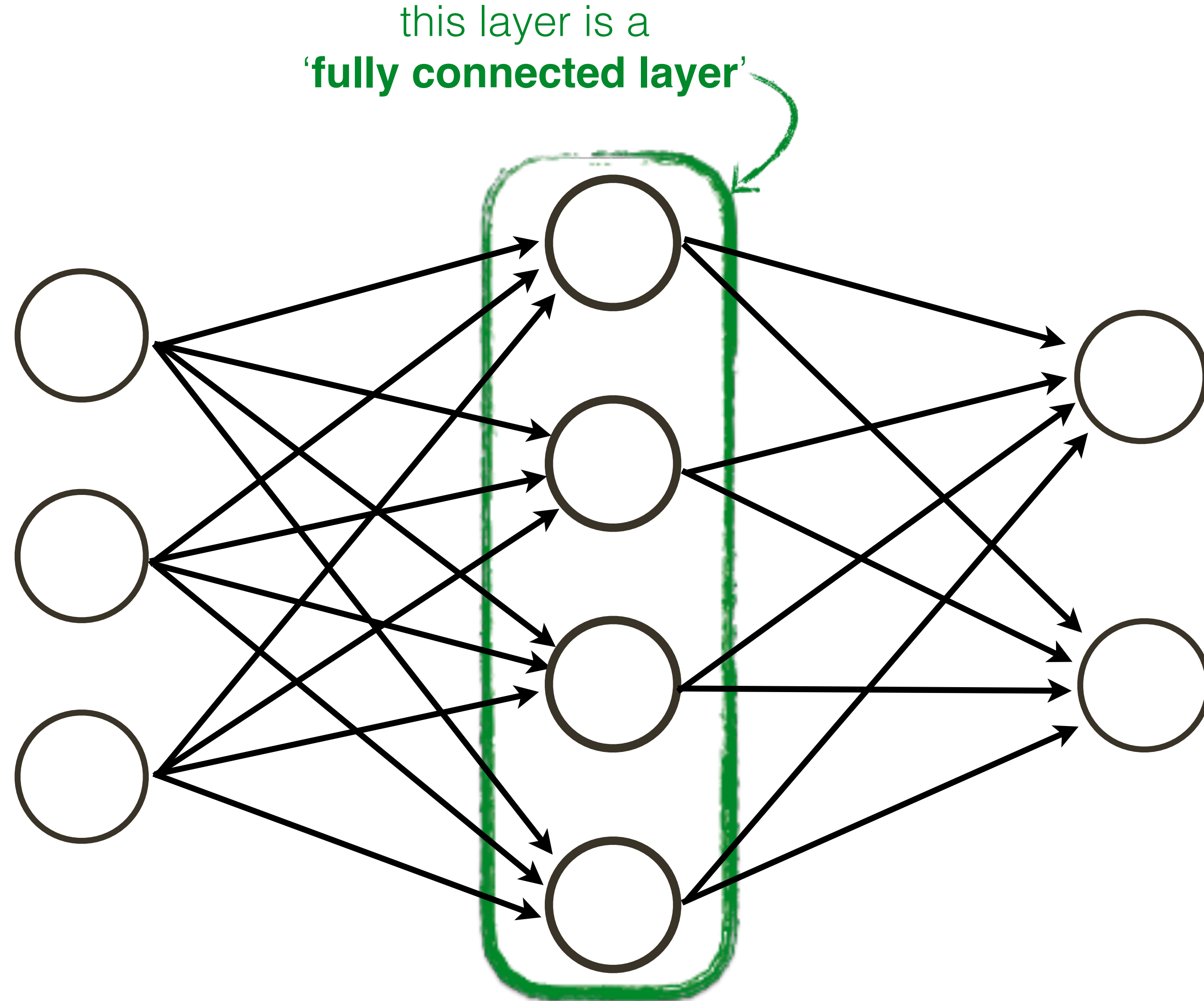
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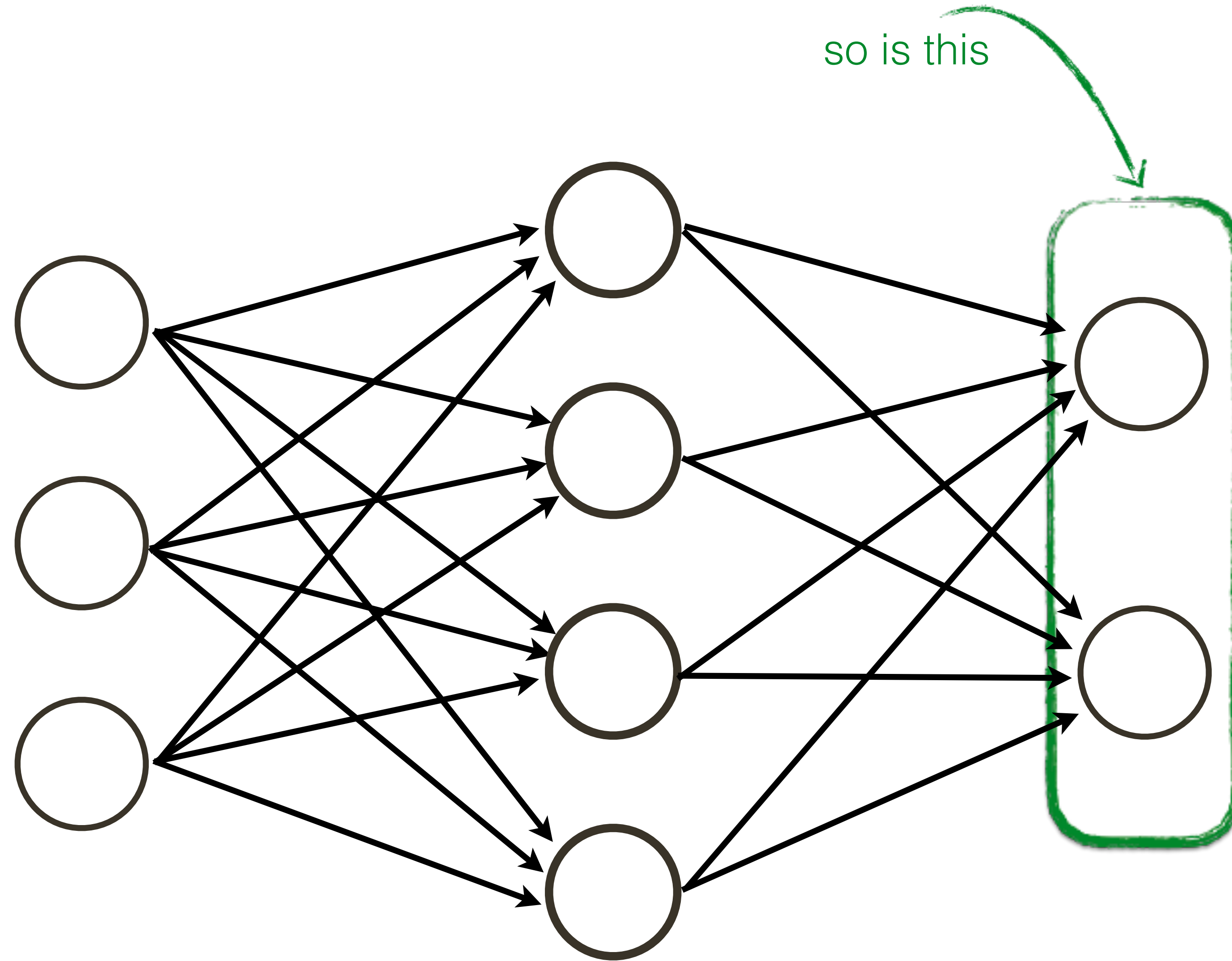
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Neural Network

A neural network comprises neurons connected in an acyclic graph

The outputs of neurons can become inputs to other neurons

Neural networks typically contain multiple layers of neurons

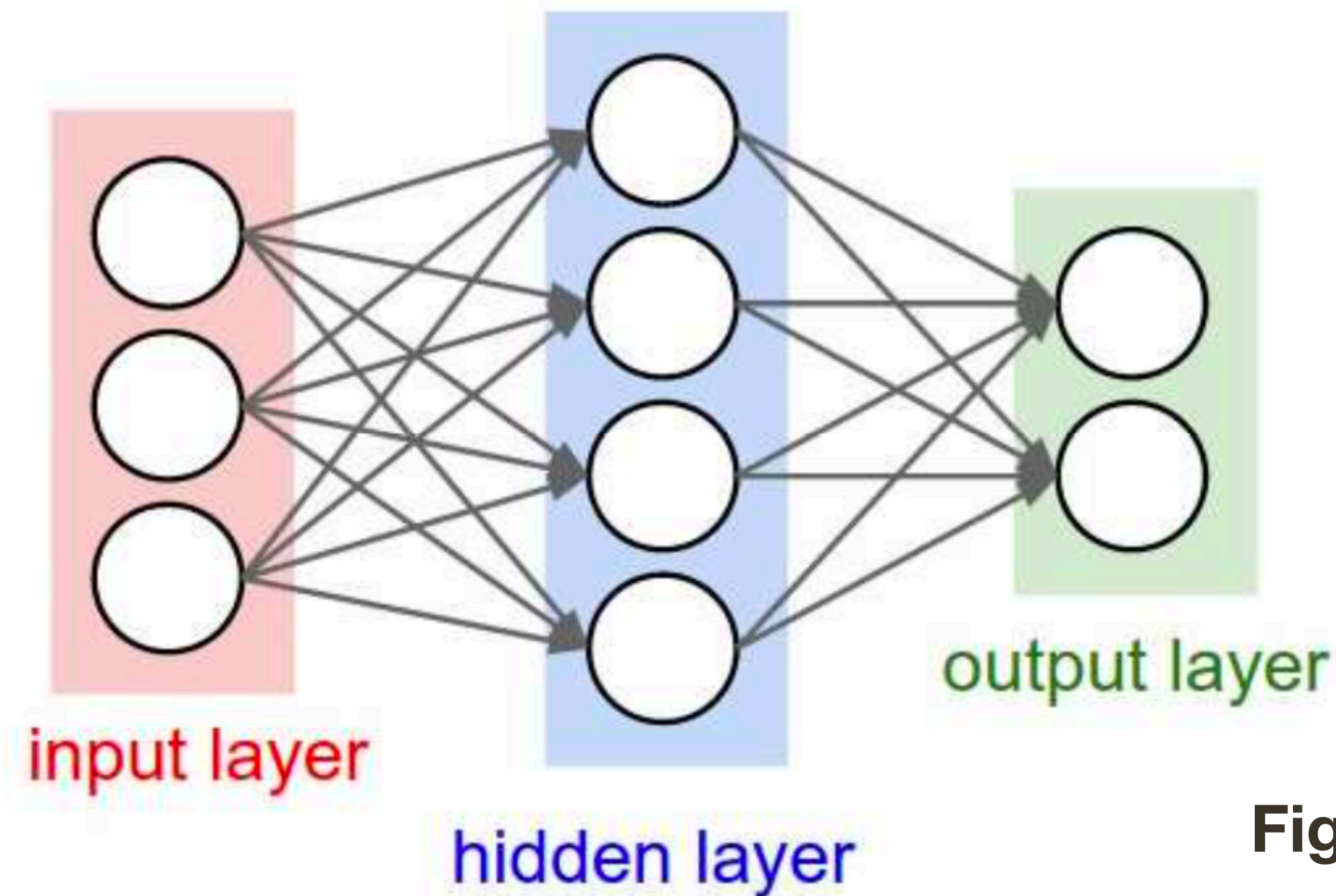


Figure credit: Fei-Fei and Karpathy

Example of a neural network with three inputs, a single hidden layer of four neurons, and an output layer of two neurons

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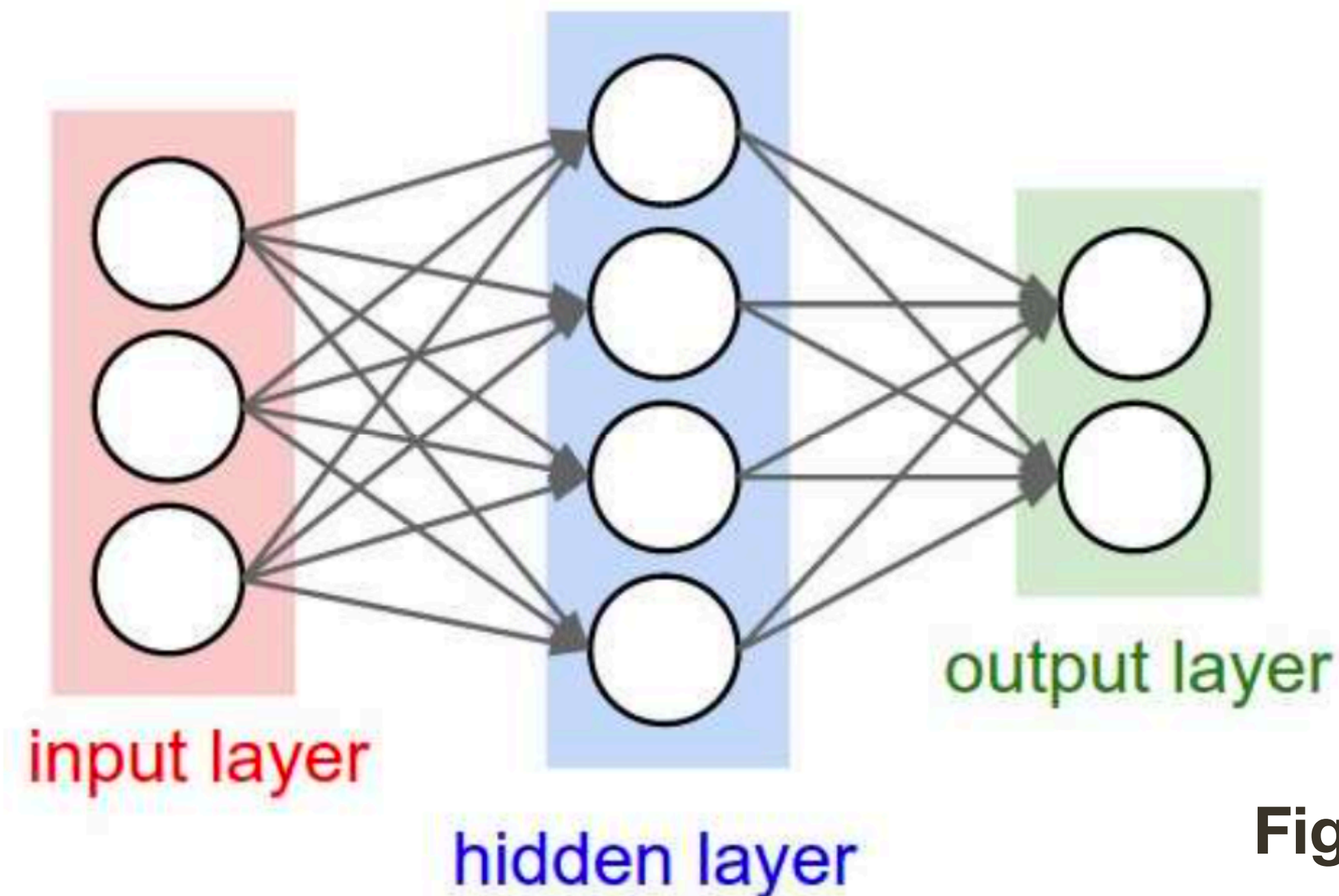


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Question: What does a hidden unit do?

Answer: It can be thought of as classifier or a feature.

Question: Why have many layers?

Answer: 1) More layers = more complex functional mapping
2) More efficient due to distributed representation

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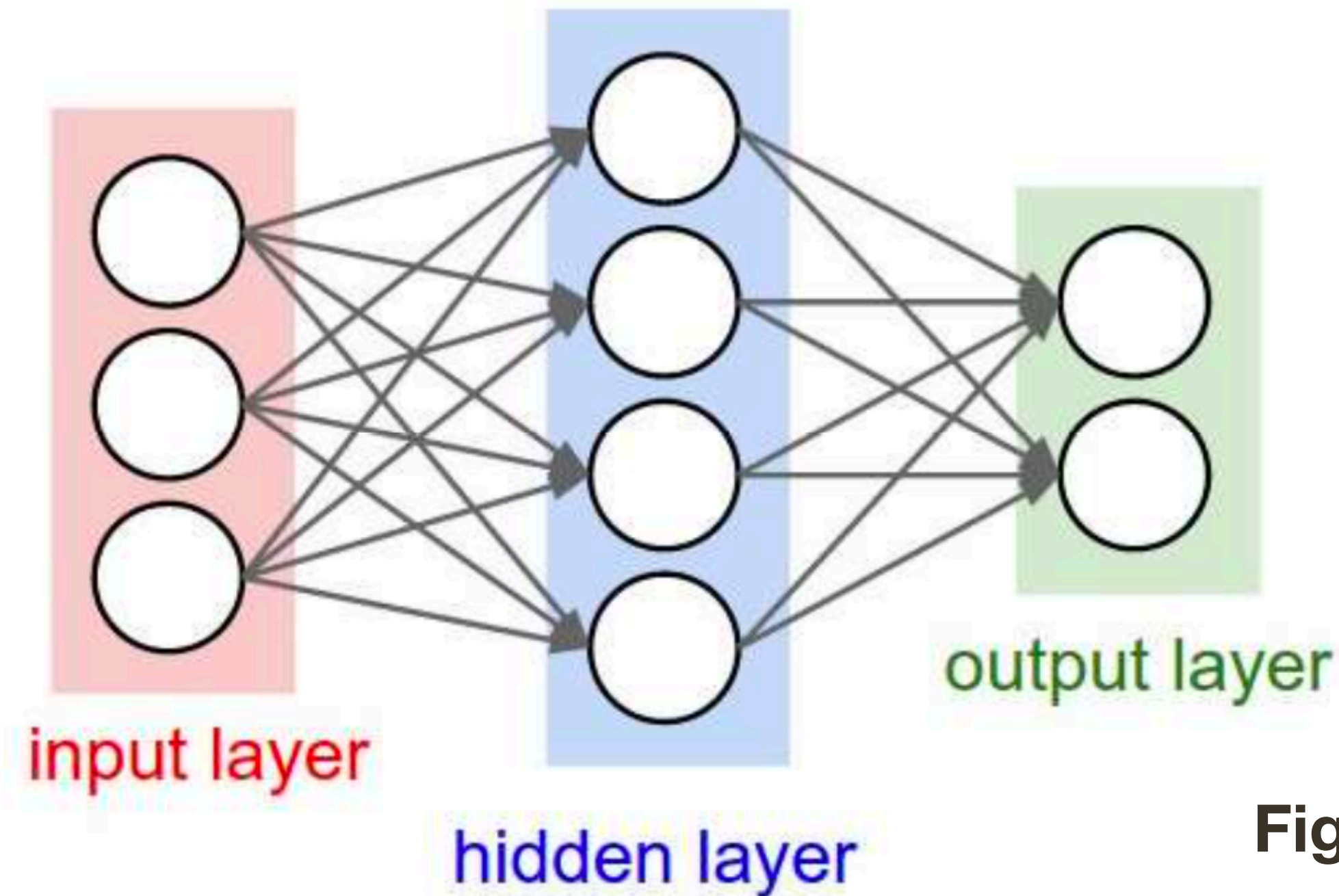


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Note: each neuron will have its own vector of weights and a bias, its easier to think of all neurons in a layer as a single entity with a matrix of weights (size = number of inputs x number of neurons) and a vector of biases (size = number of neurons)

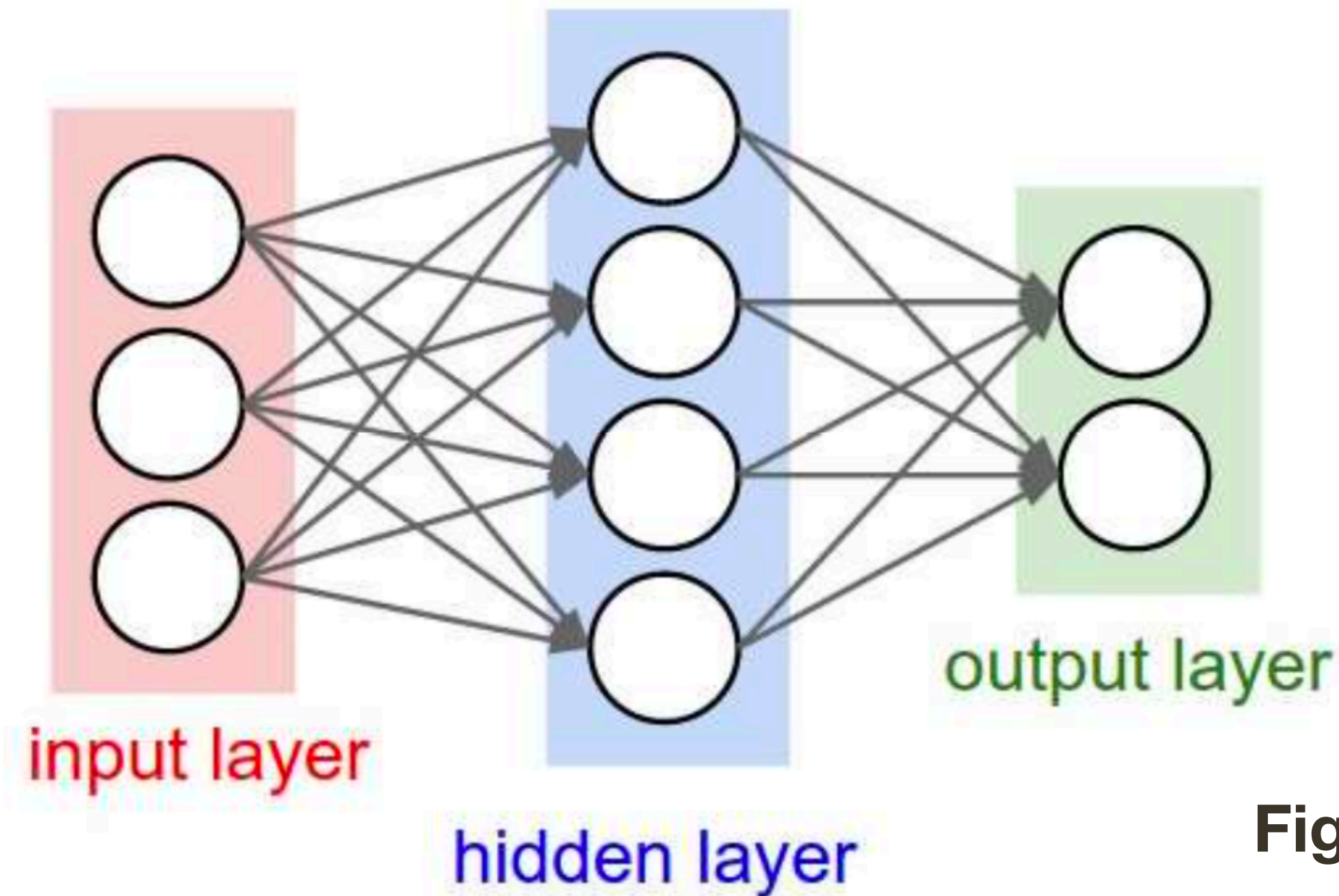


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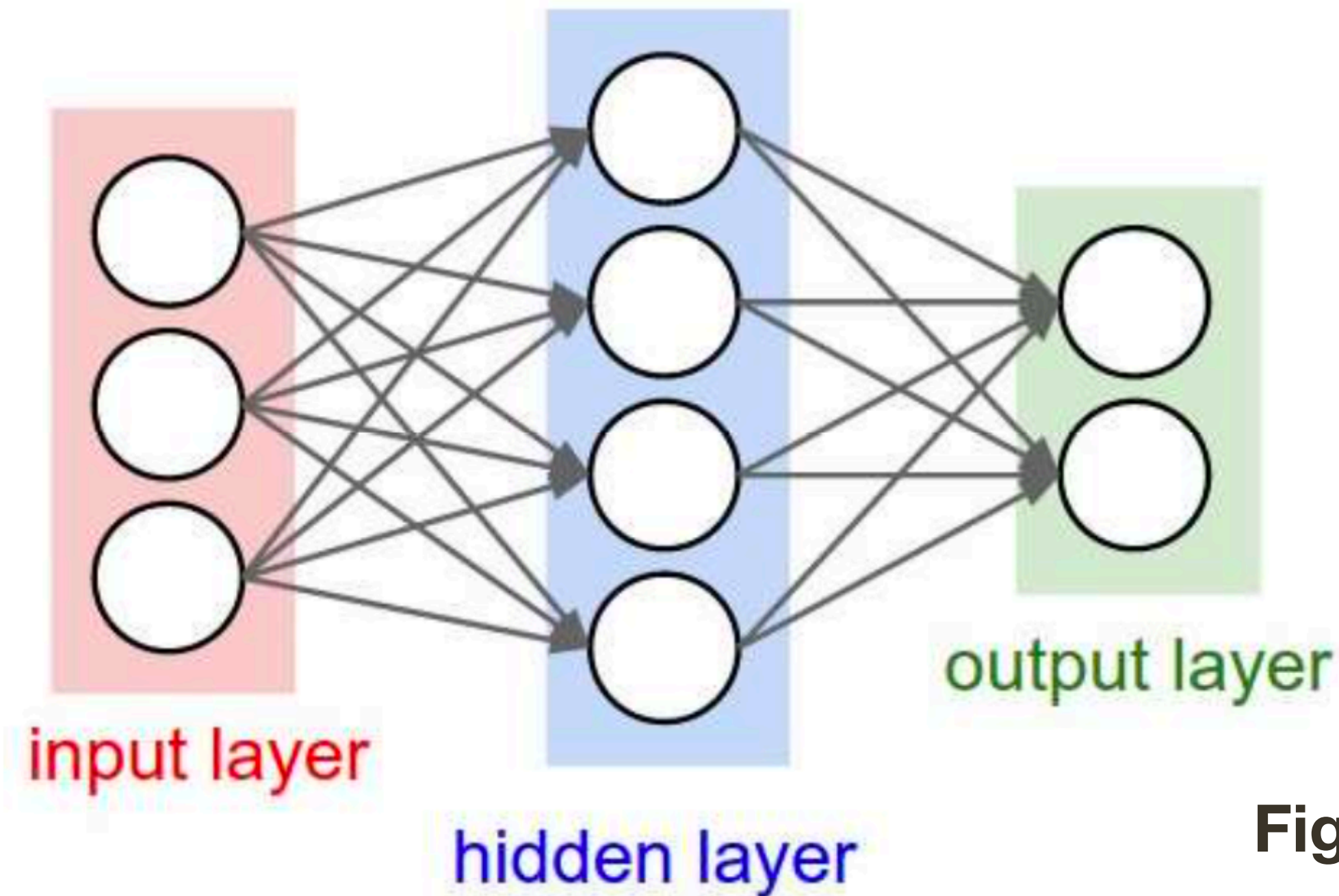
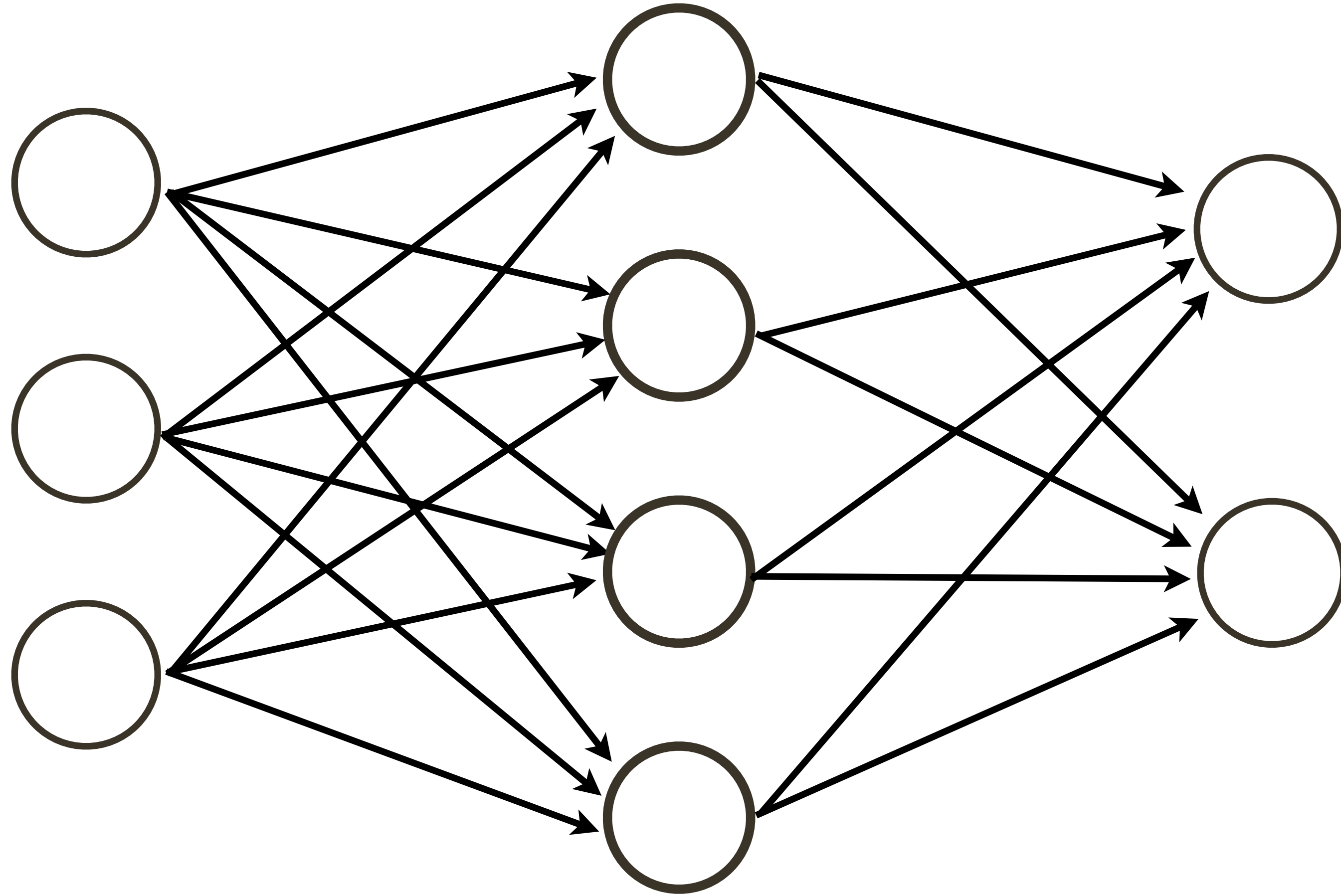


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$$\hat{y} = f(\mathbf{x}, \mathbf{W}_1, \mathbf{W}_2, \mathbf{b}_1, \mathbf{b}_2) = \sigma \left(\mathbf{W}_2^{(2 \times 4)} \sigma \left(\mathbf{W}_1^{(4 \times 3)} \mathbf{x} + \mathbf{b}_1^{(4)} \right) + \mathbf{b}_2^{(2)} \right)$$

Activation Function

Why can't we have **linear** activation functions? Why have non-linear activations?



Activation Function

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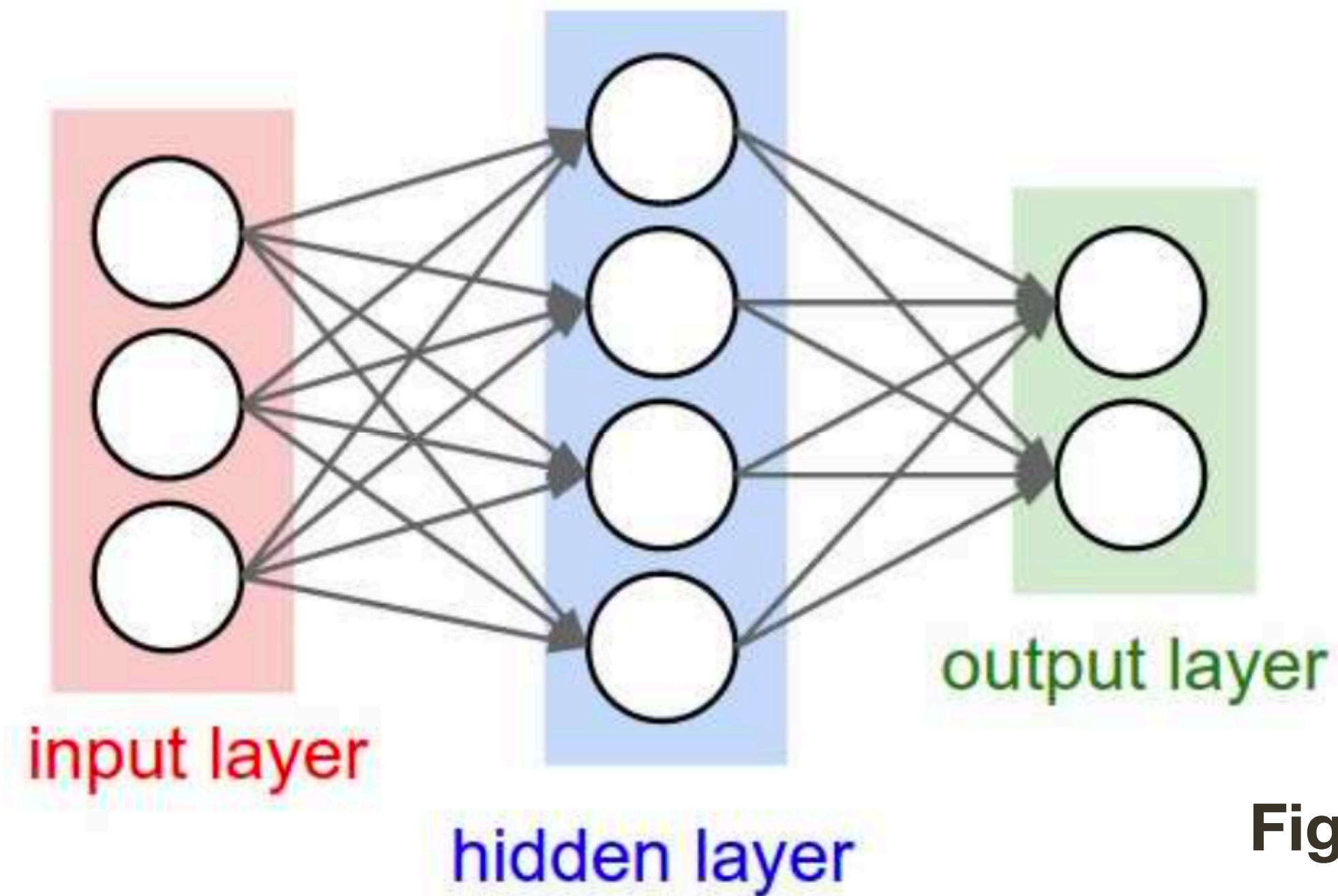


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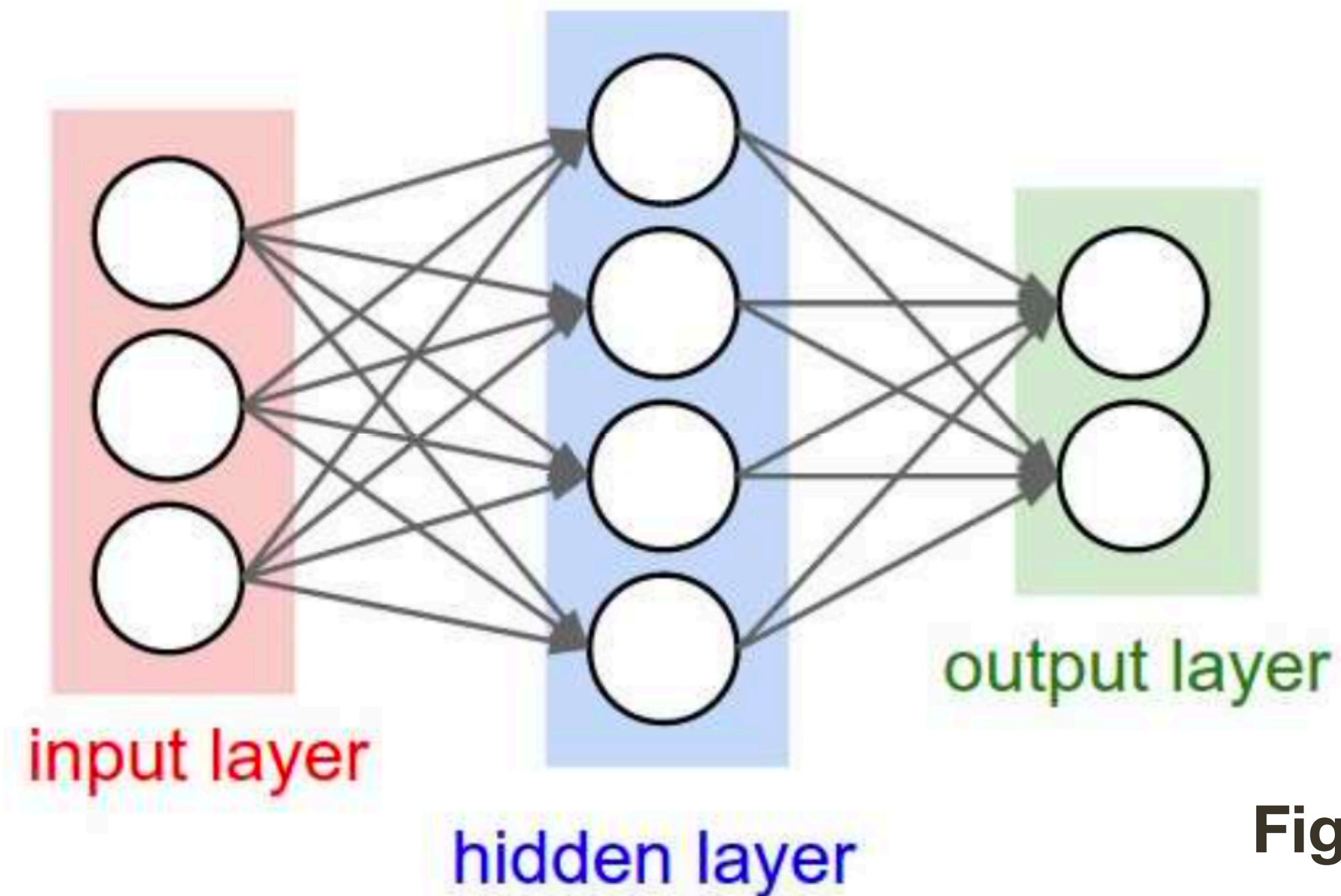


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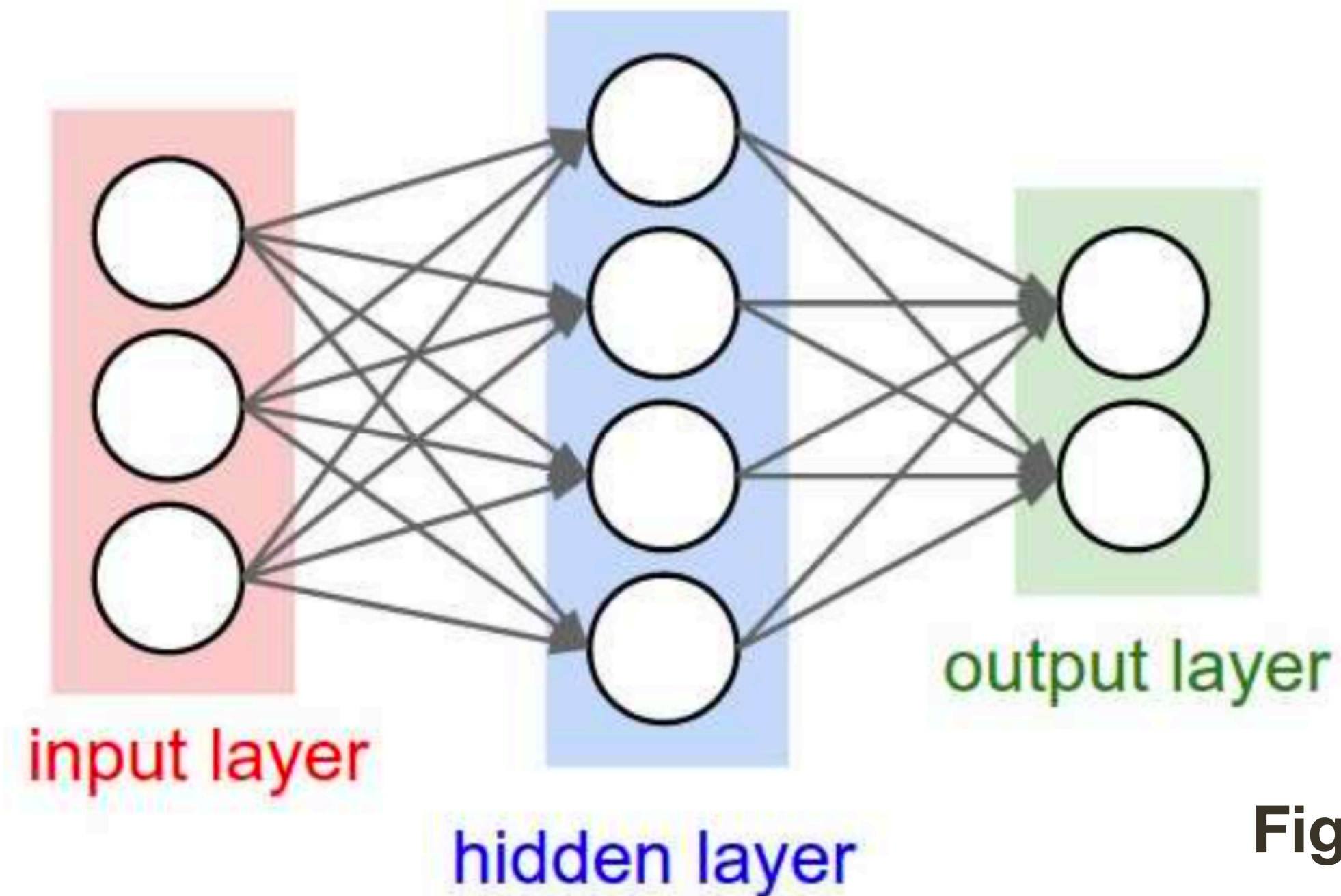


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Activation Function

$$\begin{aligned}\hat{y} &= f(\mathbf{x}, \mathbf{W}_1, \mathbf{W}_2, \mathbf{b}_1, \mathbf{b}_2) = \sigma \left(\mathbf{W}_2^{(2 \times 4)} \sigma \left(\mathbf{W}_1^{(4 \times 3)} \mathbf{x} + \mathbf{b}_1^{(4)} \right) + \mathbf{b}_2^{(2)} \right) \\ &= \mathbf{W}_2^{(2 \times 4)} \left(\mathbf{W}_1^{(4 \times 3)} \mathbf{x} + \mathbf{b}_1^{(4)} \right) + \mathbf{b}_2^{(2)} \\ &= \underbrace{\mathbf{W}_2^{(2 \times 4)} \mathbf{W}_1^{(4 \times 3)}}_{\mathbf{W}_*^{(2 \times 3)}} \mathbf{x} + \underbrace{\mathbf{W}_2^{(2 \times 4)} \mathbf{b}_1^{(4)}}_{\mathbf{b}^{(2)}} + \mathbf{b}_2^{(2)}\end{aligned}$$

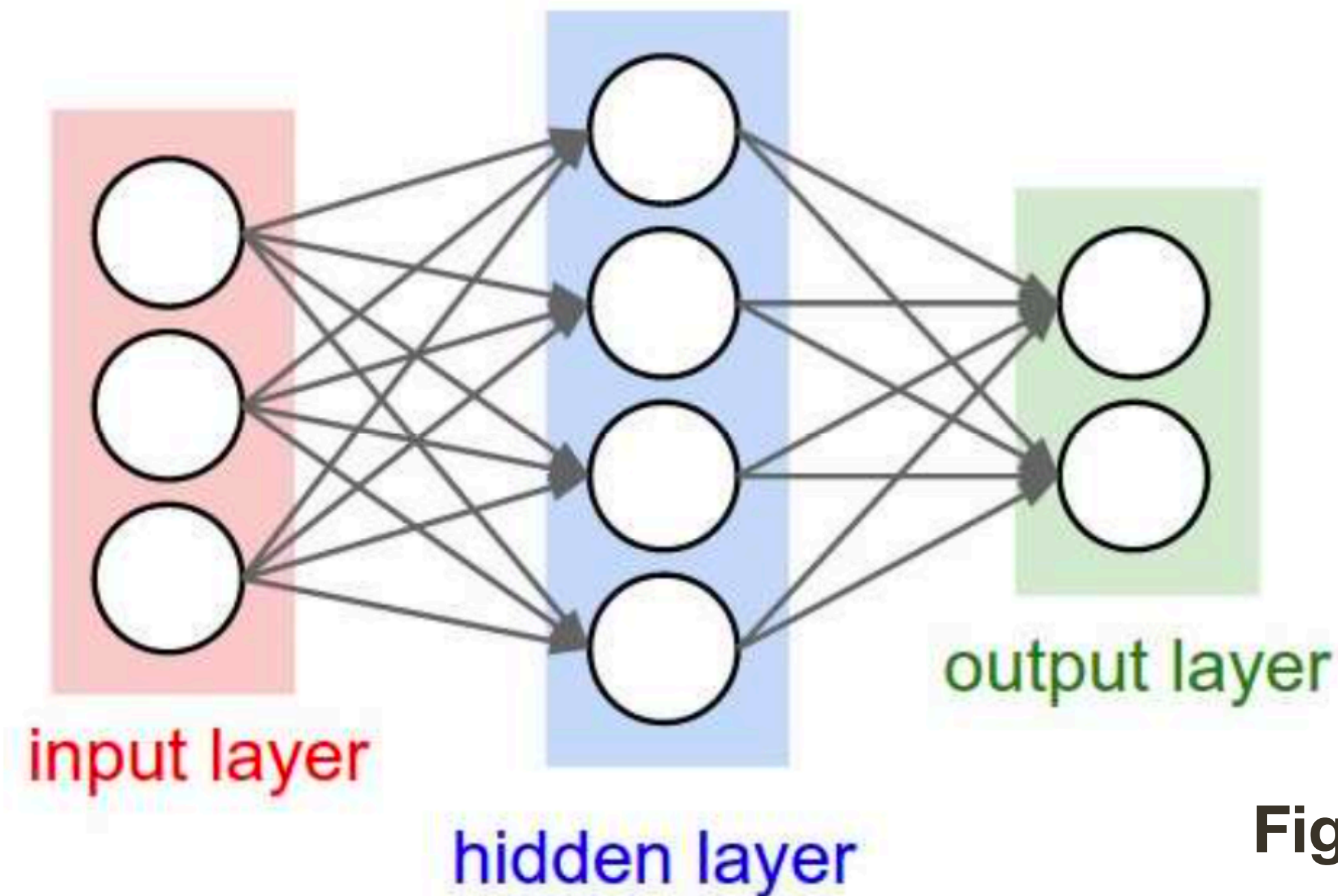
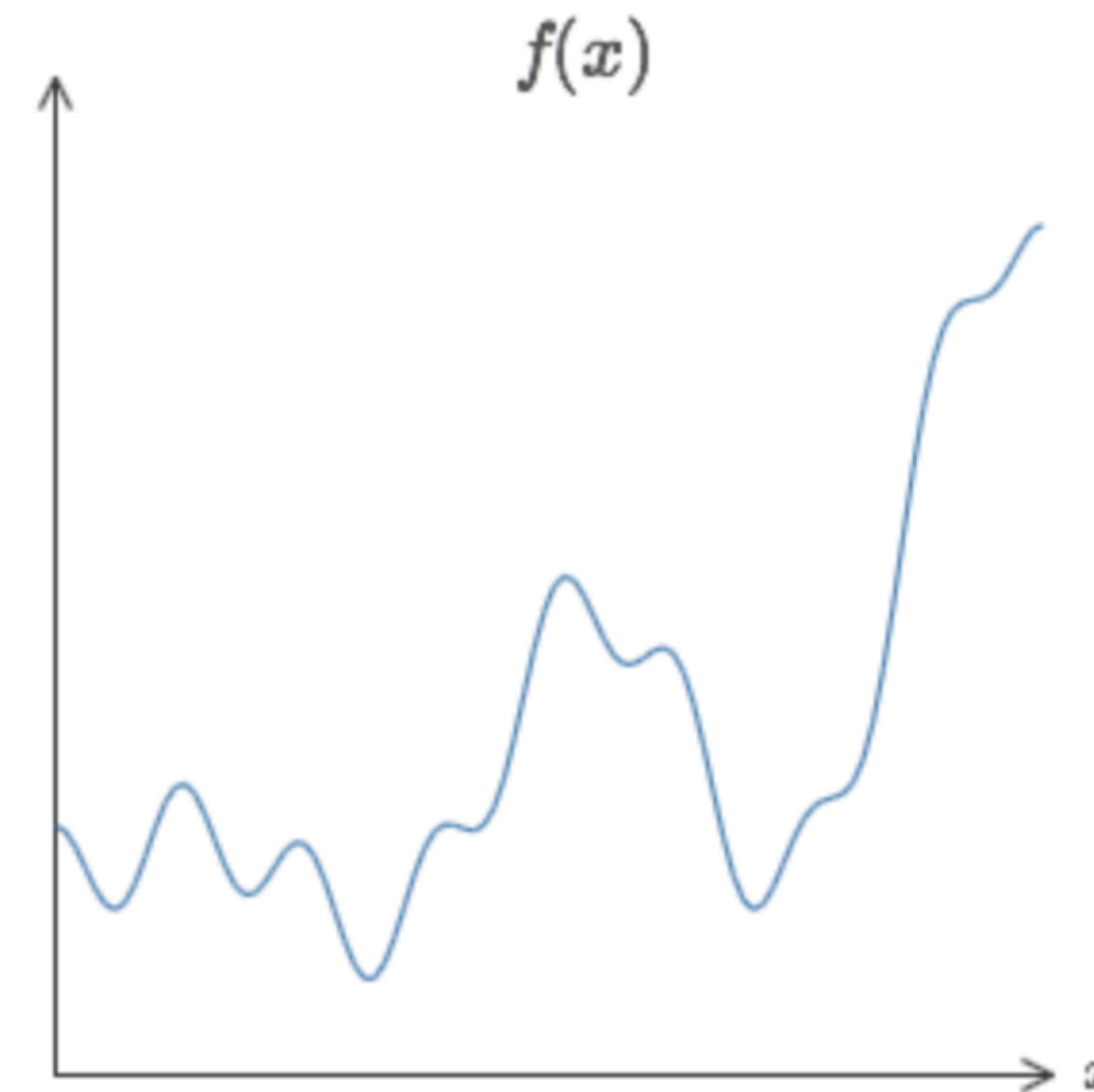


Figure credit: Fei-Fei and Karpathy

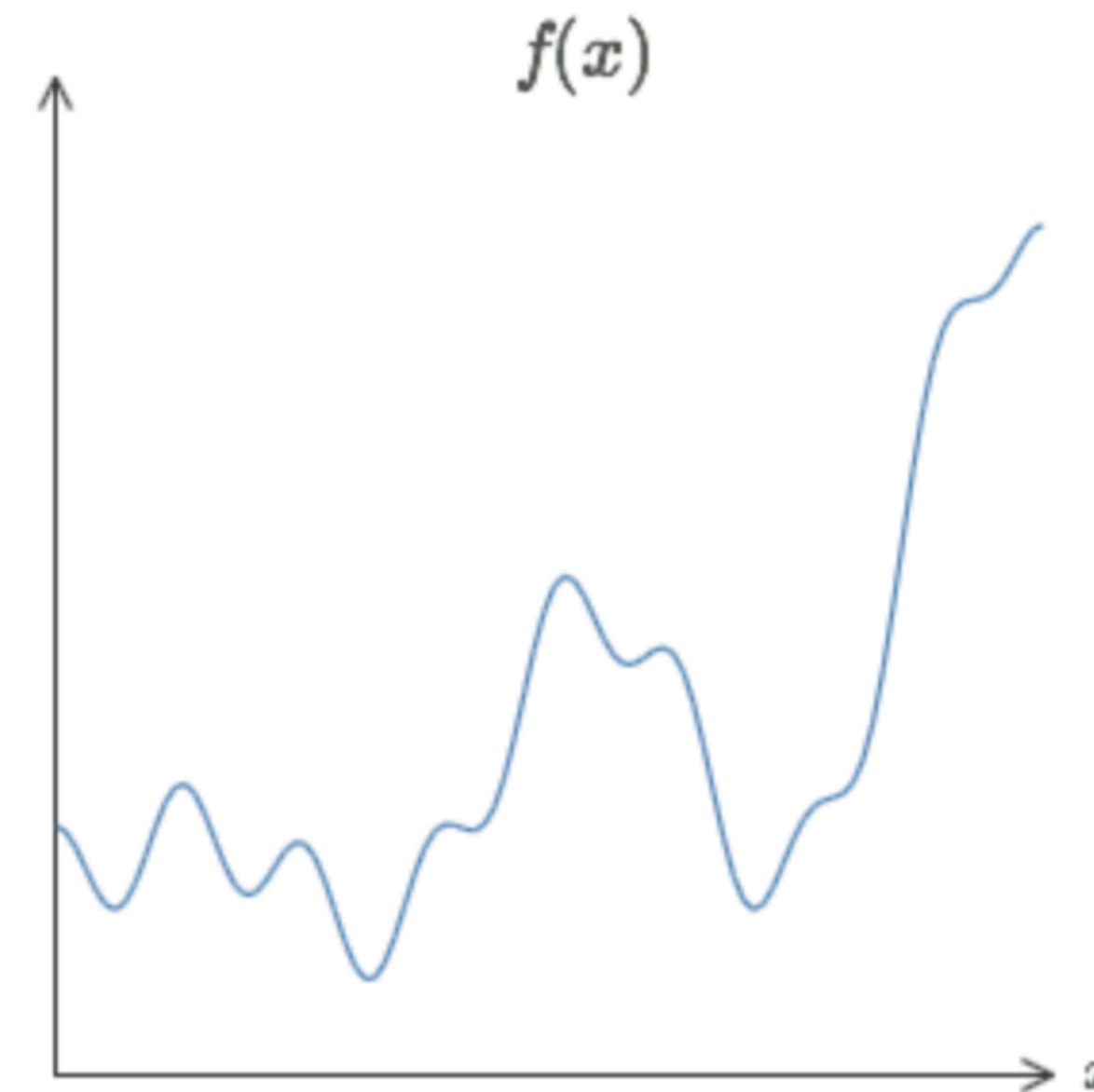
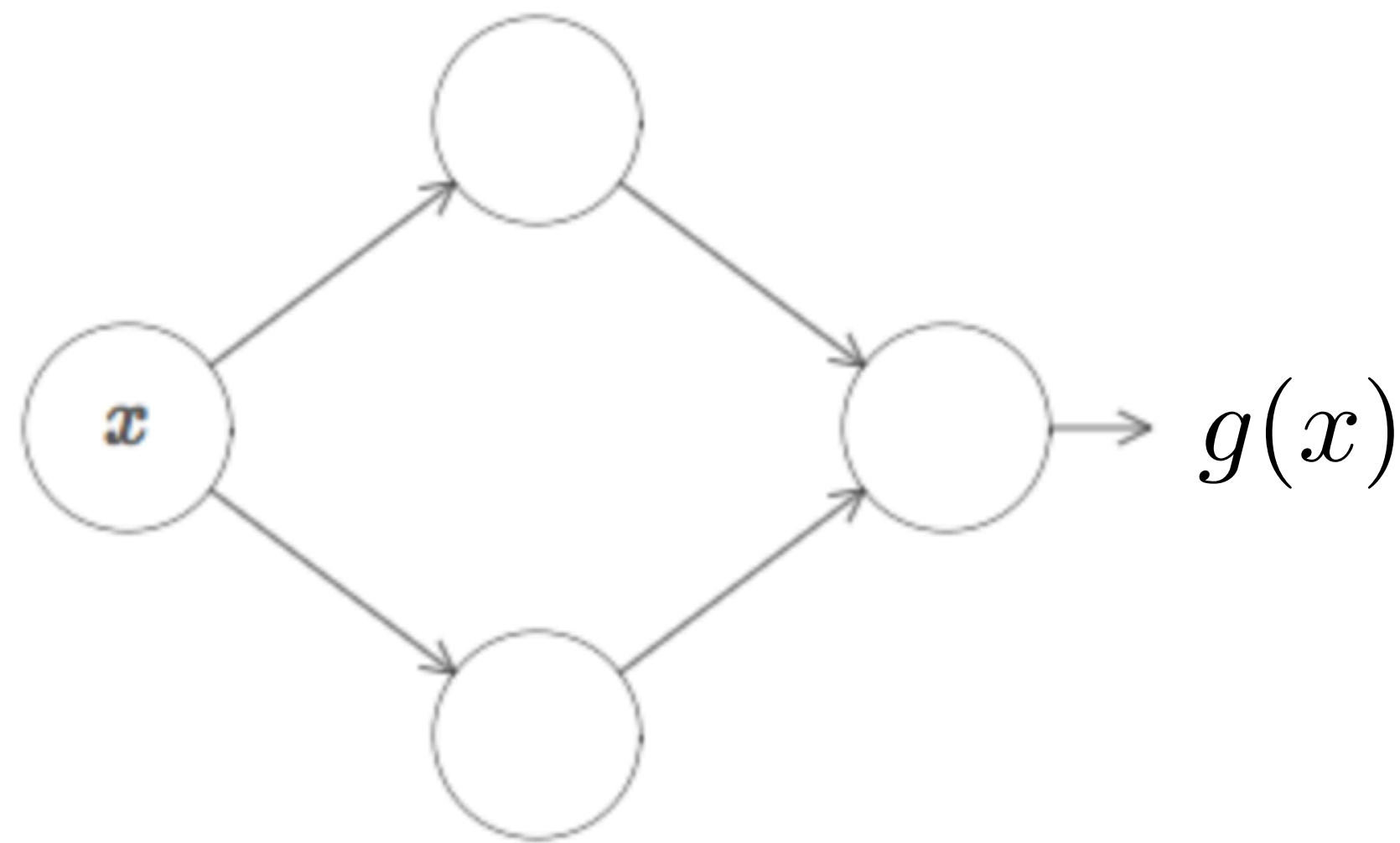
Light Theory: Neural Network as Universal Approximator

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



Light Theory: Neural Network as Universal Approximator

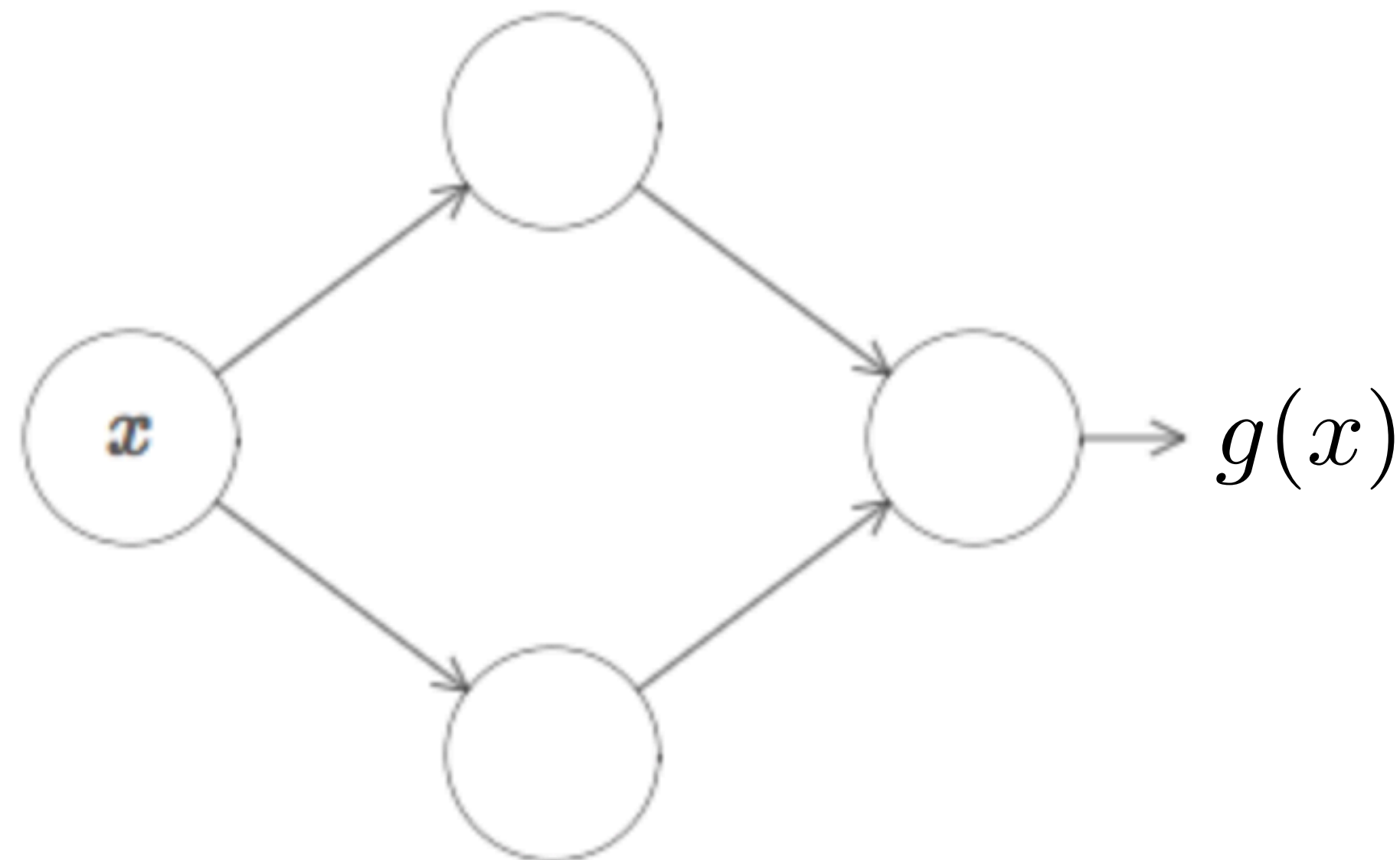
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The guarantee is that by using enough hidden neurons we can always find a neural network whose output $g(x)$ satisfies $|g(x) - f(x)| < \epsilon$ for an arbitrarily small ϵ

Light Theory: Neural Network as Universal Approximator

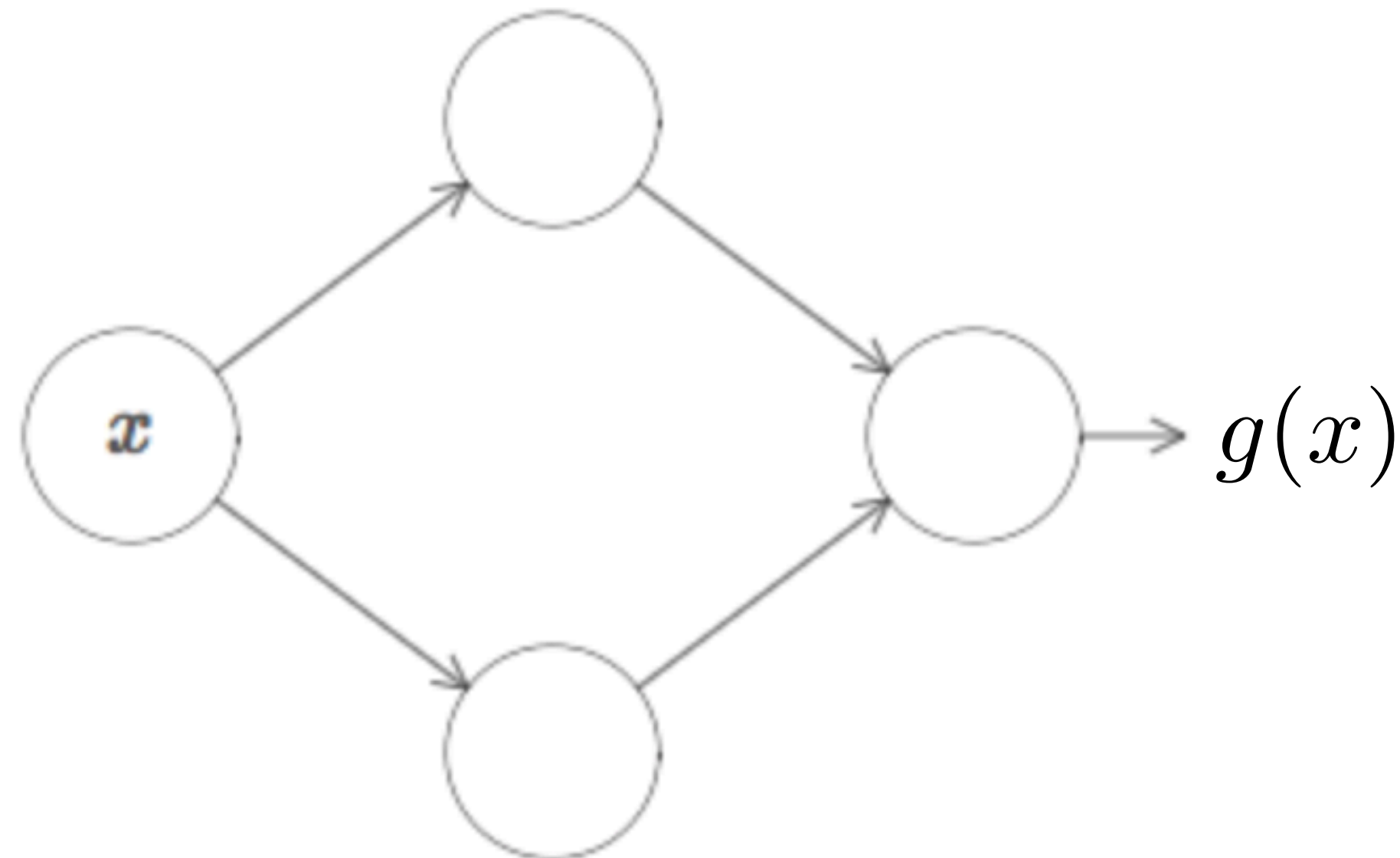
Lets start with a simple network: one hidden layer with two hidden neurons and a single output layer with one neuron (with sigmoid activations)



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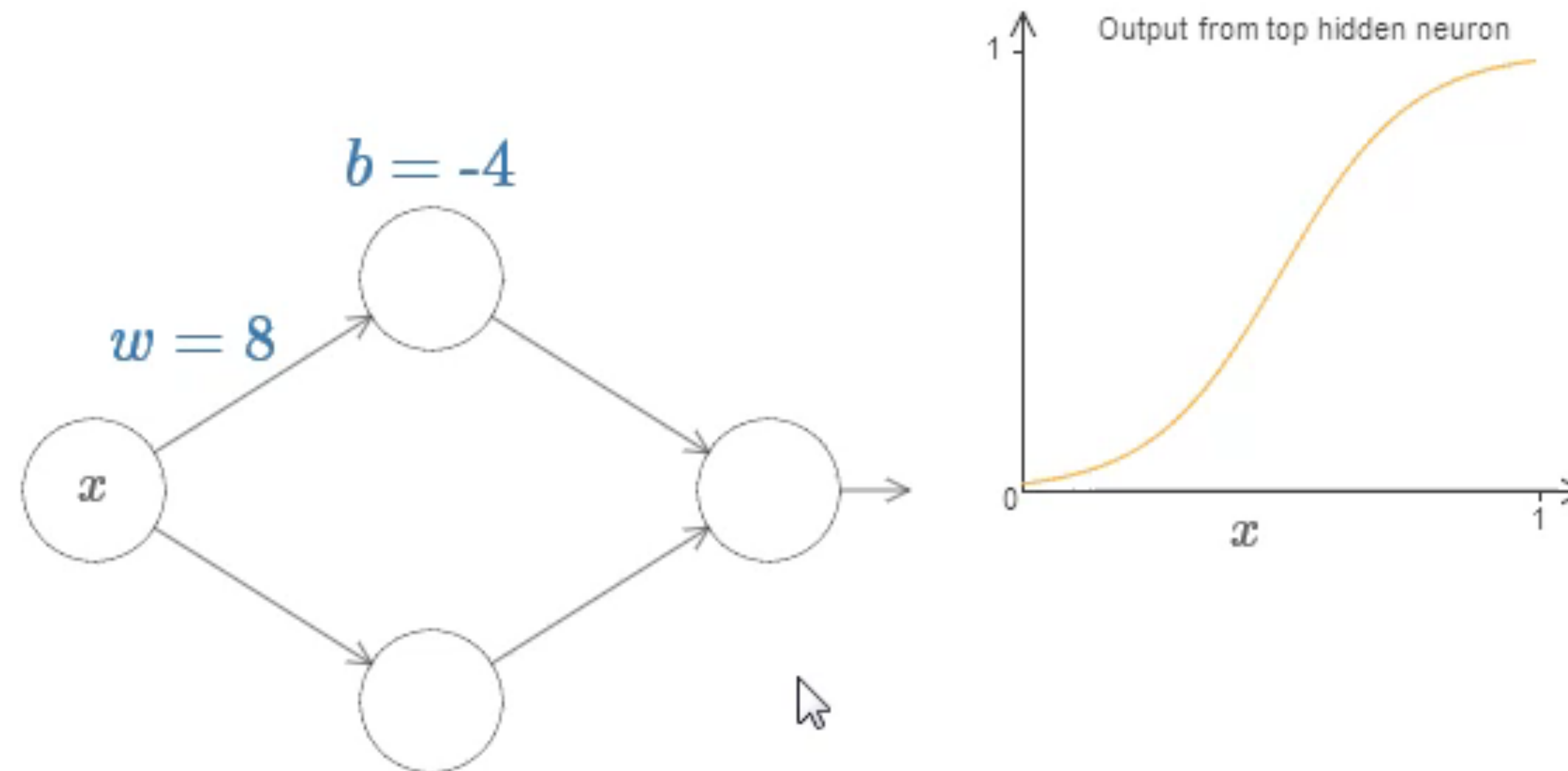
Let's look at output of this (hidden) neuron as a function of parameters (weight, bias)



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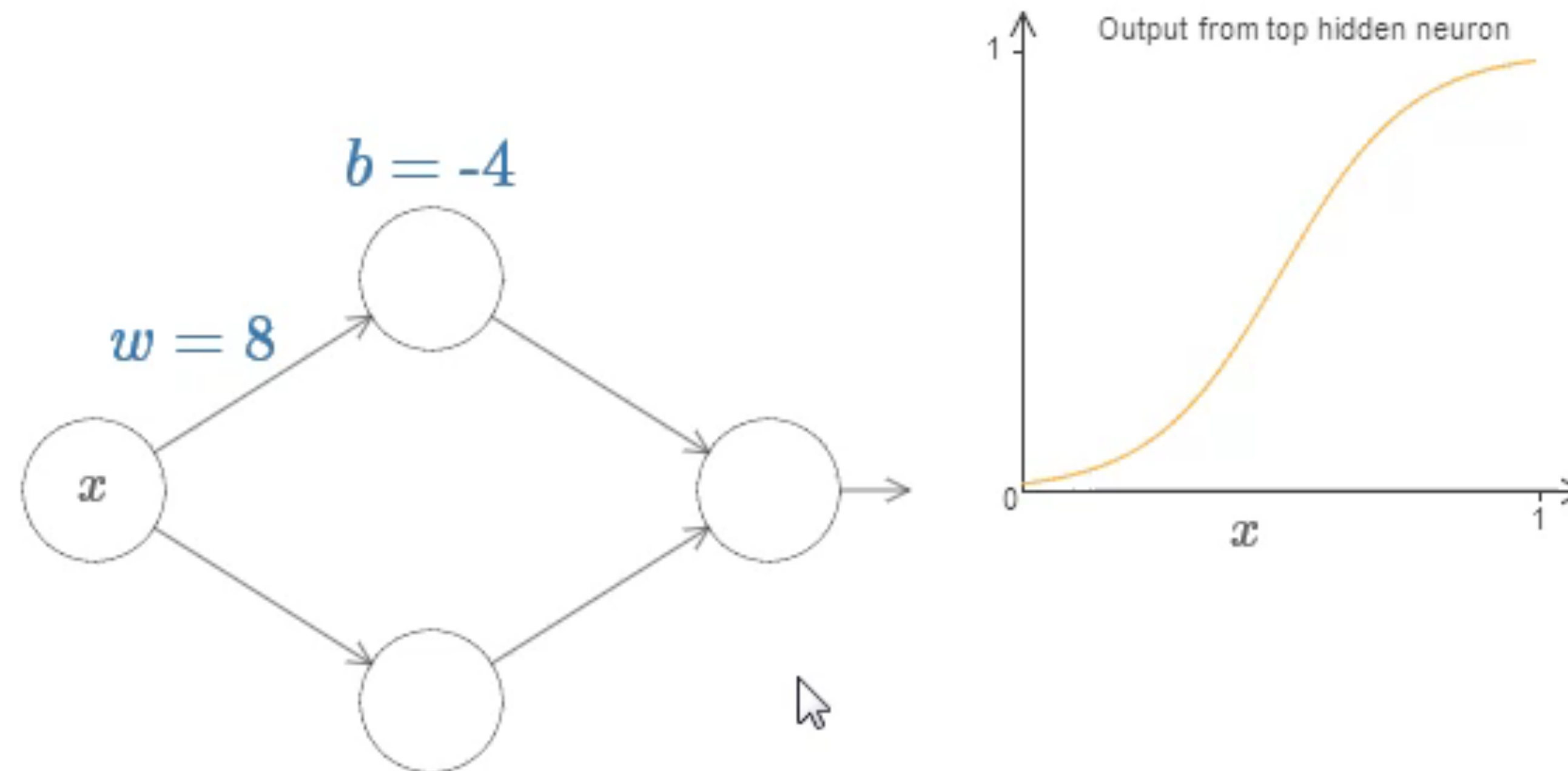
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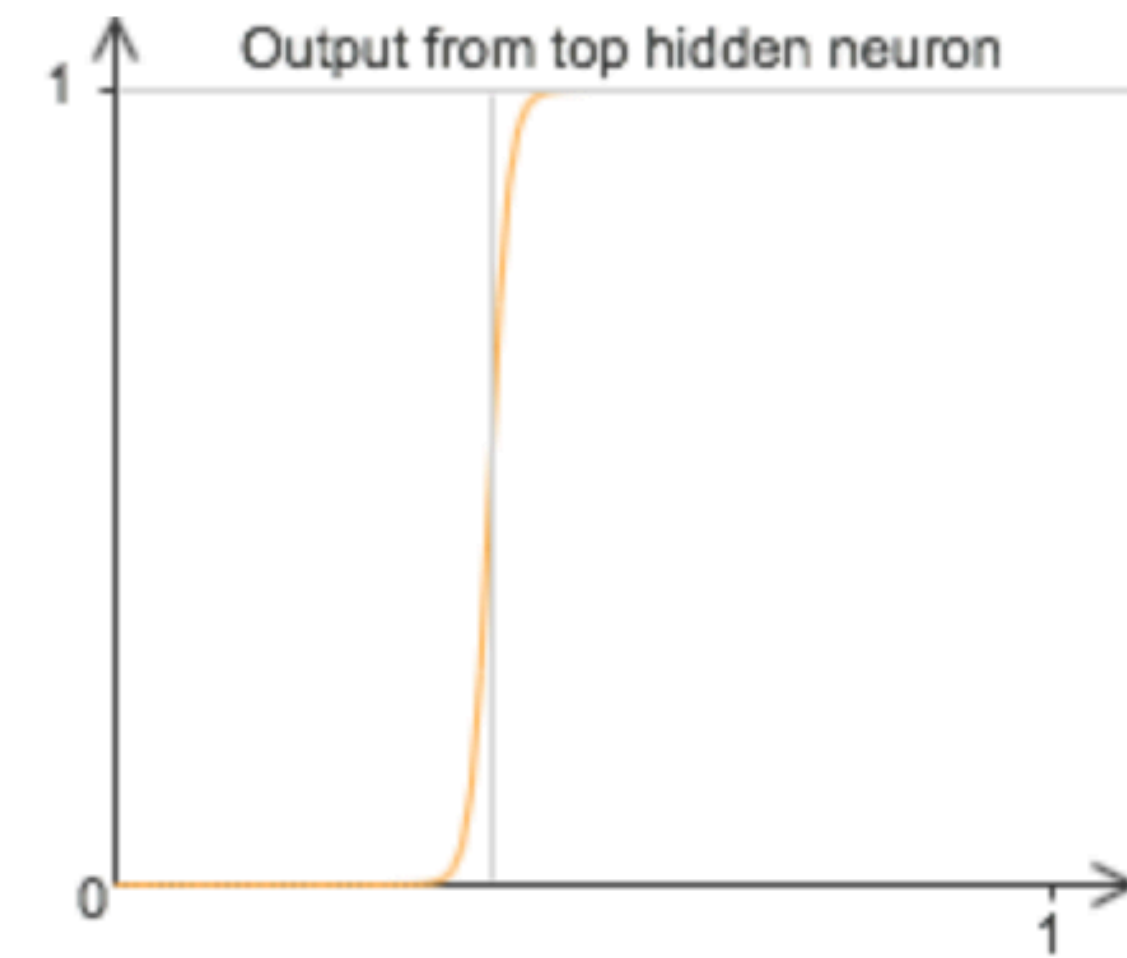
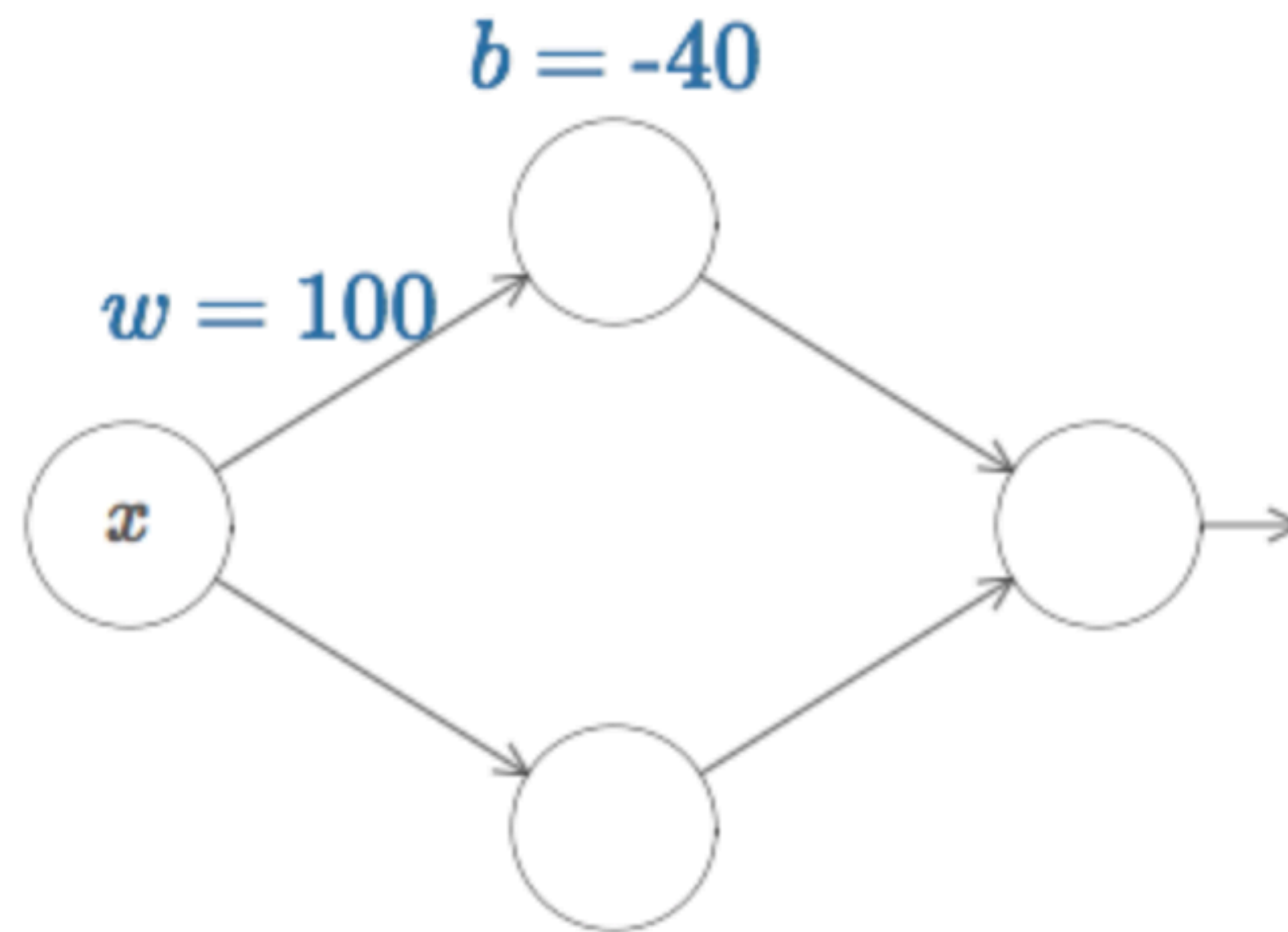
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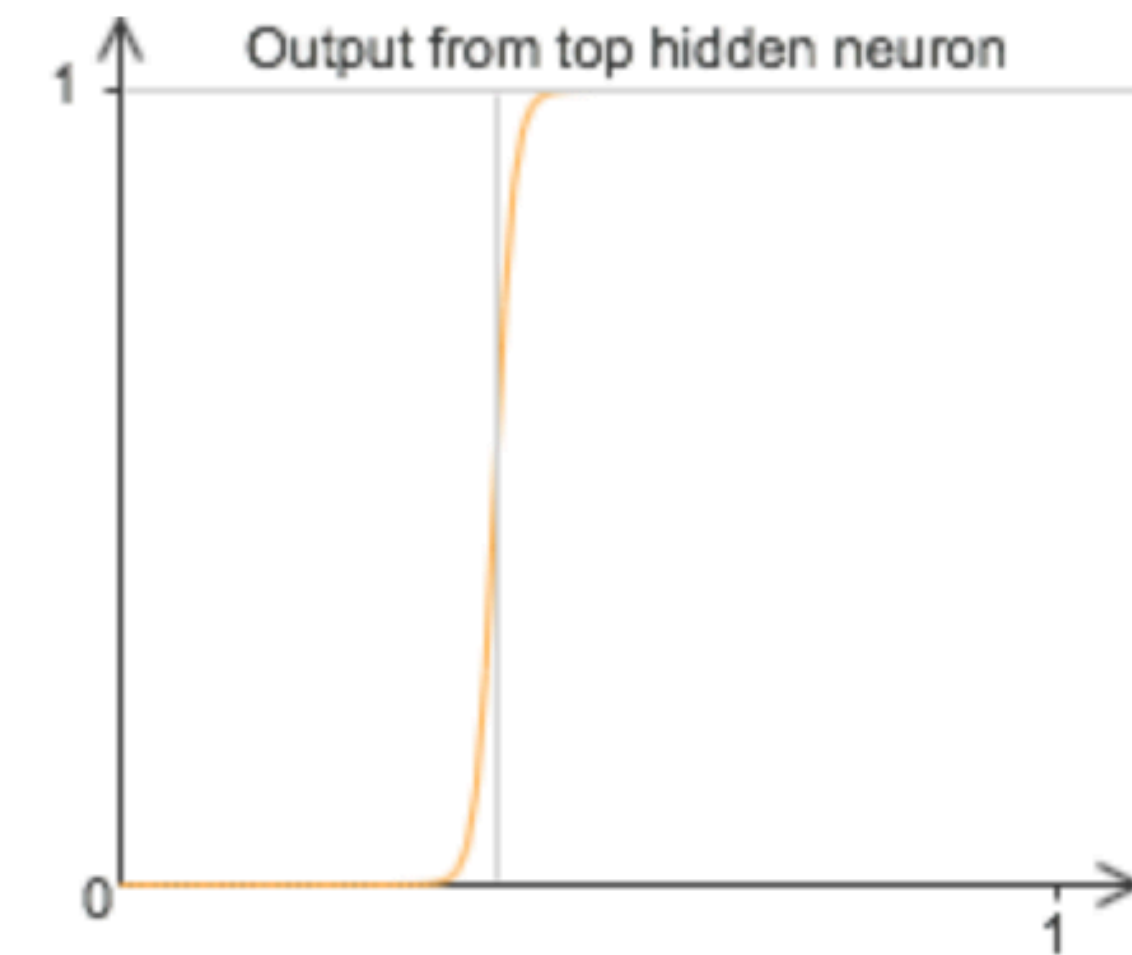
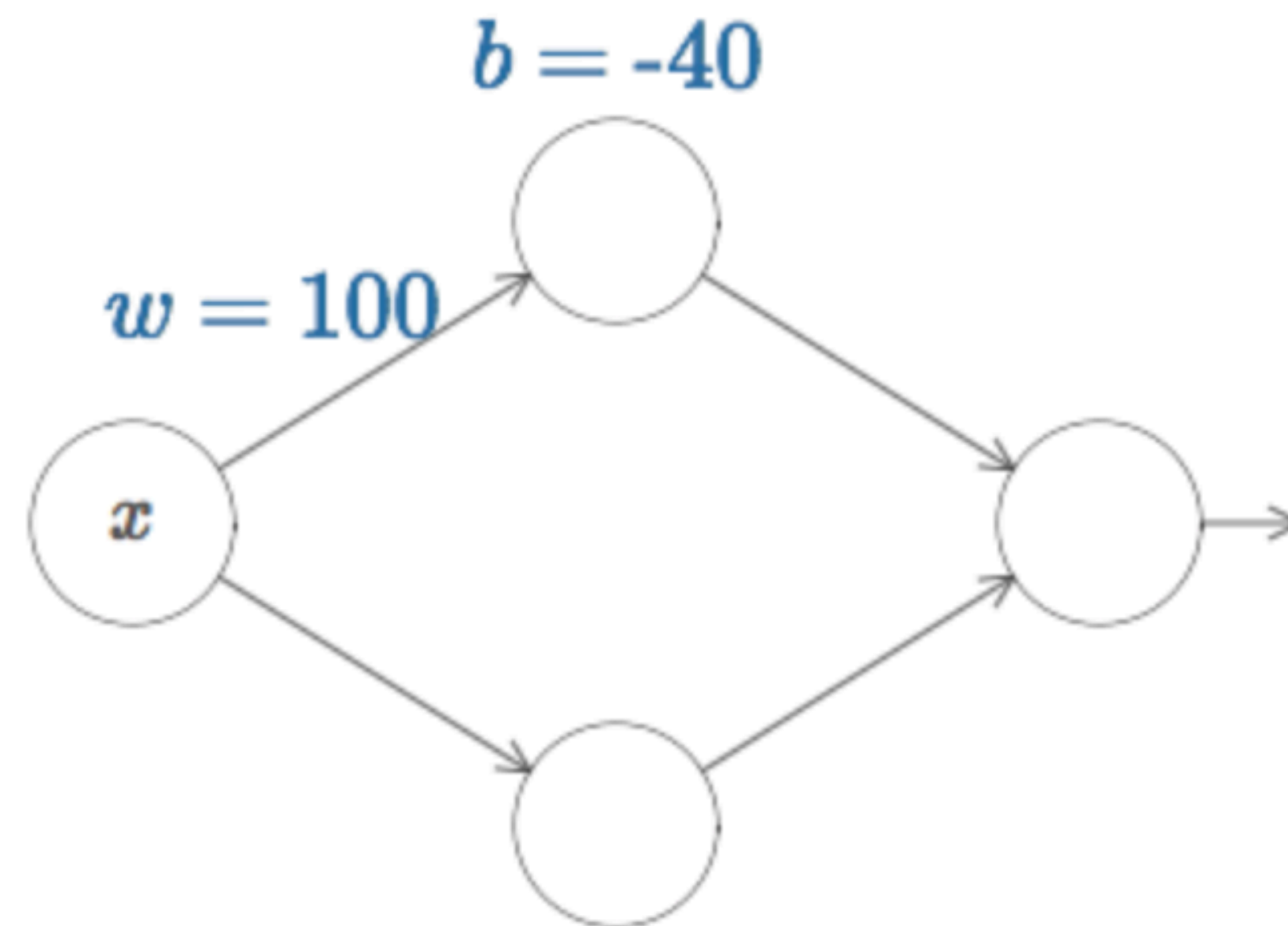
By dialing up the weight (e.g. $w = 999$) we can actually create a “step” function



Light Theory: Neural Network as Universal Approximator

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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.

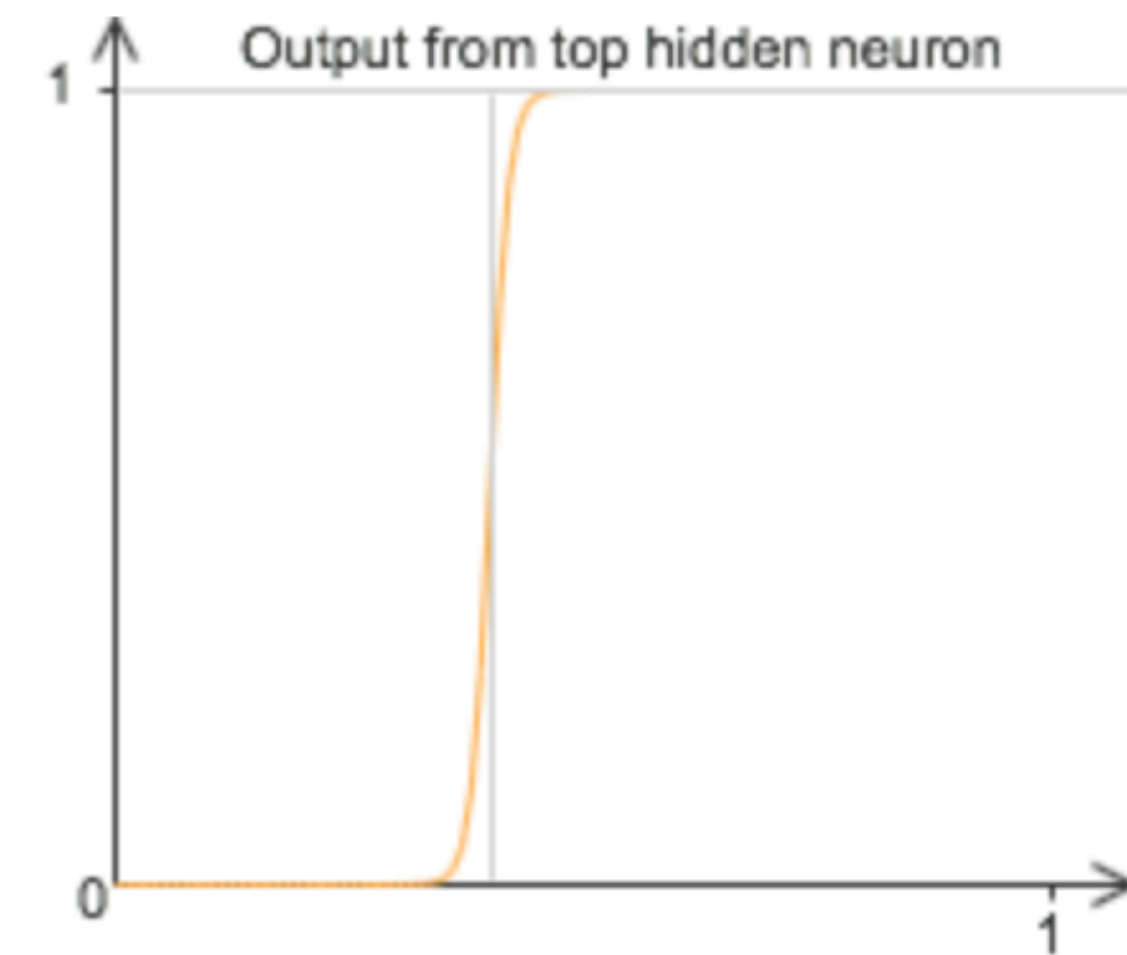
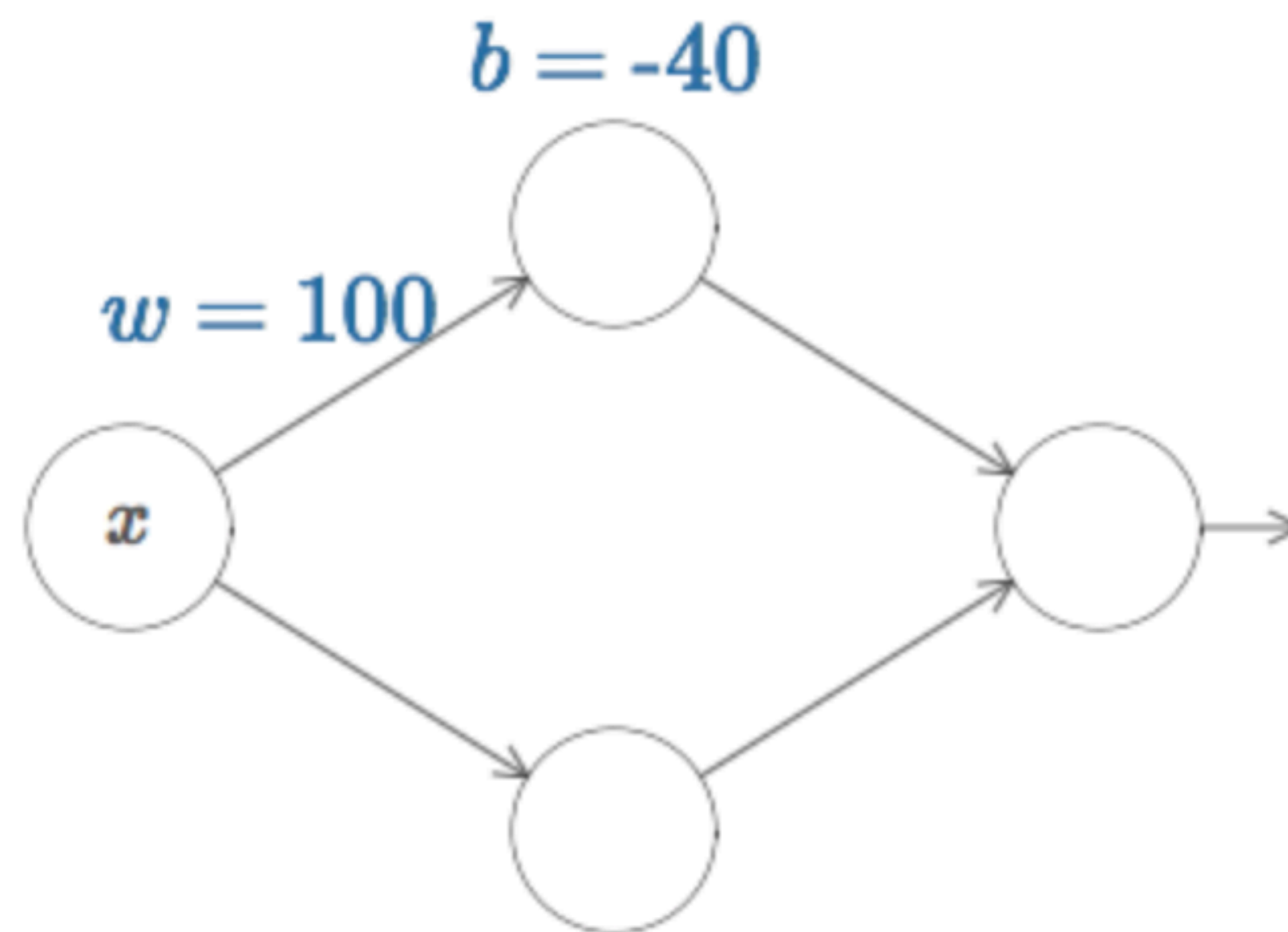


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Location of the step?



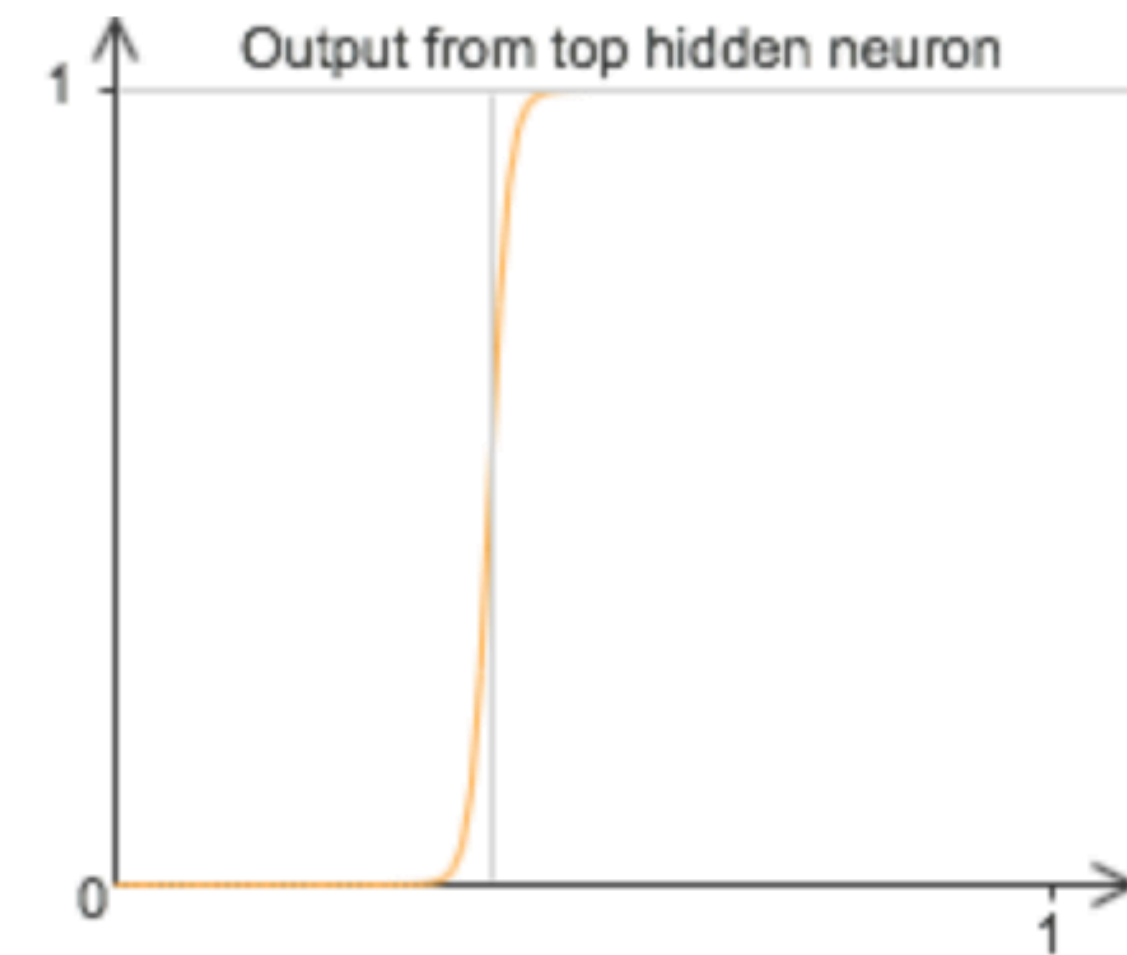
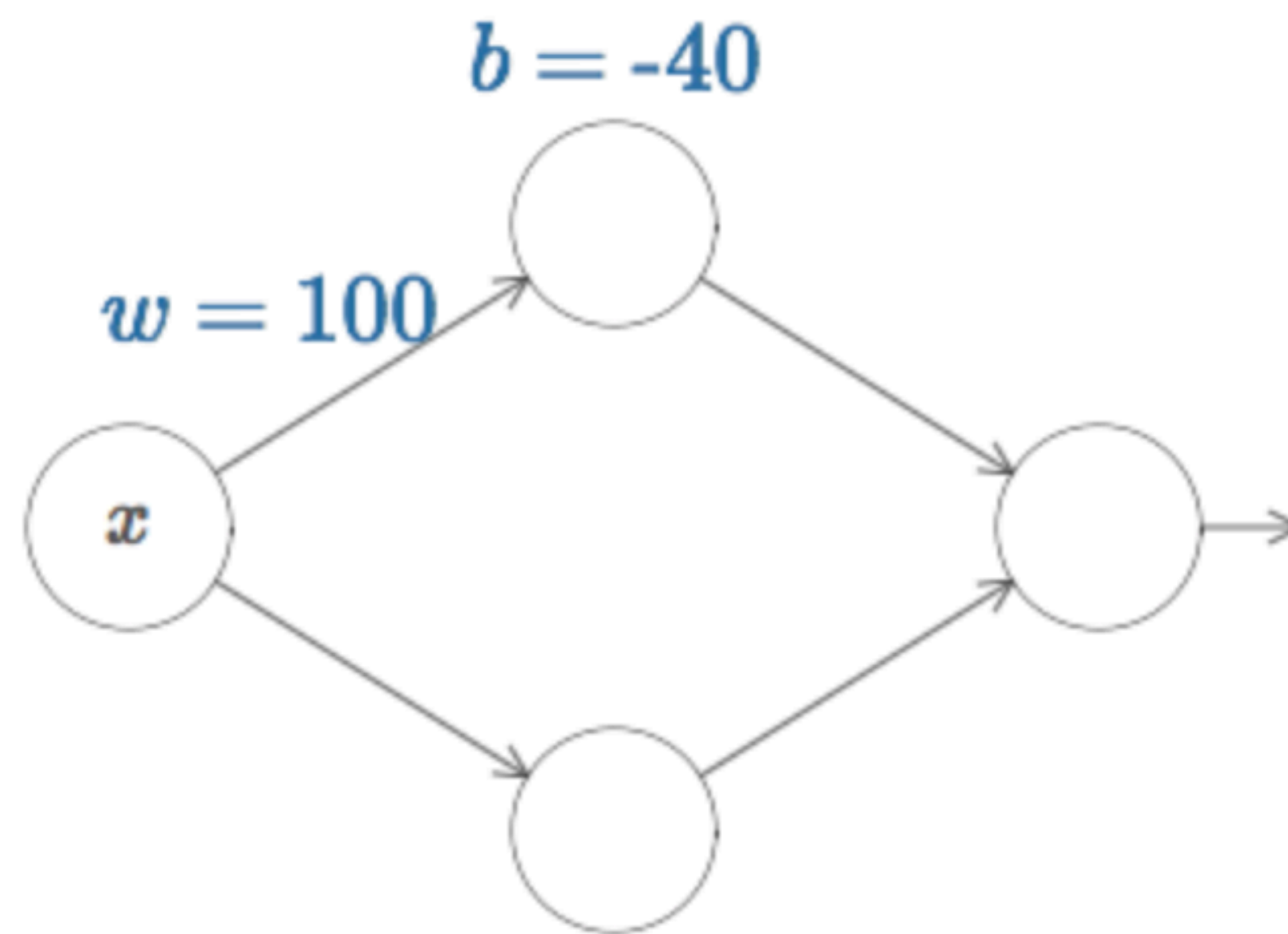
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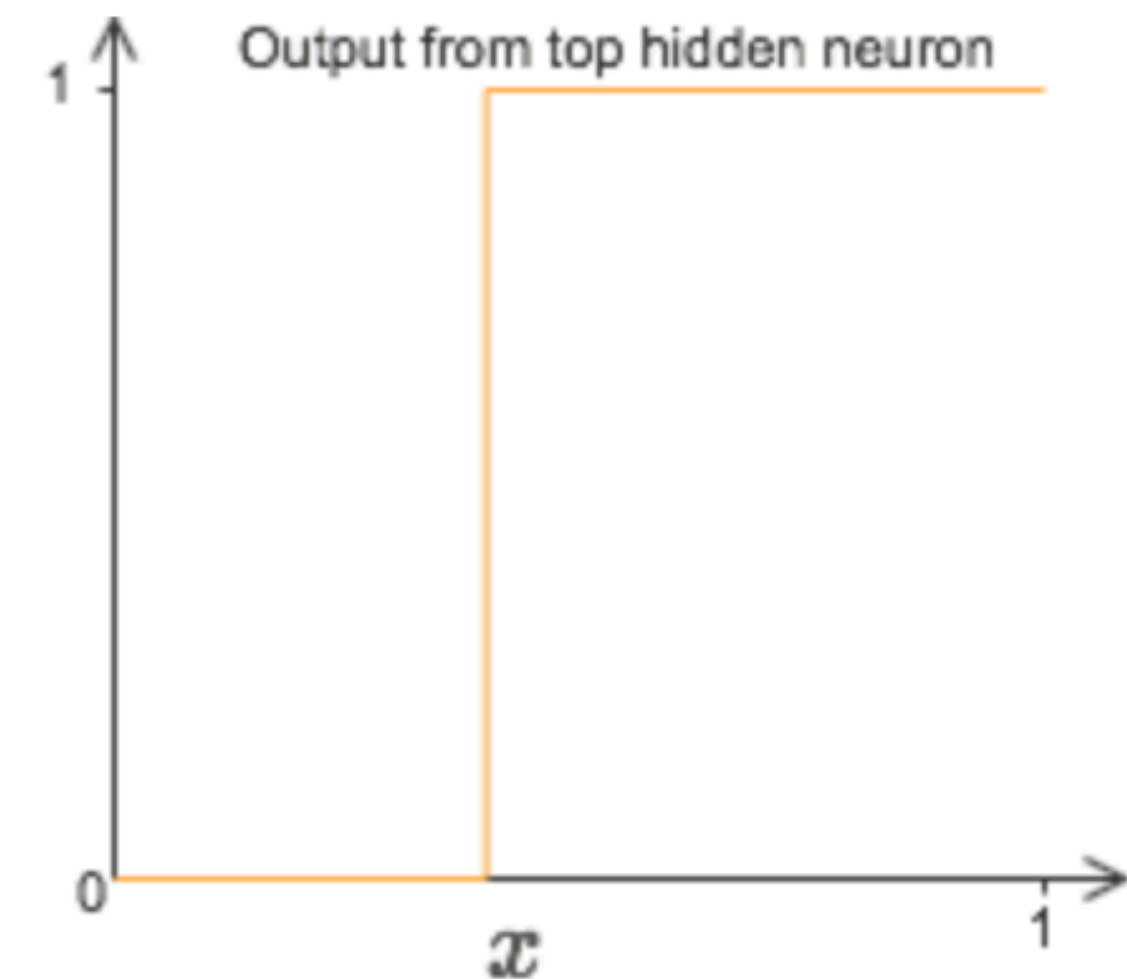
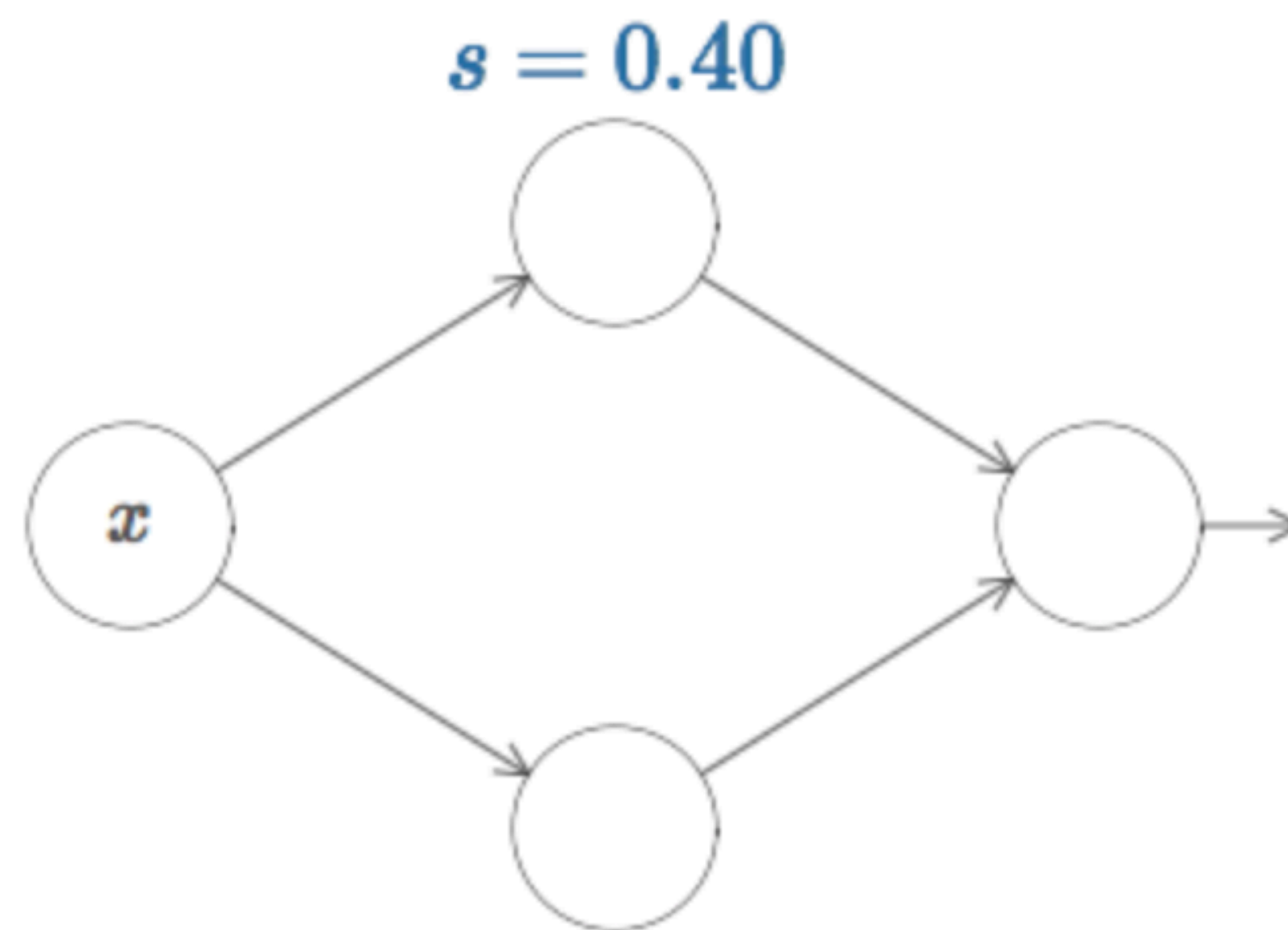
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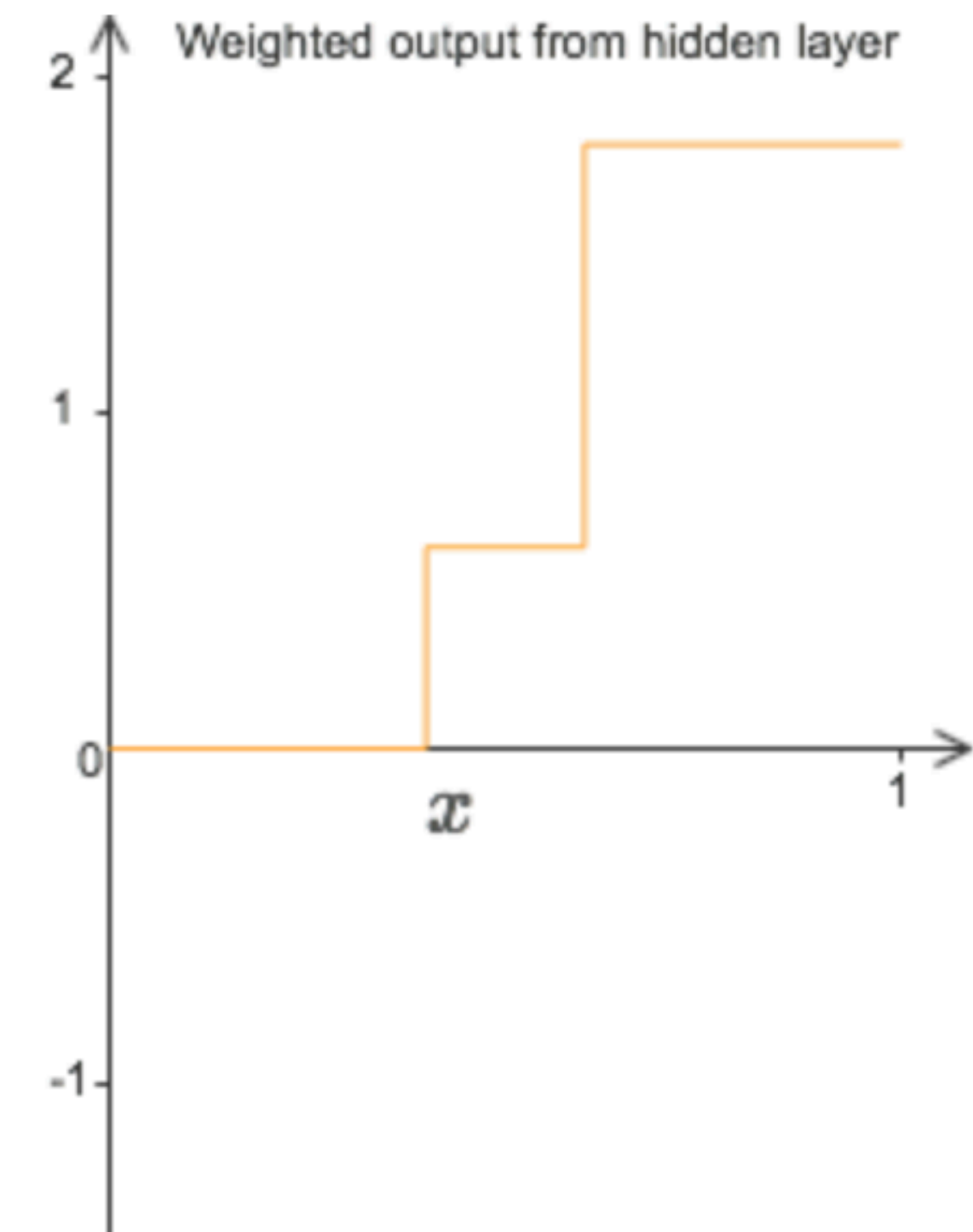
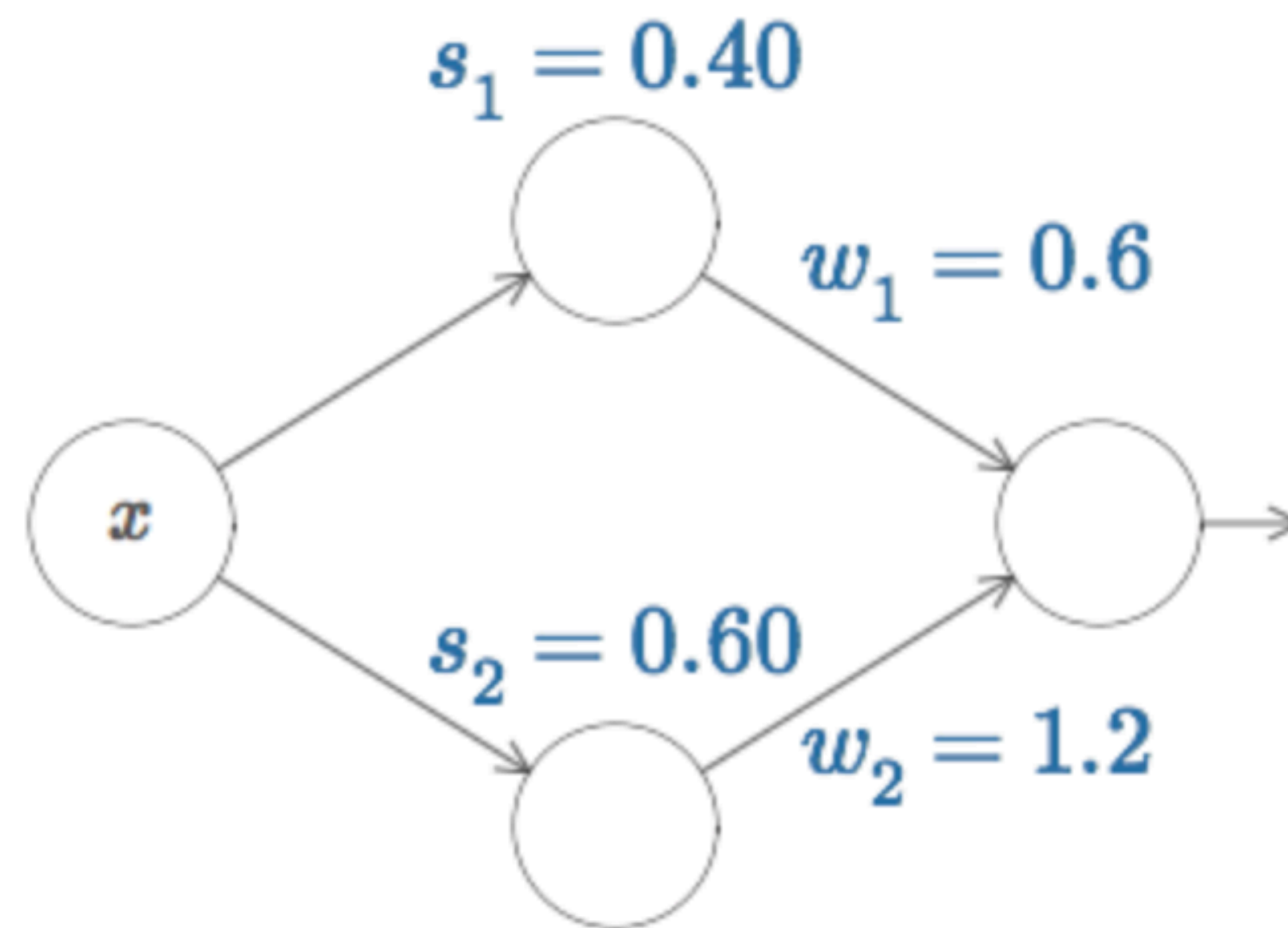
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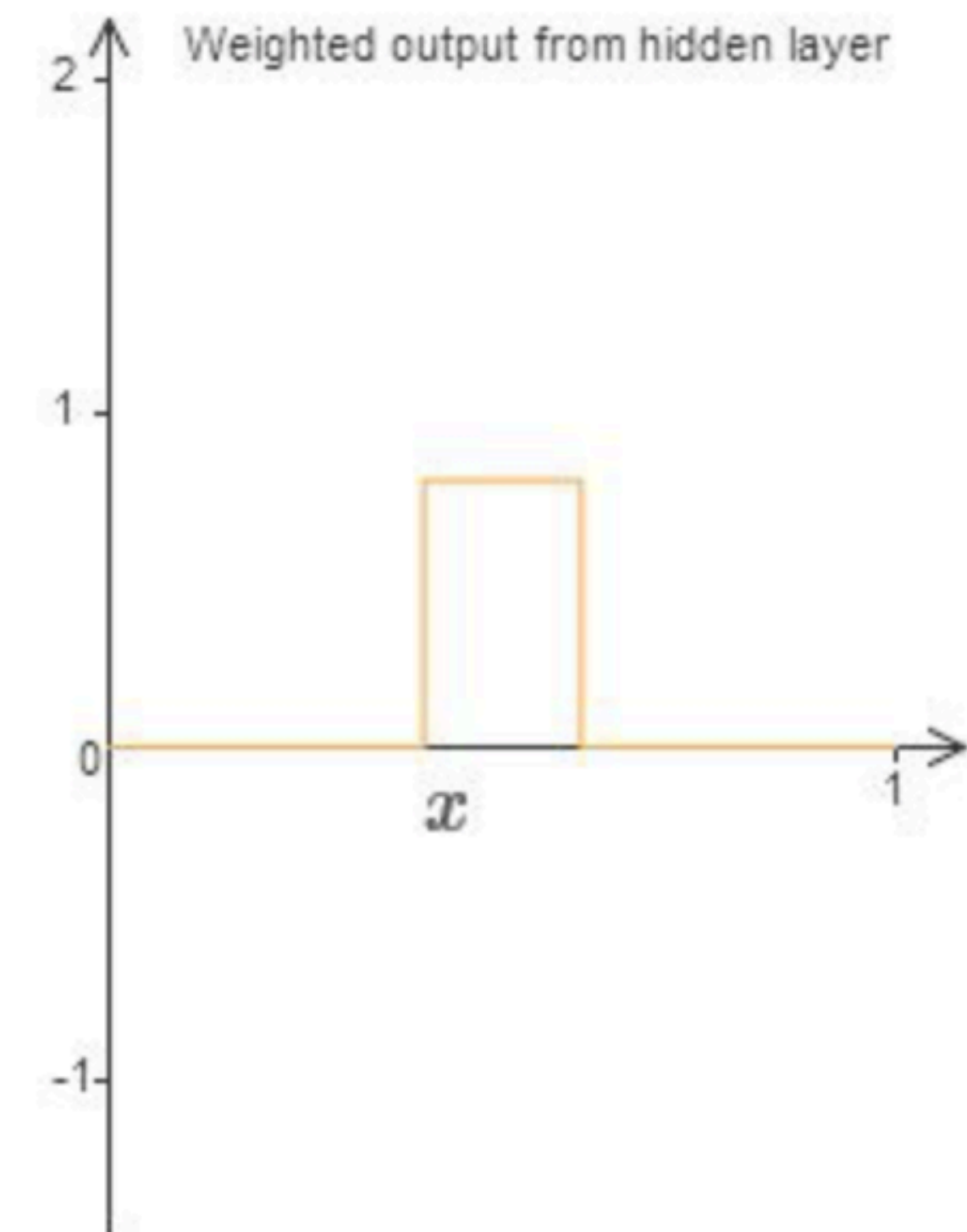
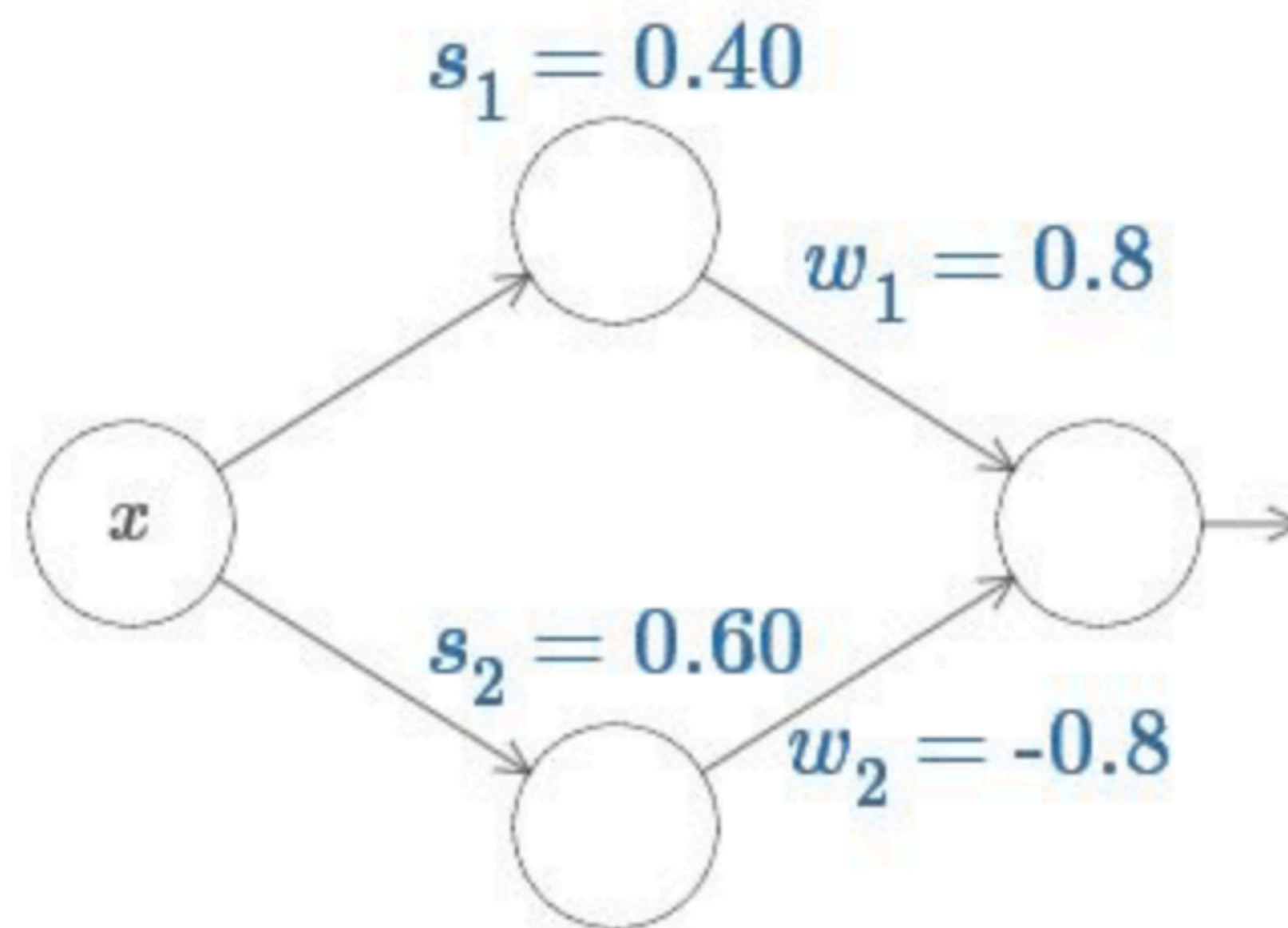
Light Theory: Neural Network as Universal Approximator

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



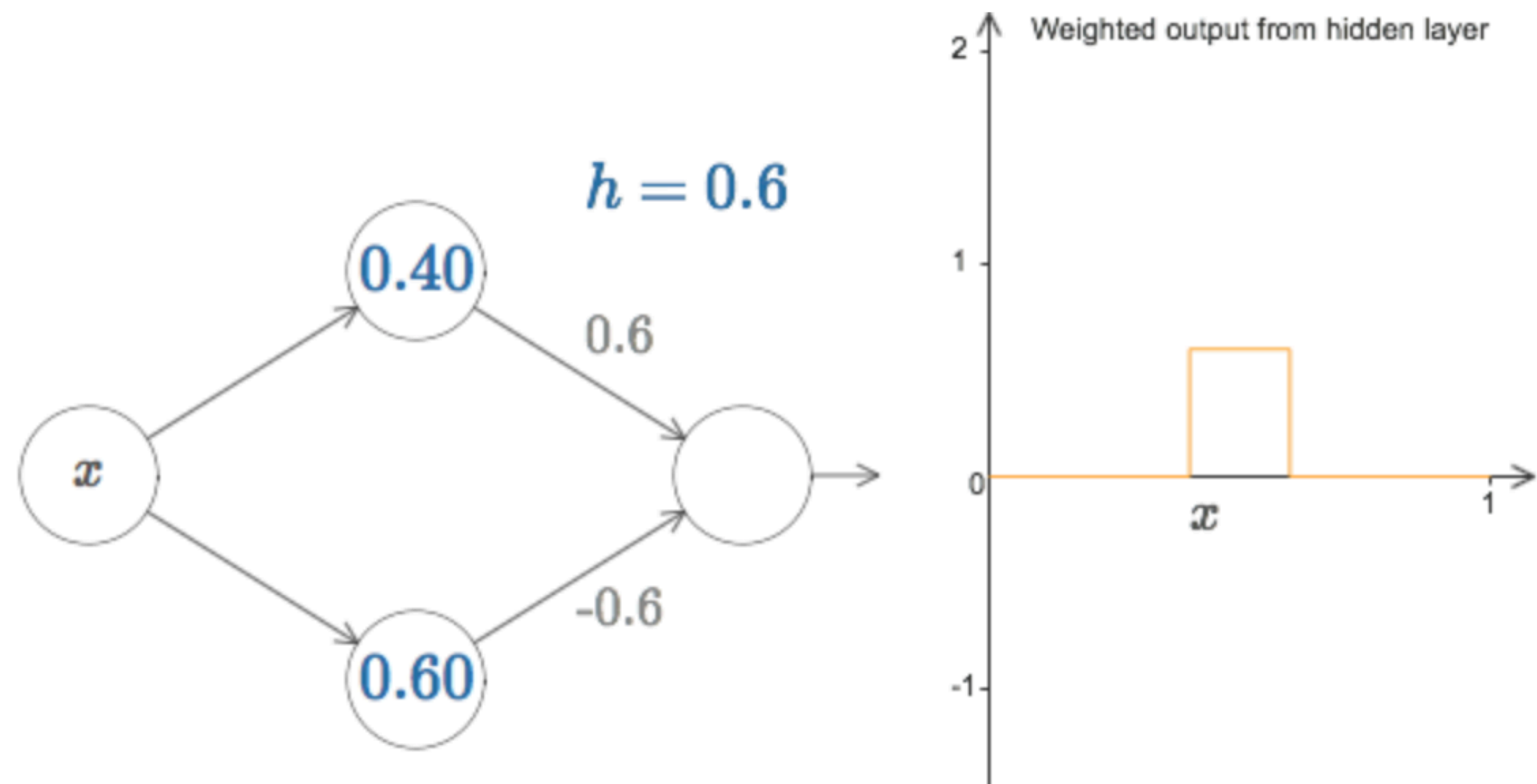
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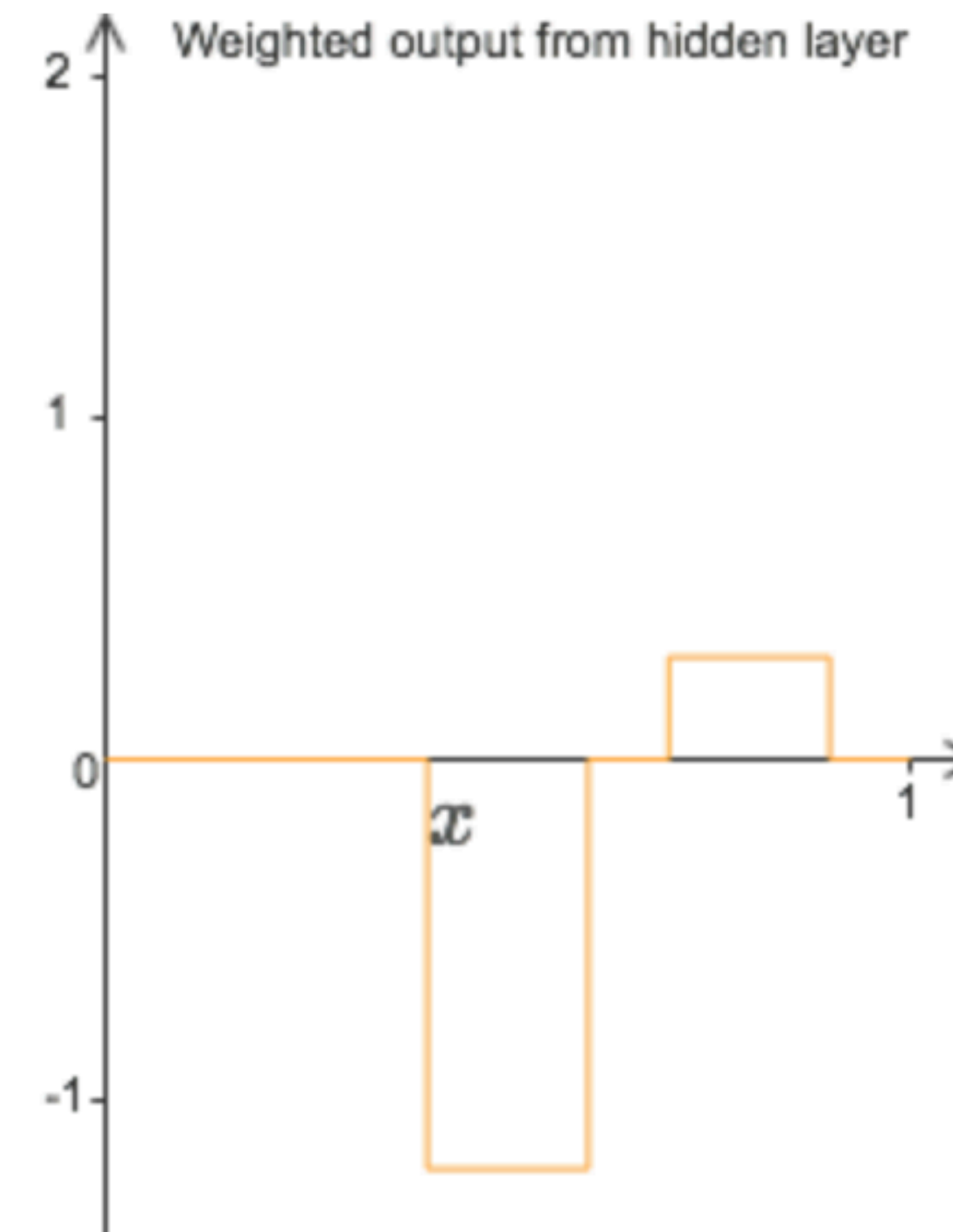
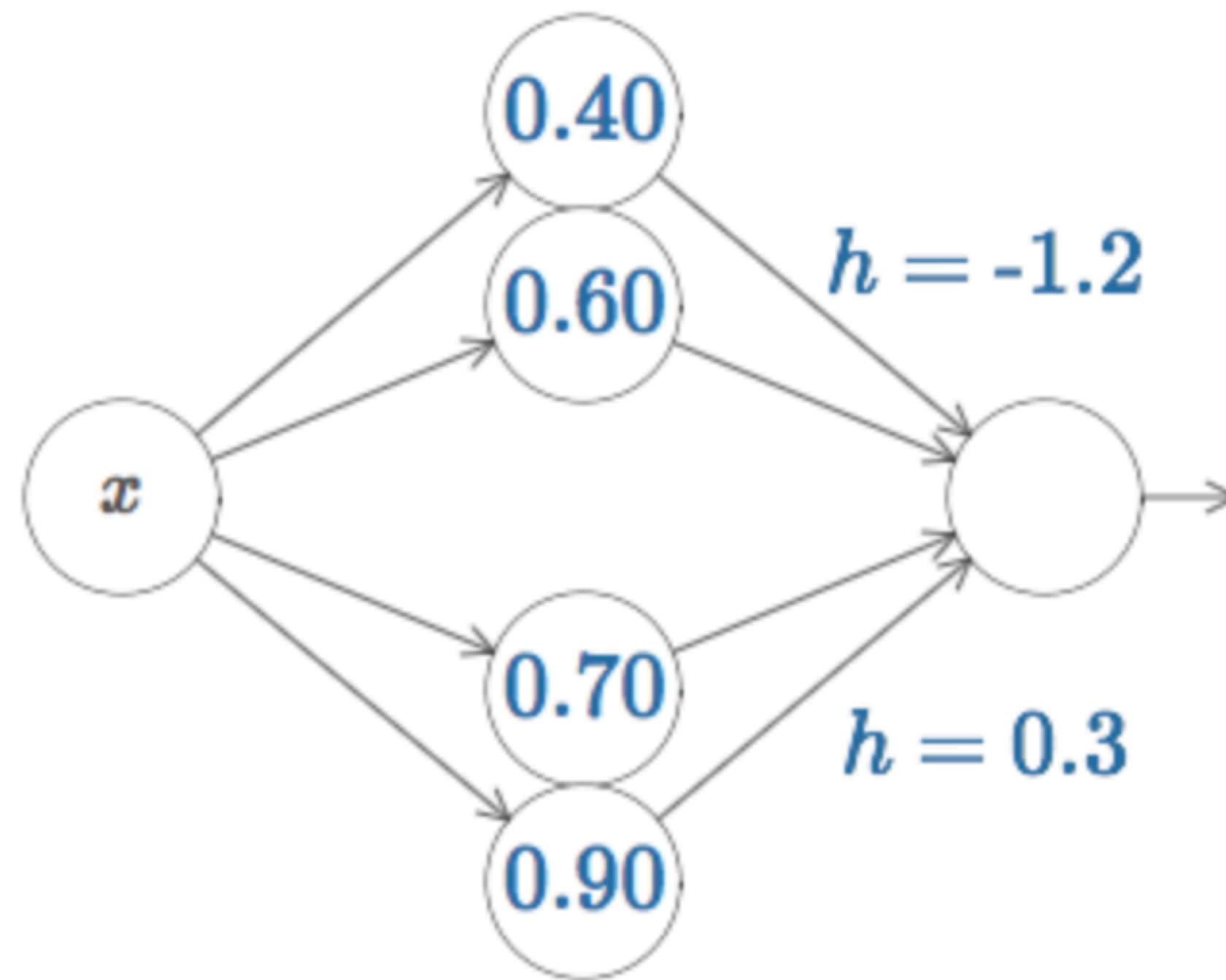


Light Theory: Neural Network as Universal Approximator

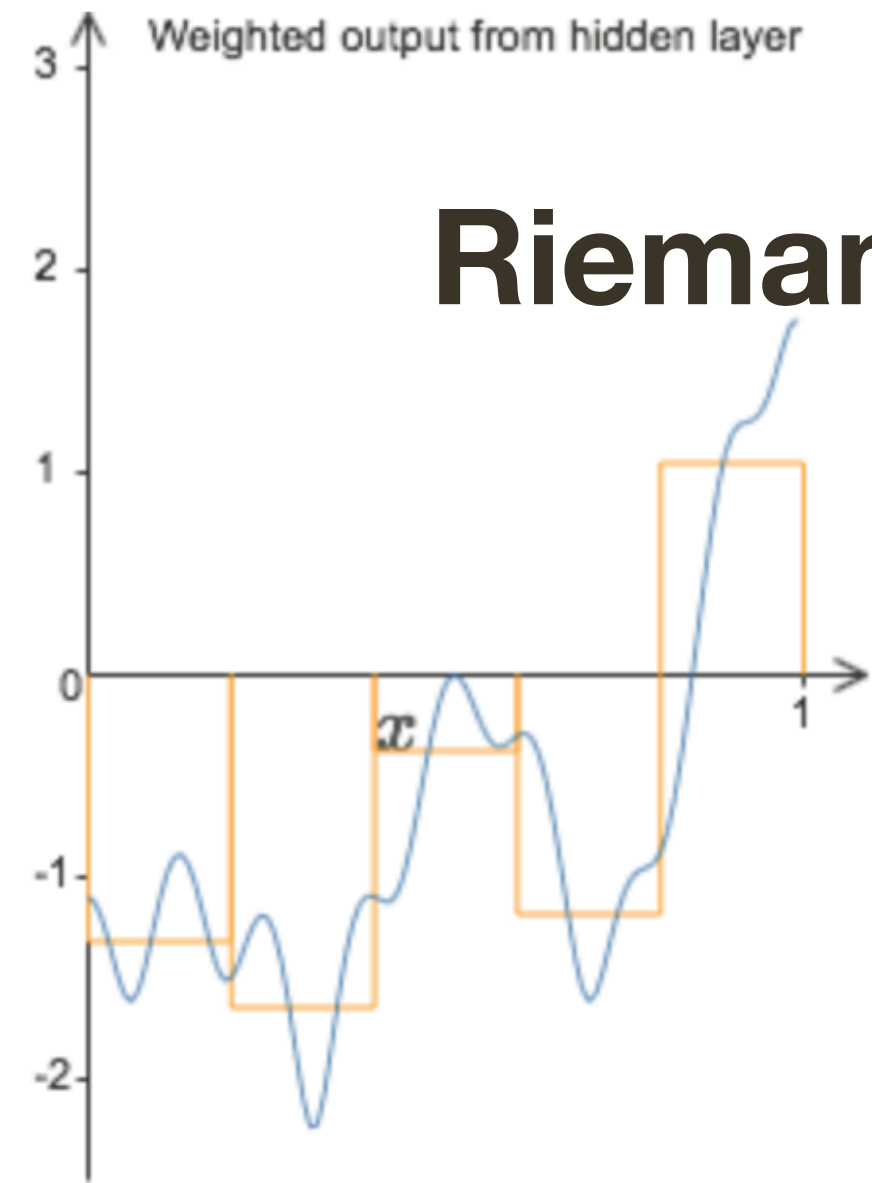
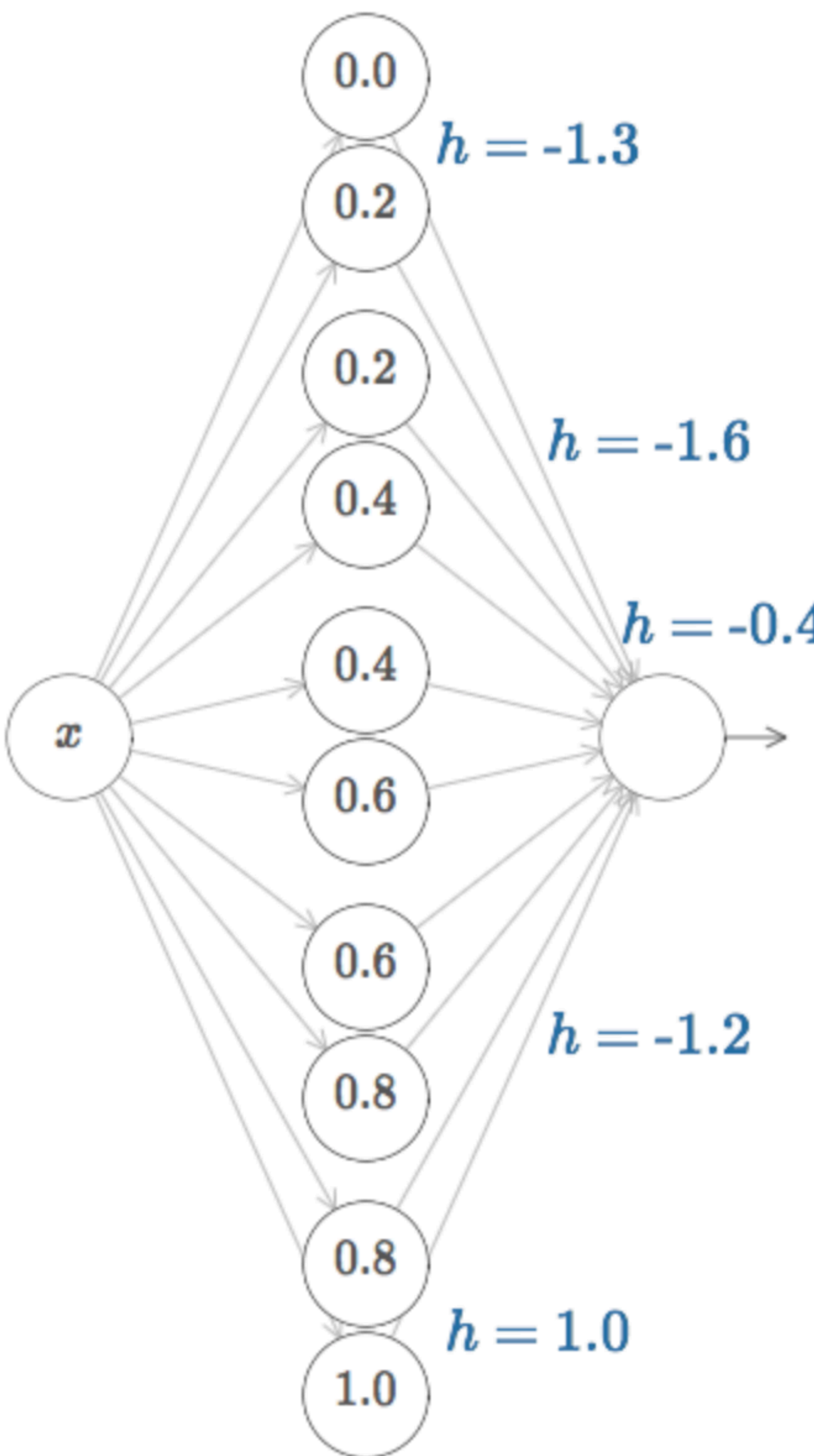
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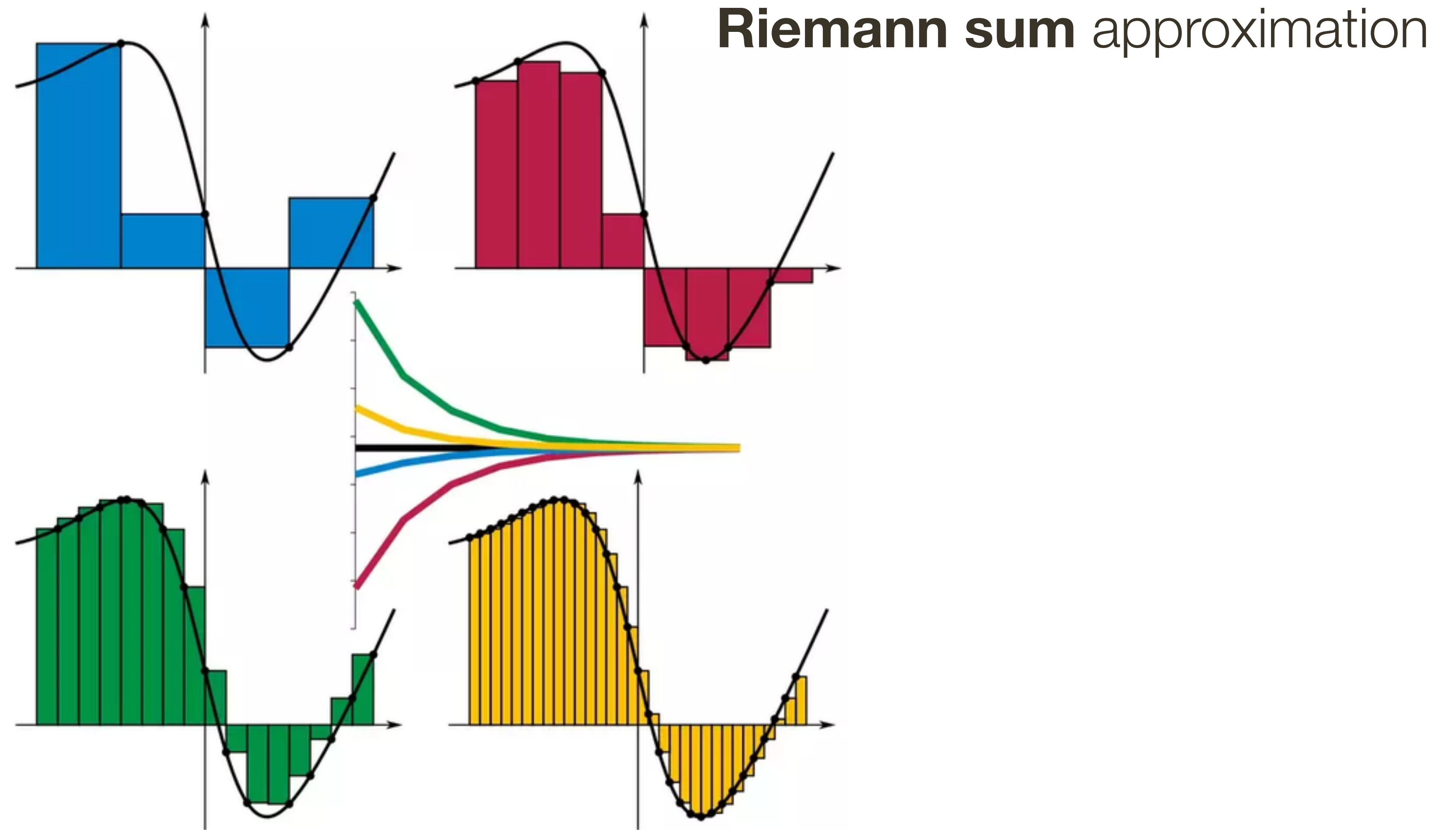


Light Theory: Neural Network as Universal Approximator



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

Light Theory: Neural Network as Universal Approximator



Light Theory: Neural Network as Universal Approximator

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

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

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

$$A \neq B$$

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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.

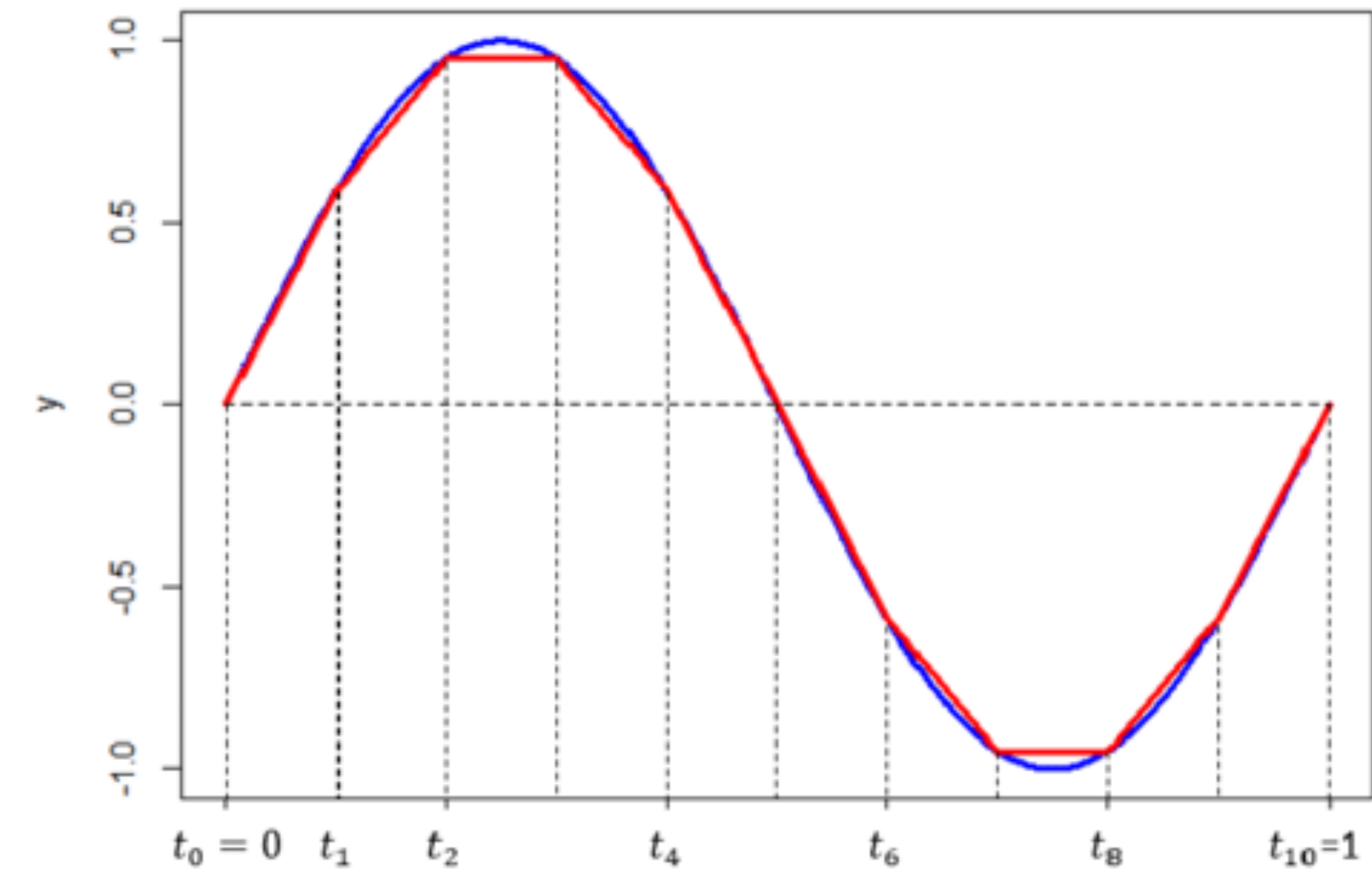
Activation Function

Non-linear activation is required to provably make the Neural Net a **universal function approximator**

Intuition: with ReLU activation, we effectively get a linear spline approximation to any function.

Optimization of neural net parameters = finding slopes and transitions of linear pieces

The quality of approximation depends on the number of linear segments



Number of linear segments for large input dimension: $\Omega(2^{\frac{2}{3}} L^n)$

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]

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.

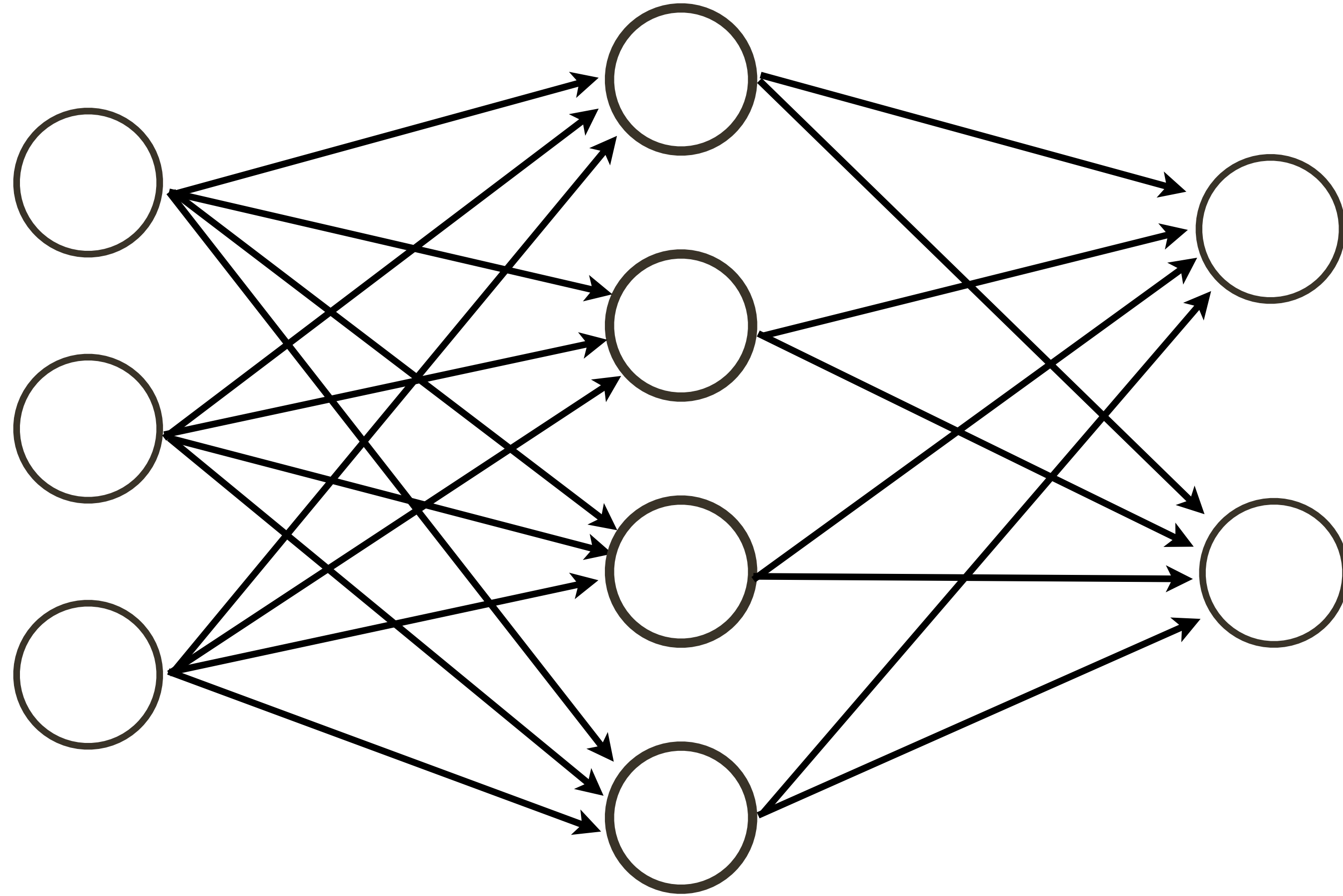
[Lu *et al.*, NIPS 2017]

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

[Lin and Jegelka, NIPS 2018]

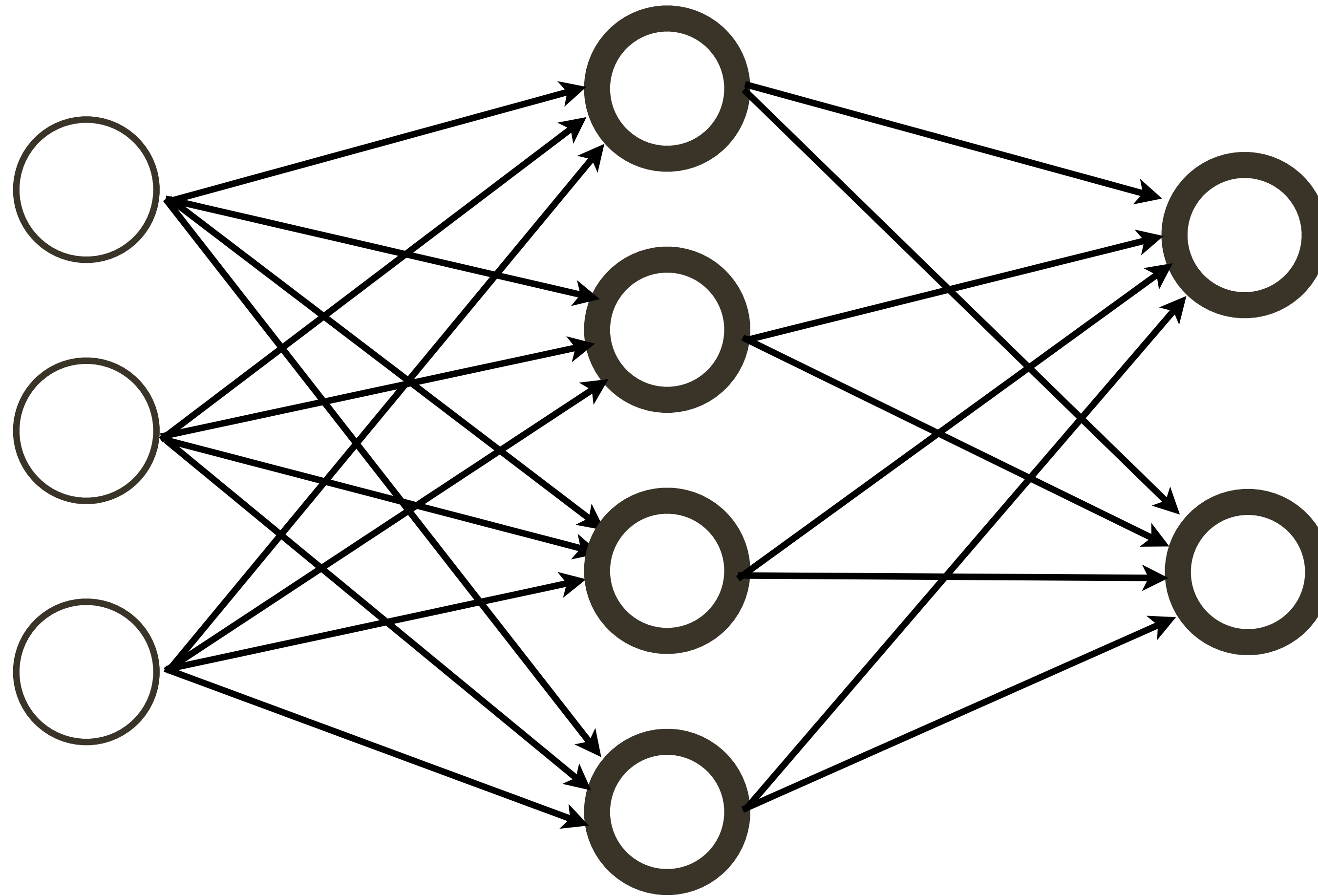
Neural Network

How many neurons?



Neural Network

How many neurons? $4+2 = 6$

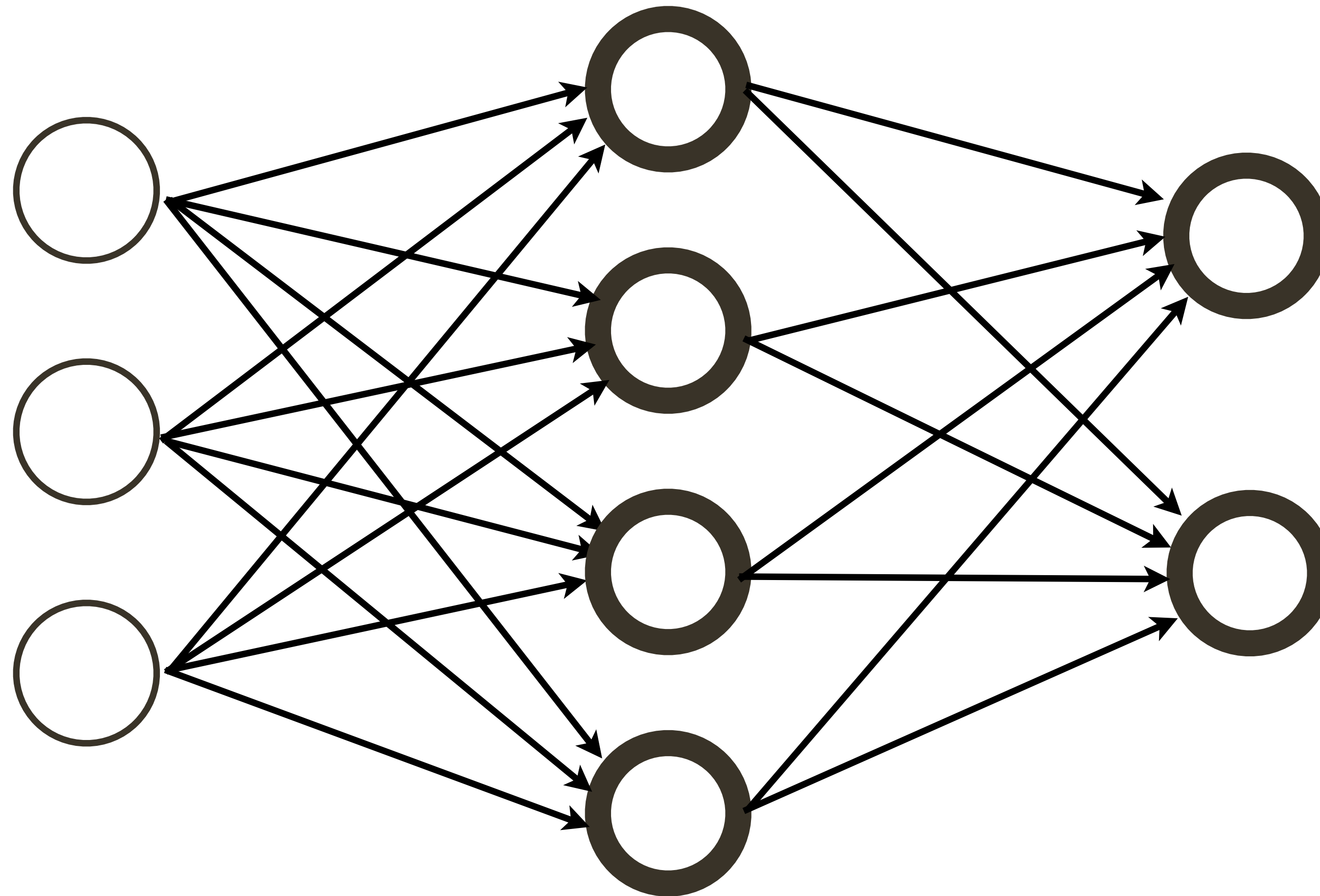


Neural Network

How many neurons?

$$4 + 2 = 6$$

How many weights?

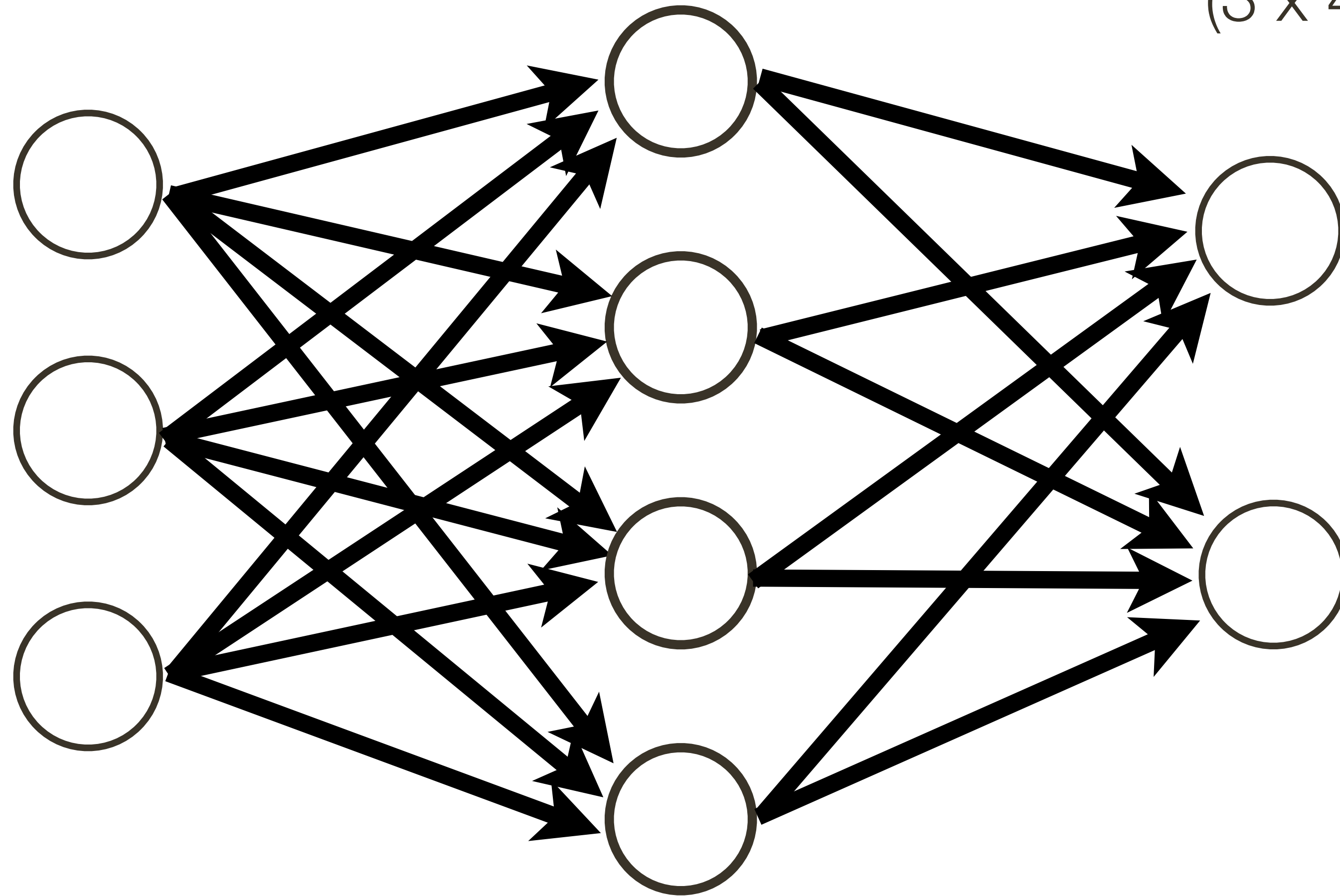


Neural Network

How many neurons? $4+2 = 6$

How many weights?

$$(3 \times 4) + (4 \times 2) = 20$$

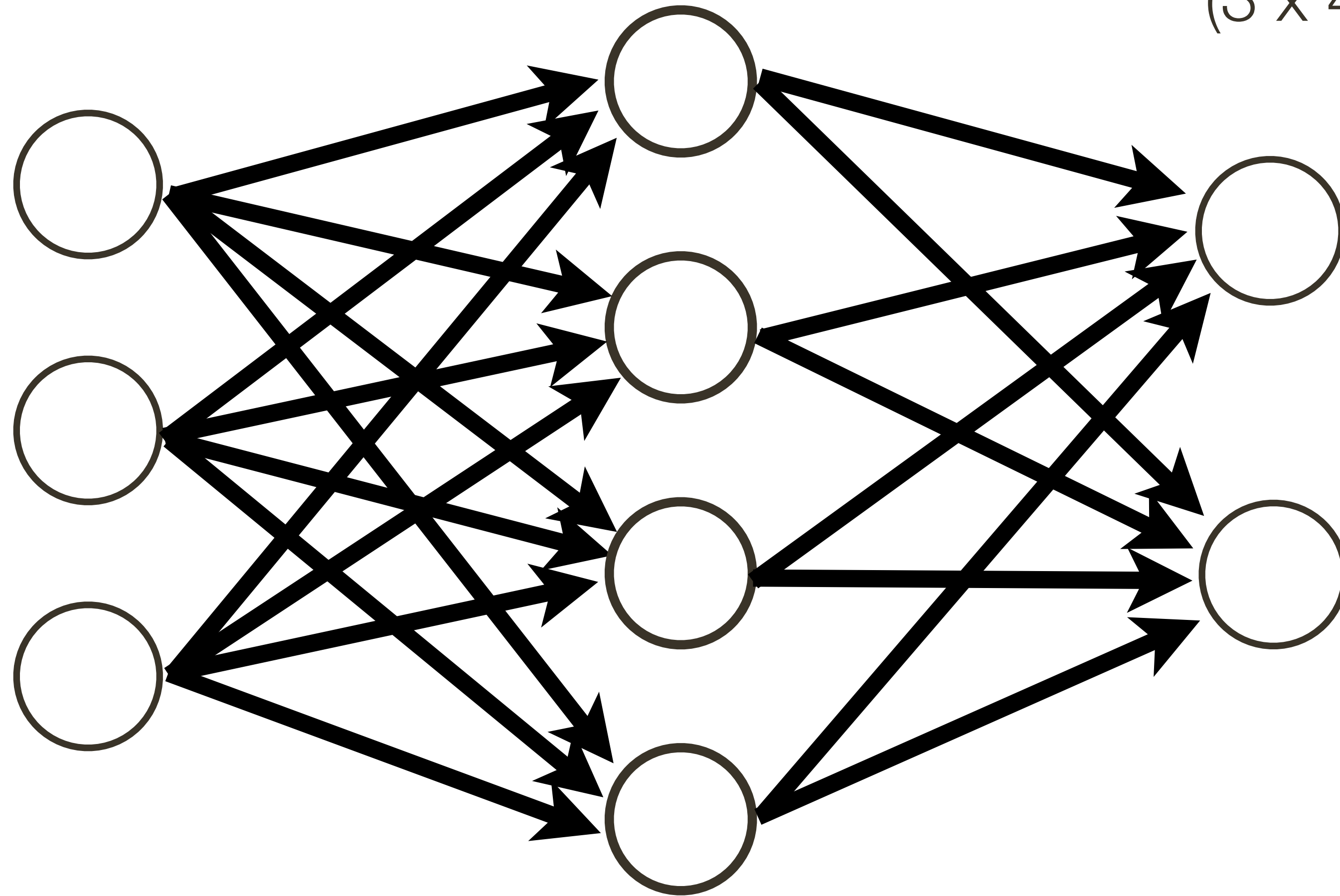


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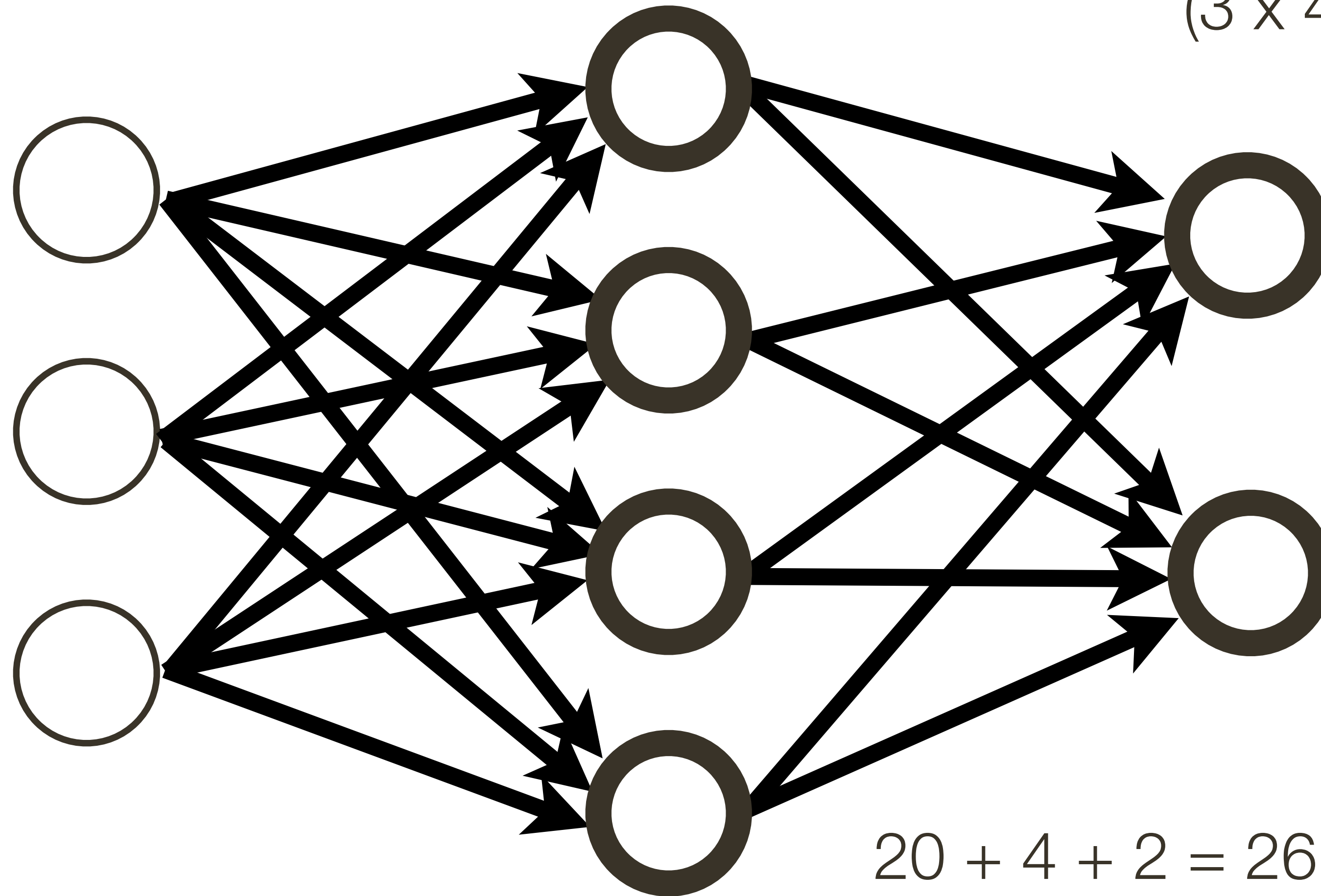
How many learnable parameters?

Neural Network

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How many learnable parameters?

$$20 + 4 + 2 = 26$$

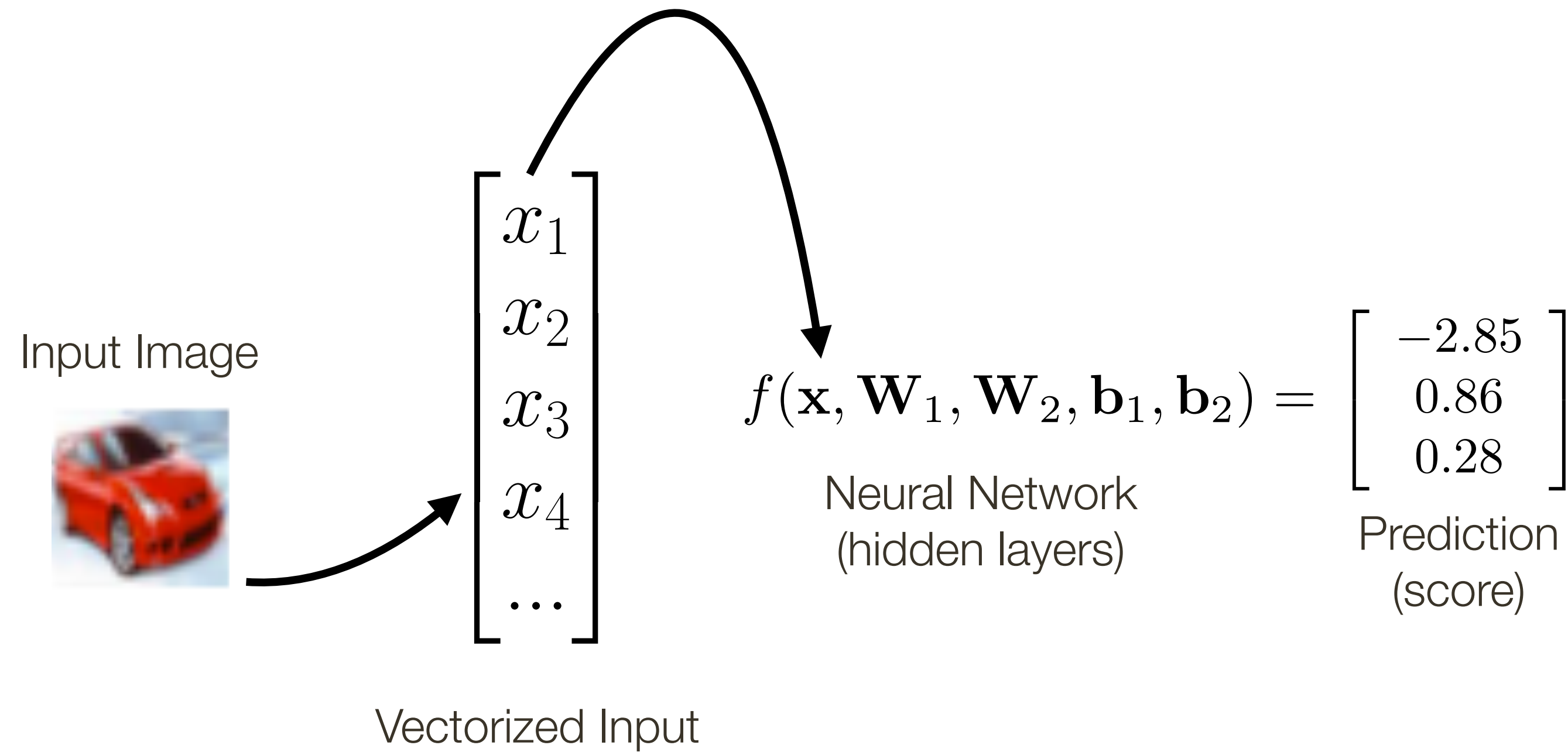
bias terms

Neural Networks

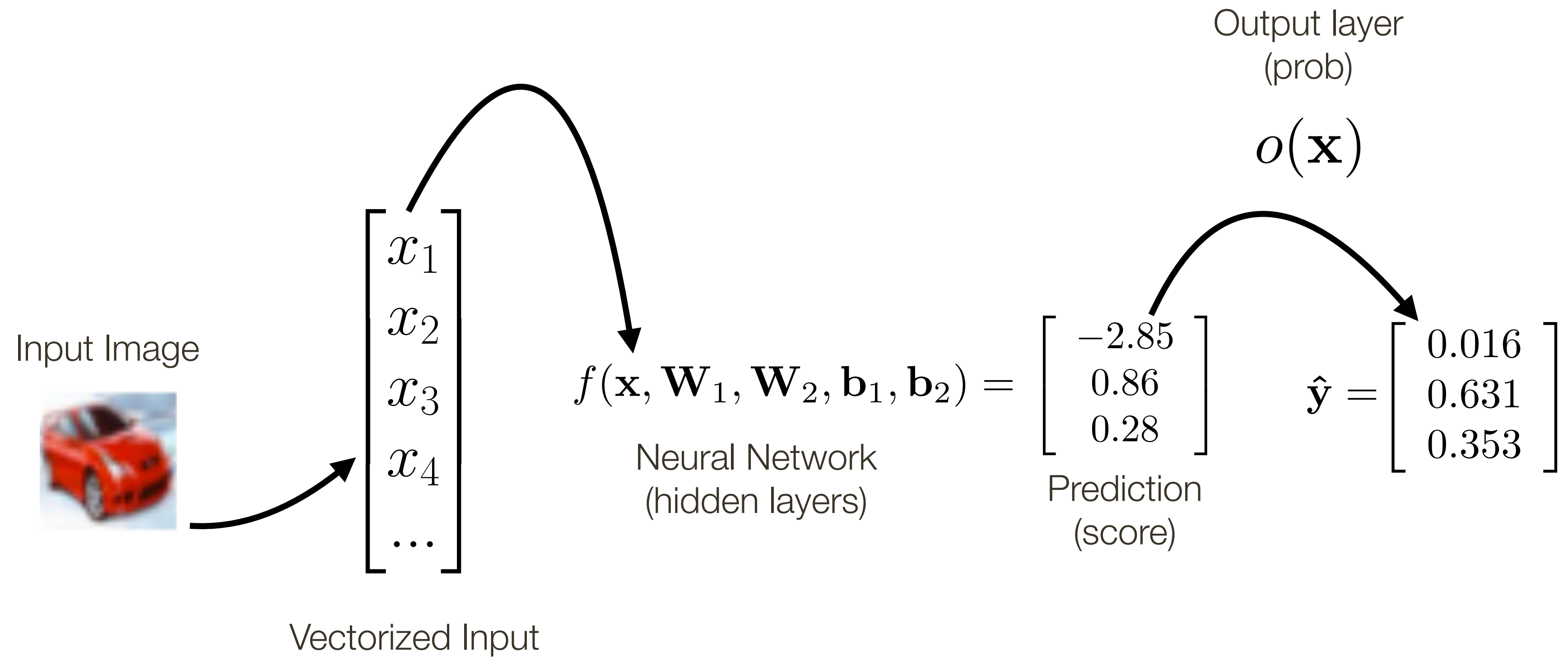
Modern **convolutional neural networks** contain 10-20 layers and on the order of 100 million parameters

Training a neural network requires estimating a large number of parameters

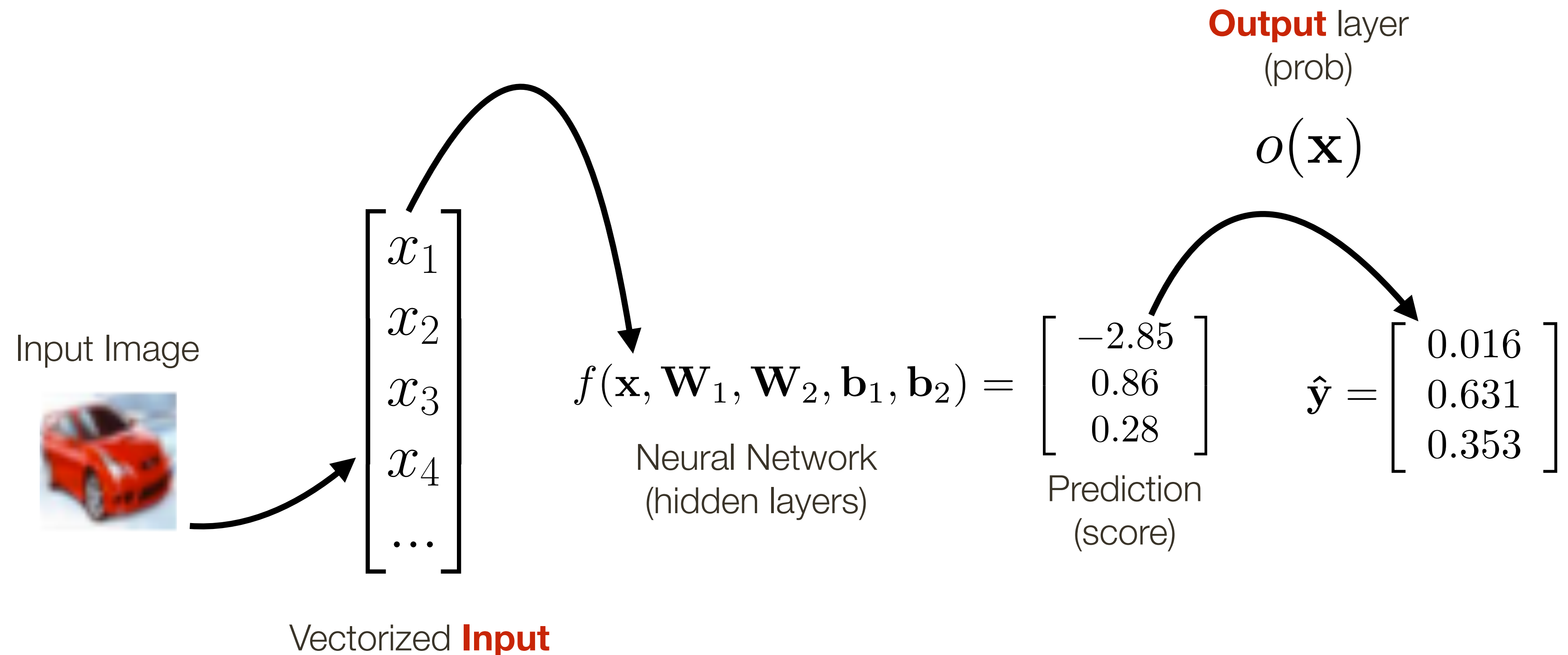
Training a Neural Network



Training a Neural Network

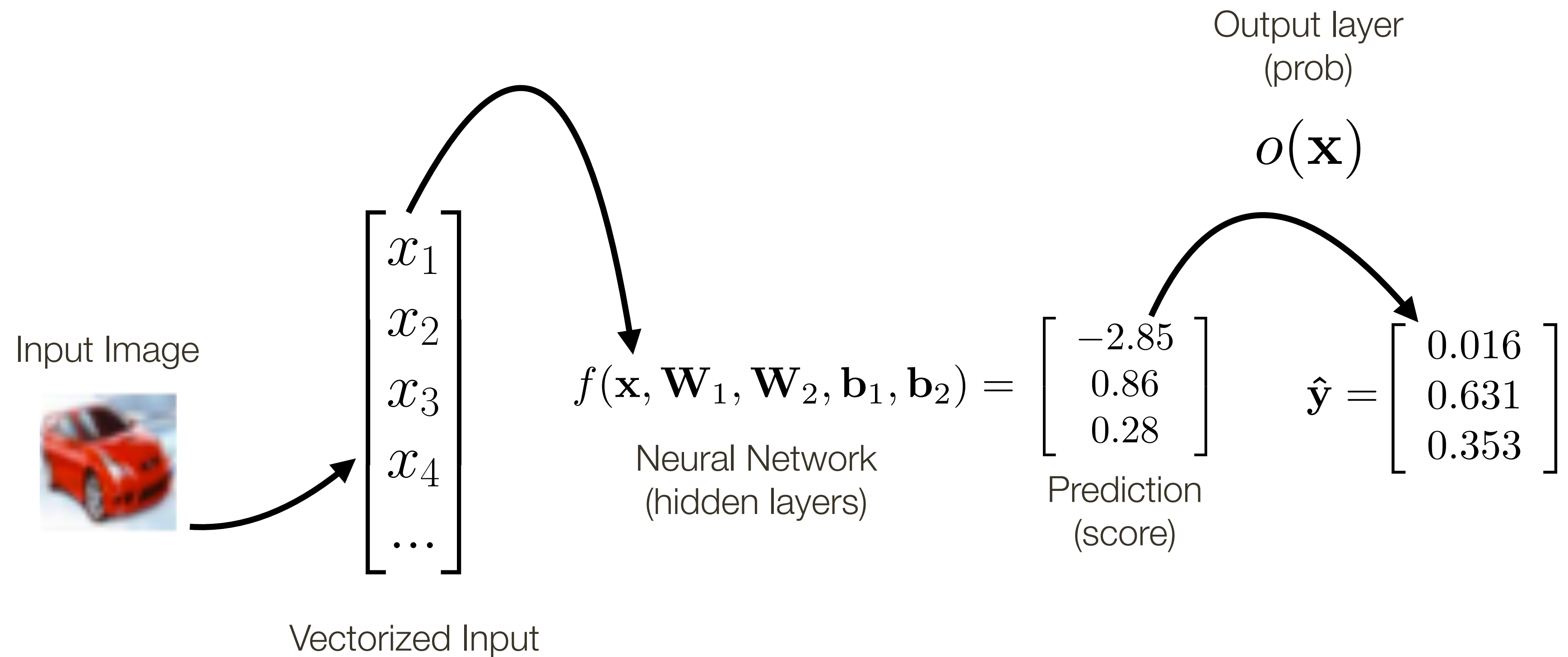


Training a Neural Network



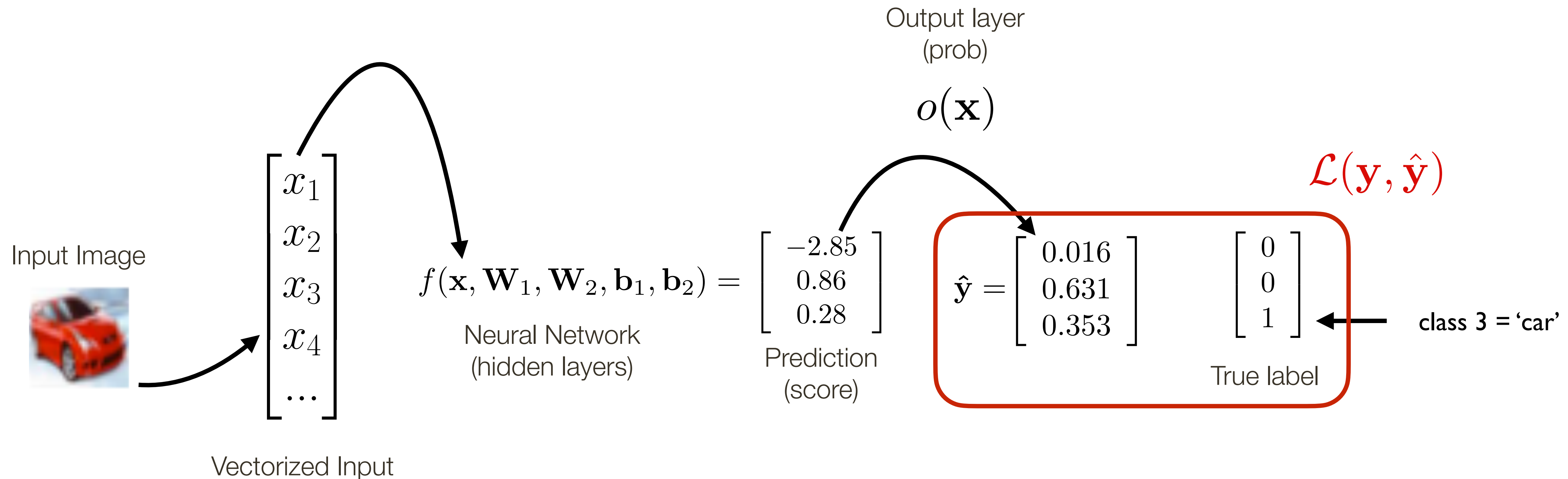
Input and **output** layers (size and form) are dictated by the problem, intermediate hidden layers have few constraints and can be *anything*

Training a Neural Network



Inference: $o(f(\mathbf{x}, \dots))$

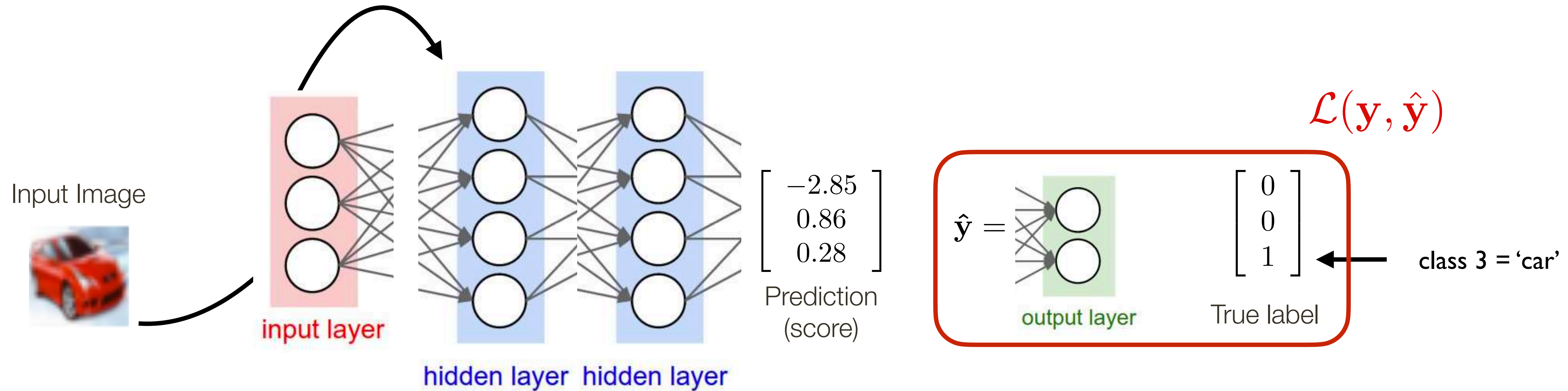
Training a Neural Network



Inference: $o(f(\mathbf{x}, \dots))$

Learning: $\mathcal{L}(\mathbf{y}, o(f(\mathbf{x}, \dots)))$

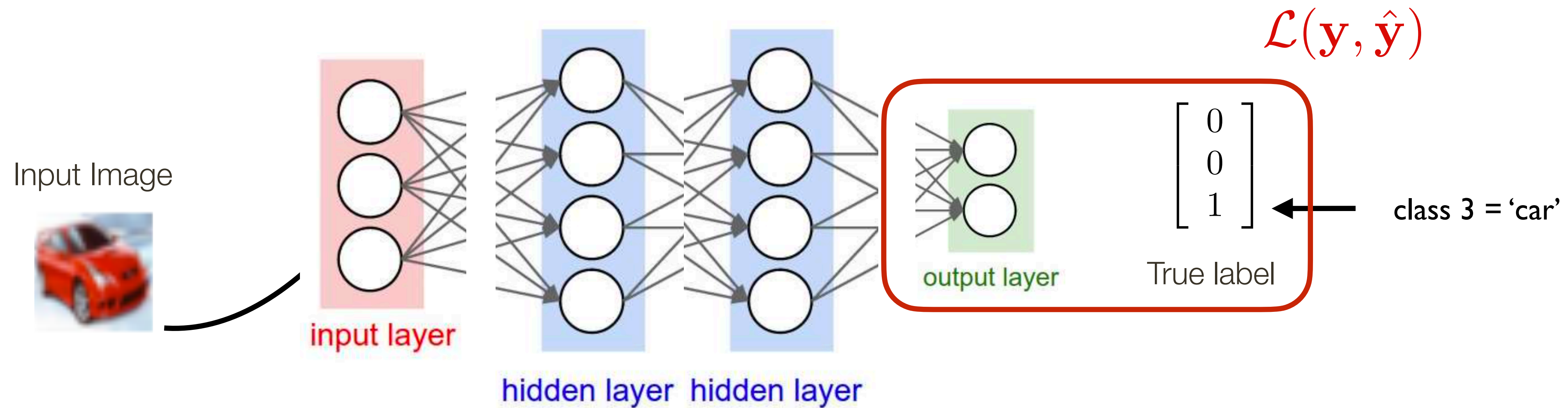
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Backpropagation

When training a neural network, the final output will be some loss (error) function

— e.g. cross-entropy loss: $\mathcal{L} = - \sum_i y_i \log(\hat{y}_i)$ $\hat{y}_i = \frac{e^{f_{y_i}}}{\sum_j e^{f_{y_j}}}$

which defines loss for i-th training example with true class index y_i ; and f_j is the j-th element of the vector of class scores coming from neural net.

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Consider neural net which takes input vector \mathbf{x}_i and predicts scores for 3 classes, with true class being class 3:

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f

$$c_1 = -2.85$$

$$c_2 = 0.86$$

$$c_3 = 0.28$$

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Backpropagation

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multi-class classifier

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$\mathcal{L} = -\log(0.353) = 1.04$

Backpropagation

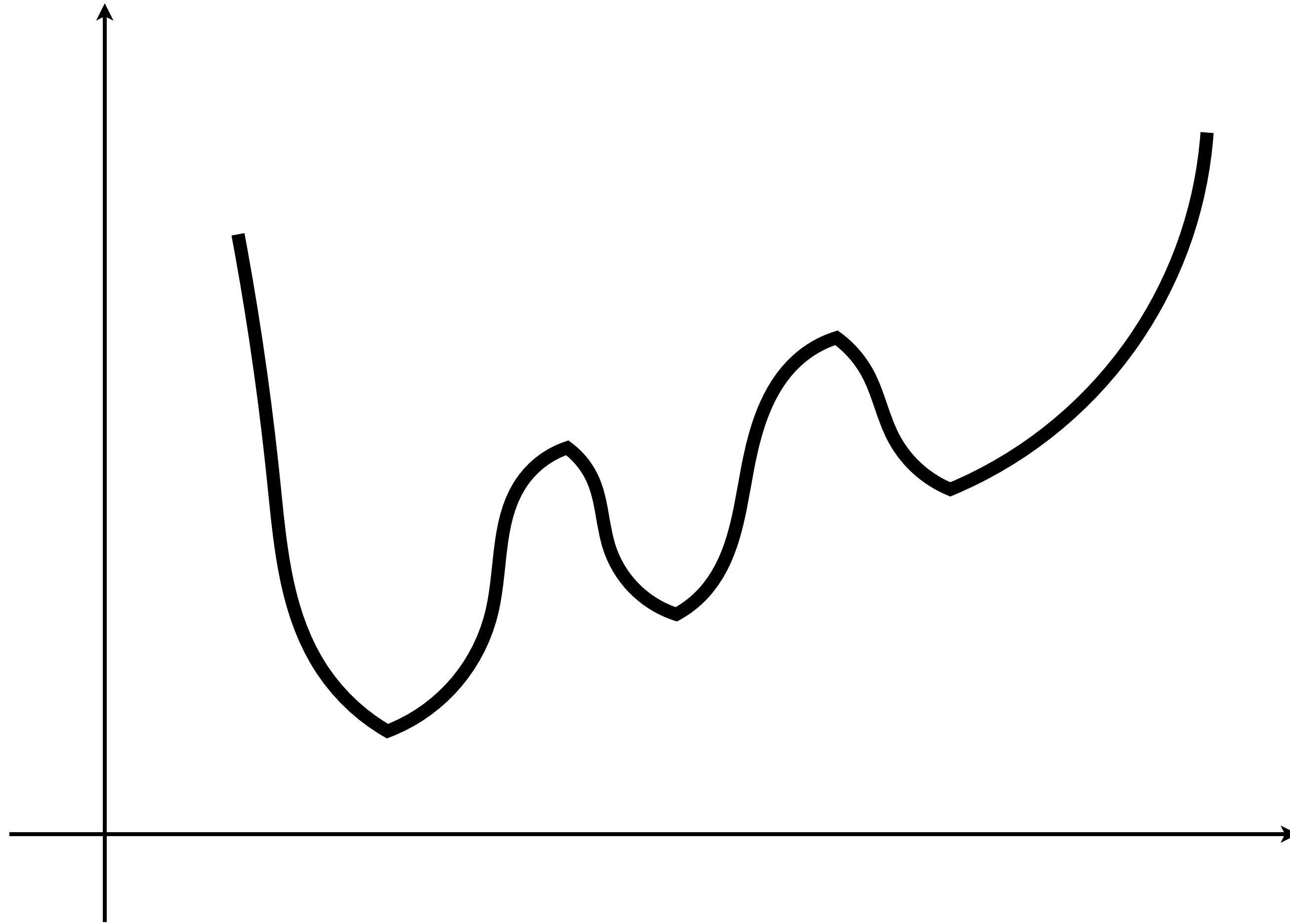
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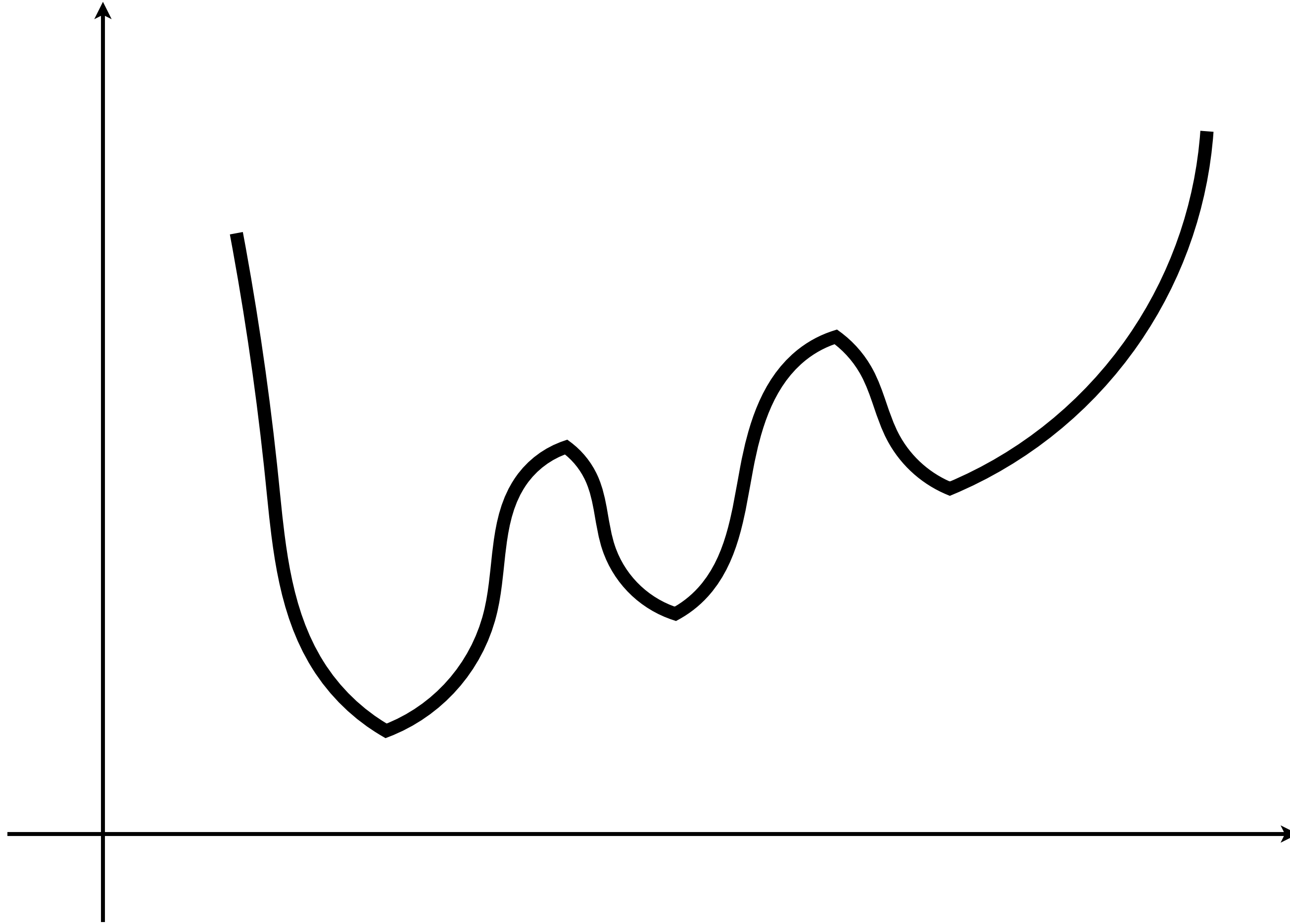
We want to compute the **gradient** of the loss with respect to the network parameters so that we can incrementally adjust the network parameters

Gradient Descent



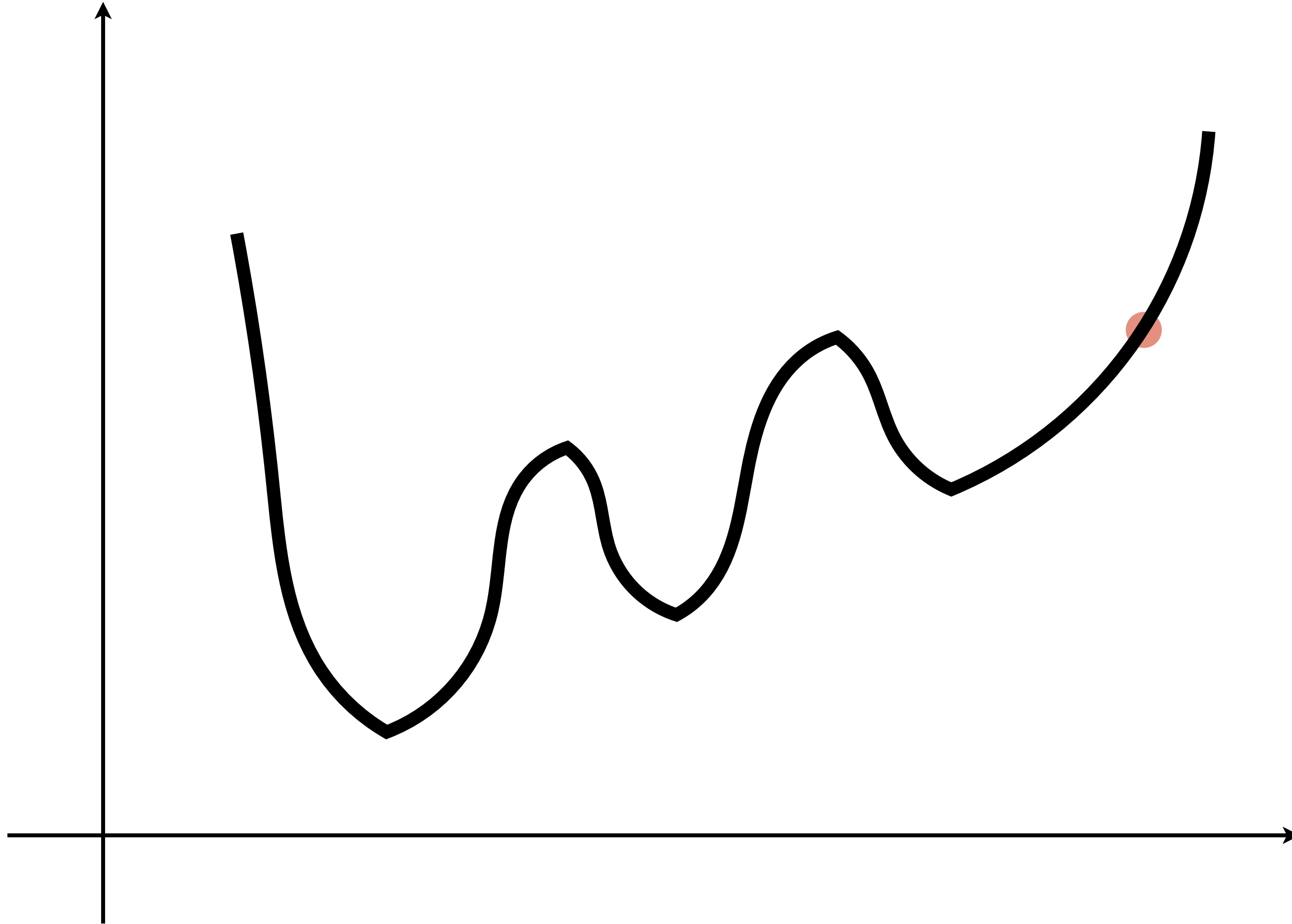
Gradient Descent

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

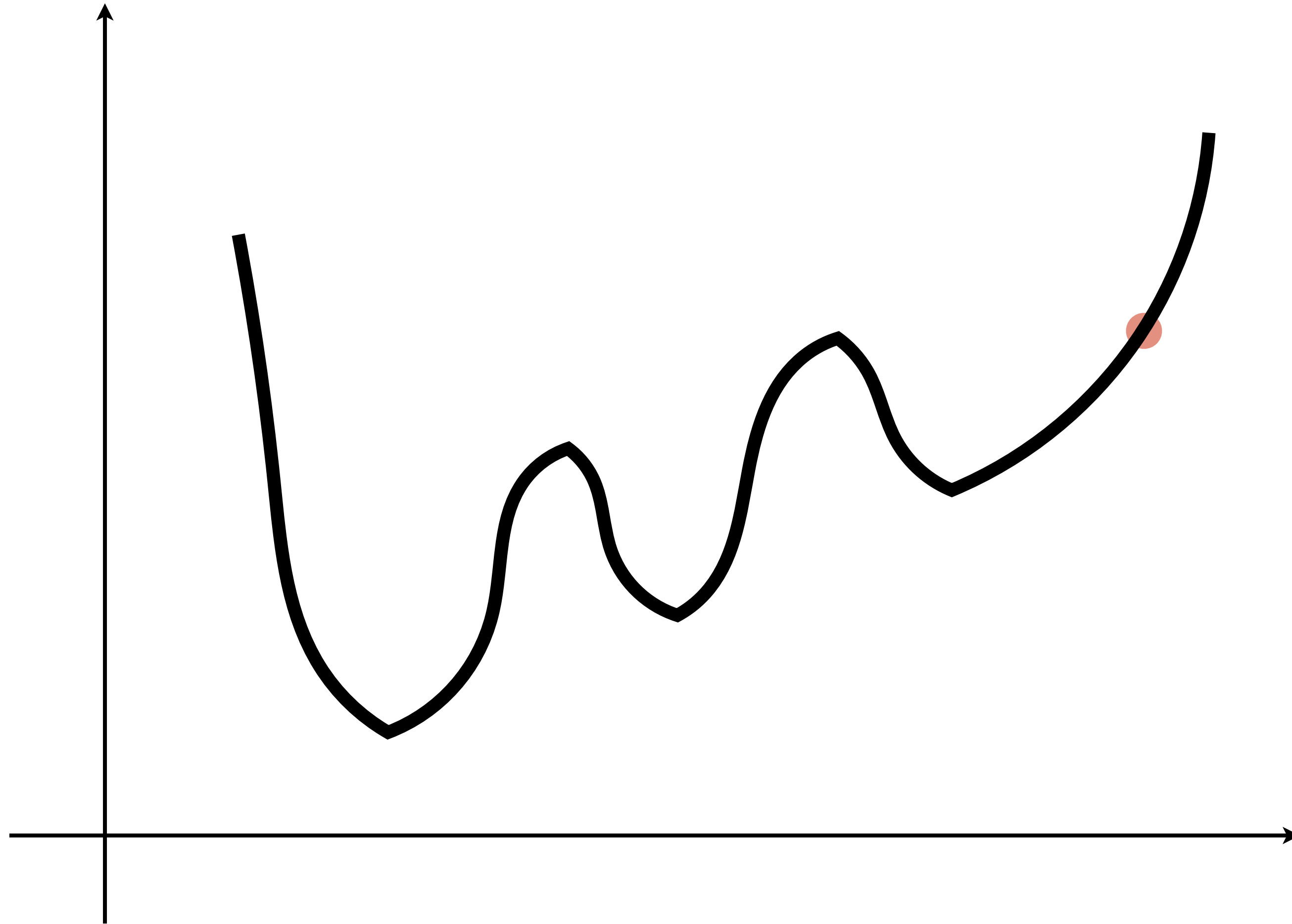


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Gradient Descent



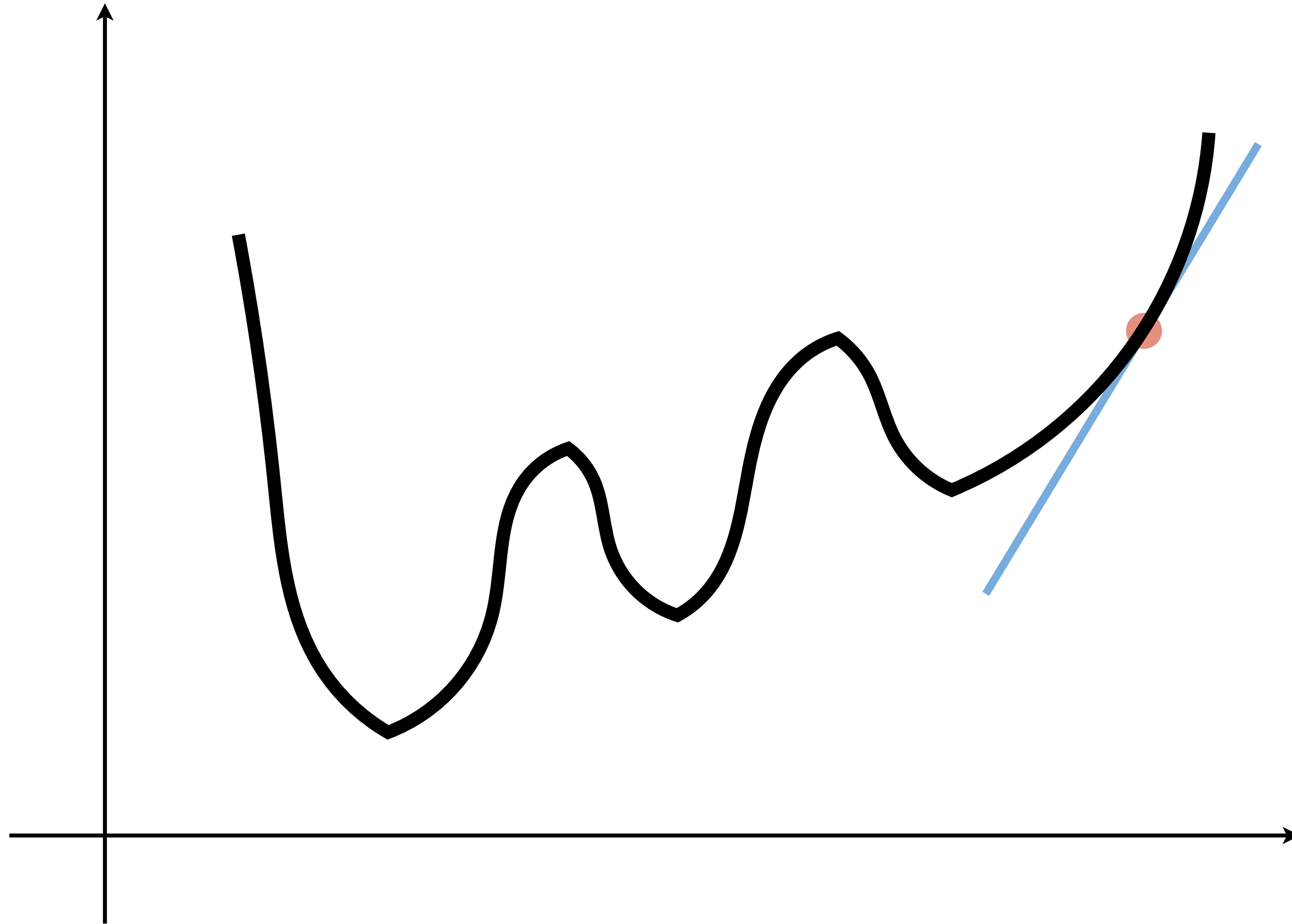
1. Start from random value of $\mathbf{W}_0, \mathbf{b}_0$

For $k = 0$ to max number of iterations

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

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

Gradient Descent



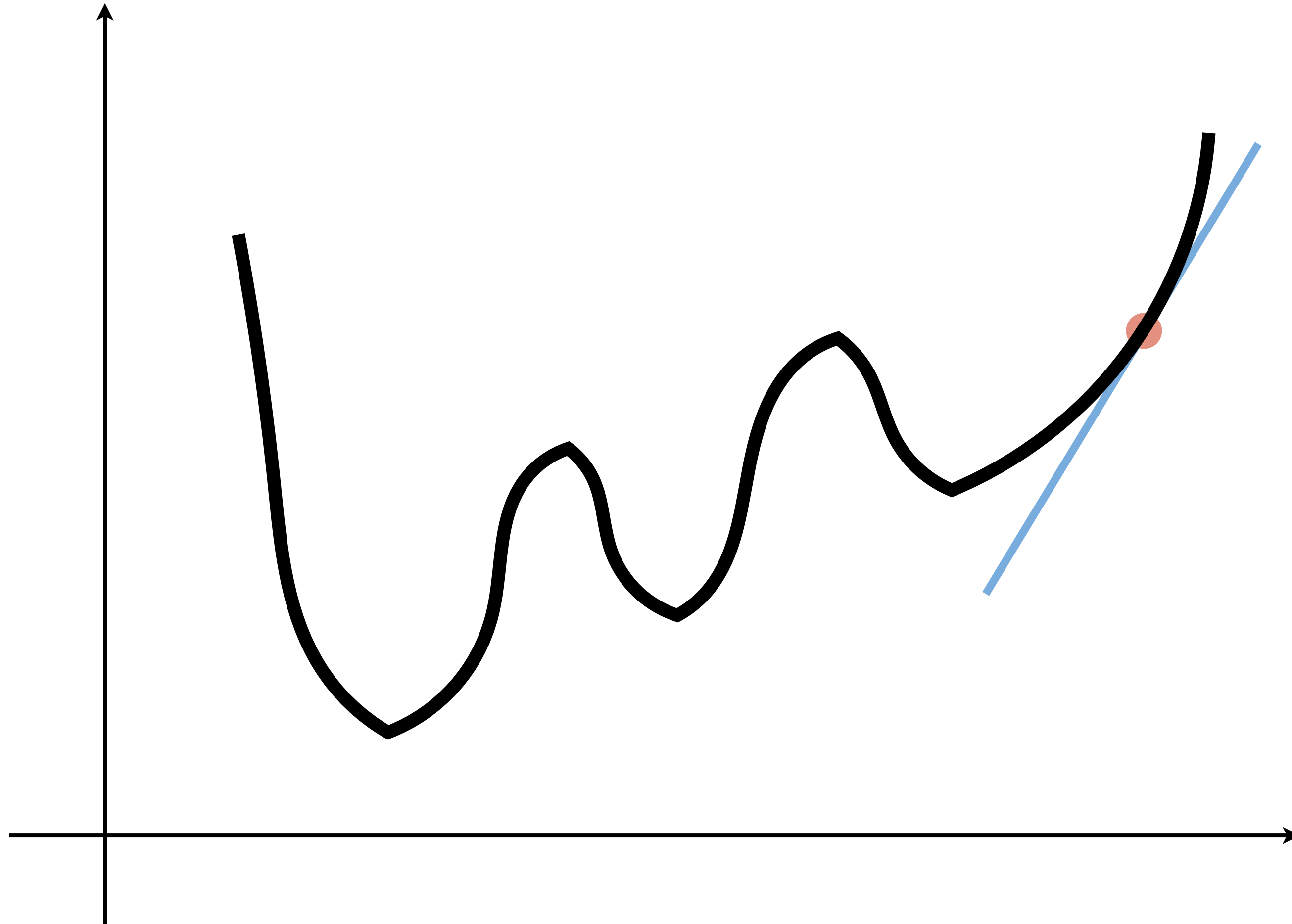
1. Start from random value of $\mathbf{W}_0, \mathbf{b}_0$

For $k = 0$ to max number of iterations

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

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

Gradient Descent



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:

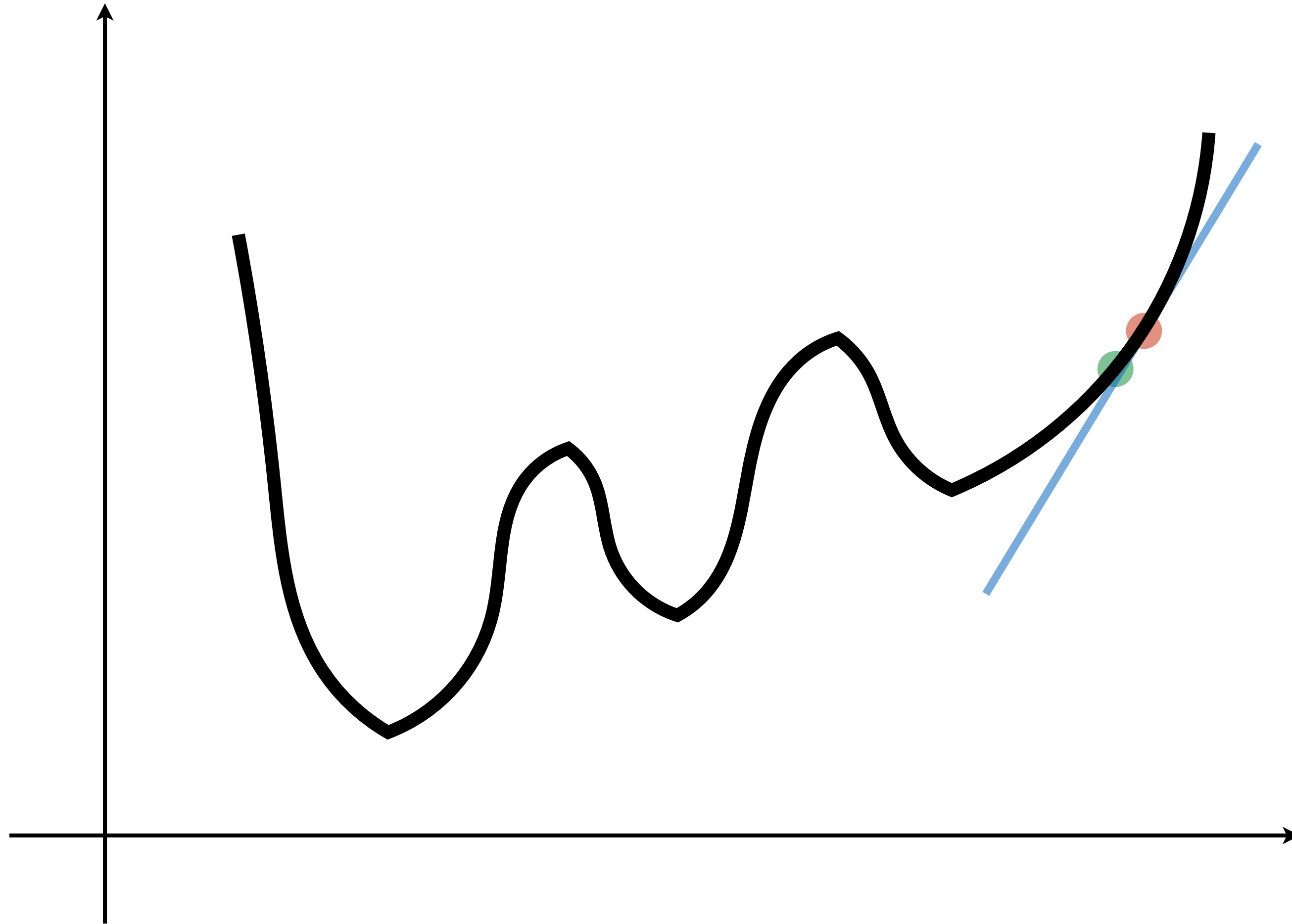
$$\nabla \mathcal{L}(\mathbf{W}, \mathbf{b}) \Big|_{\mathbf{W}=\mathbf{W}_k, \mathbf{b}=\mathbf{b}_k}$$

3. Re-estimate the parameters

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

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

Gradient Descent



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:

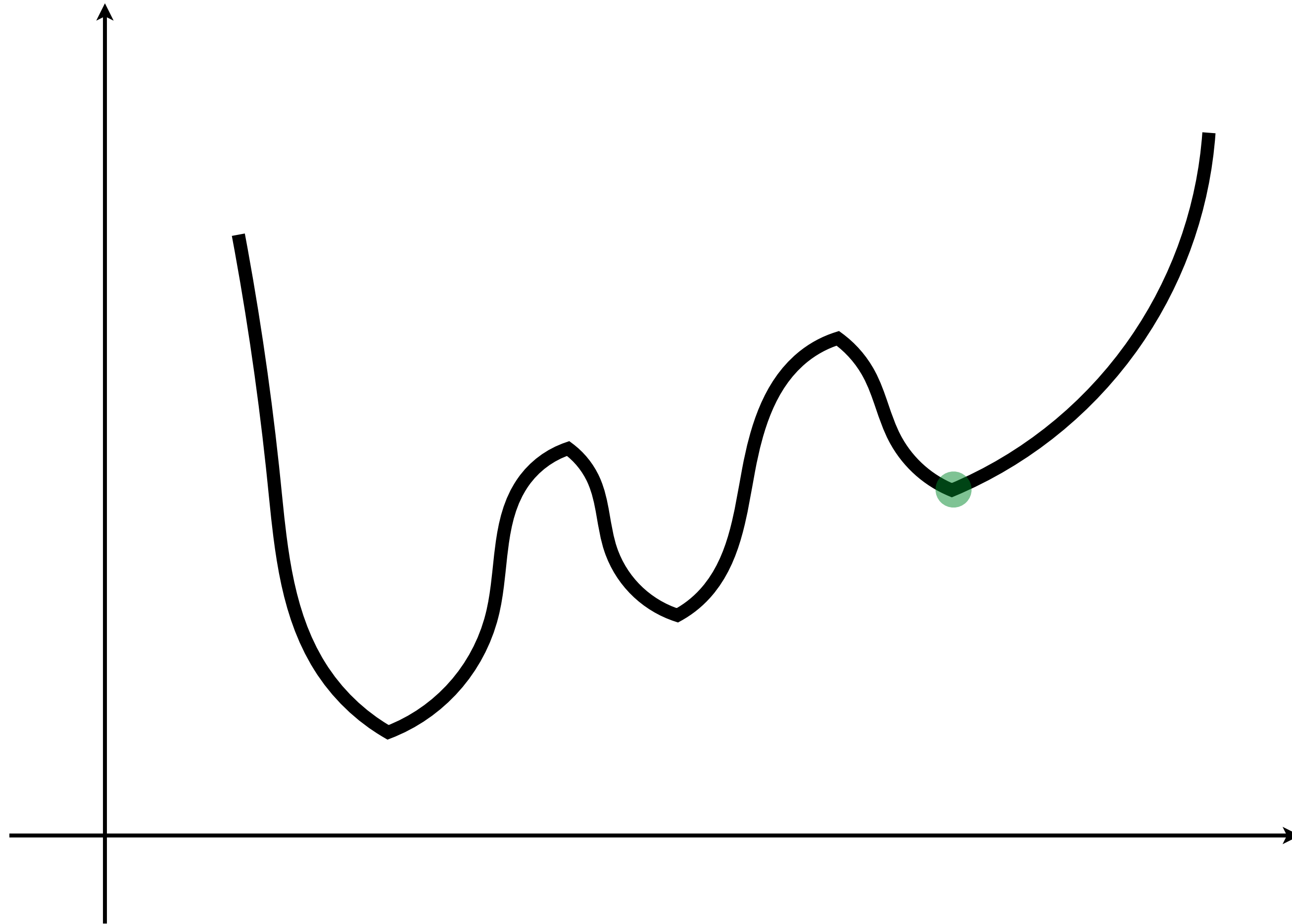
$$\nabla \mathcal{L}(\mathbf{W}, \mathbf{b}) \Big|_{\mathbf{W}=\mathbf{W}_k, \mathbf{b}=\mathbf{b}_k}$$

3. Re-estimate the parameters

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

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Gradient Descent



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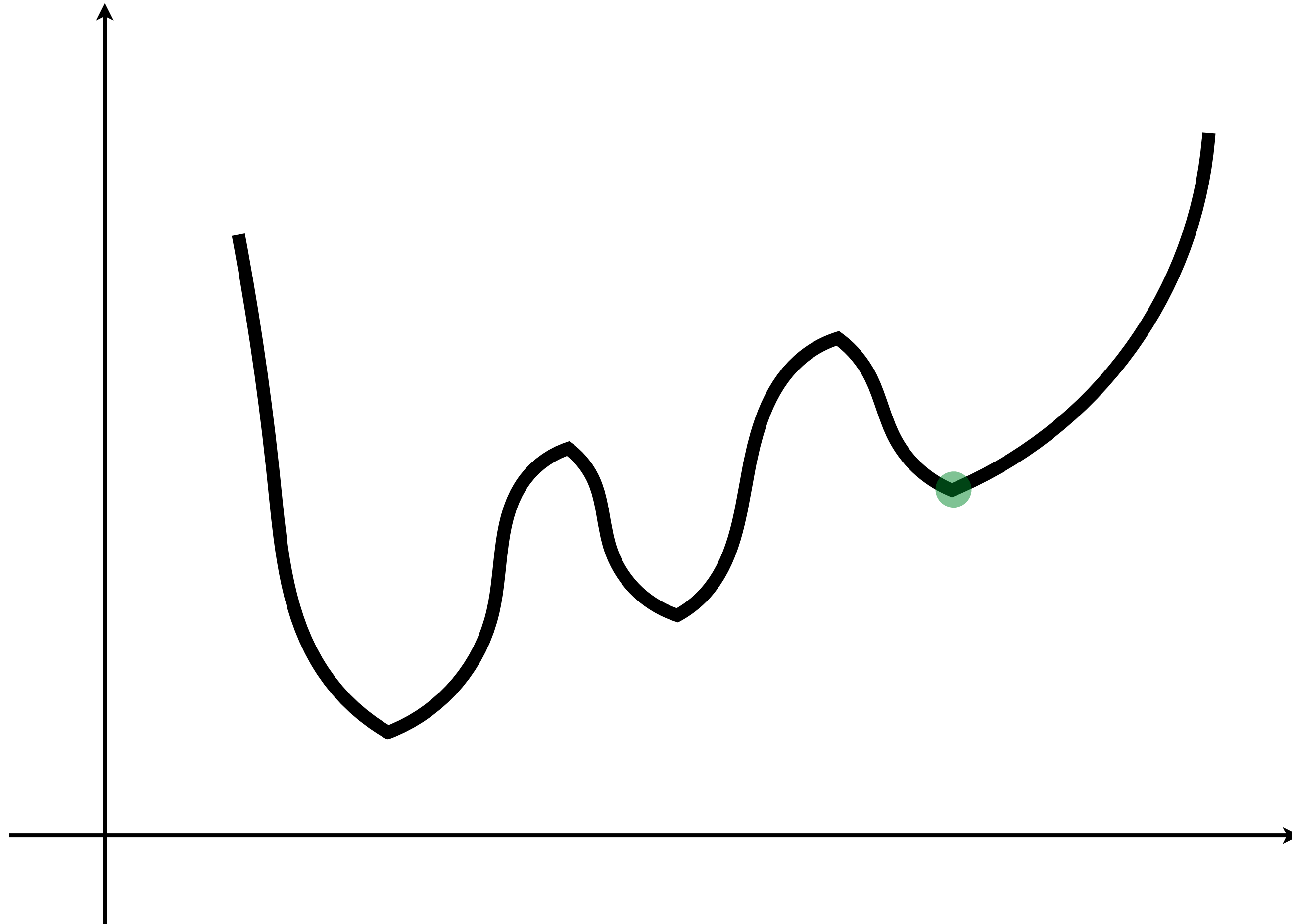
$$\nabla \mathcal{L}(\mathbf{W}, \mathbf{b}) \Big|_{\mathbf{W}=\mathbf{W}_k, \mathbf{b}=\mathbf{b}_k}$$

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

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Gradient Descent



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:

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

3. Re-estimate the parameters

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

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

Gradient Descent

Loss: $\mathcal{L} = \sum_{i=1}^{|\mathcal{D}_{train}|} ||\mathbf{y}_i - \hat{\mathbf{y}}_i|| = \sum_{i=1}^{|\mathcal{D}_{train}|} ||\mathbf{y}_i - f(\mathbf{x}_i, \mathbf{W}_1, \mathbf{W}_2, \mathbf{b}_1, \mathbf{b}_2)||$

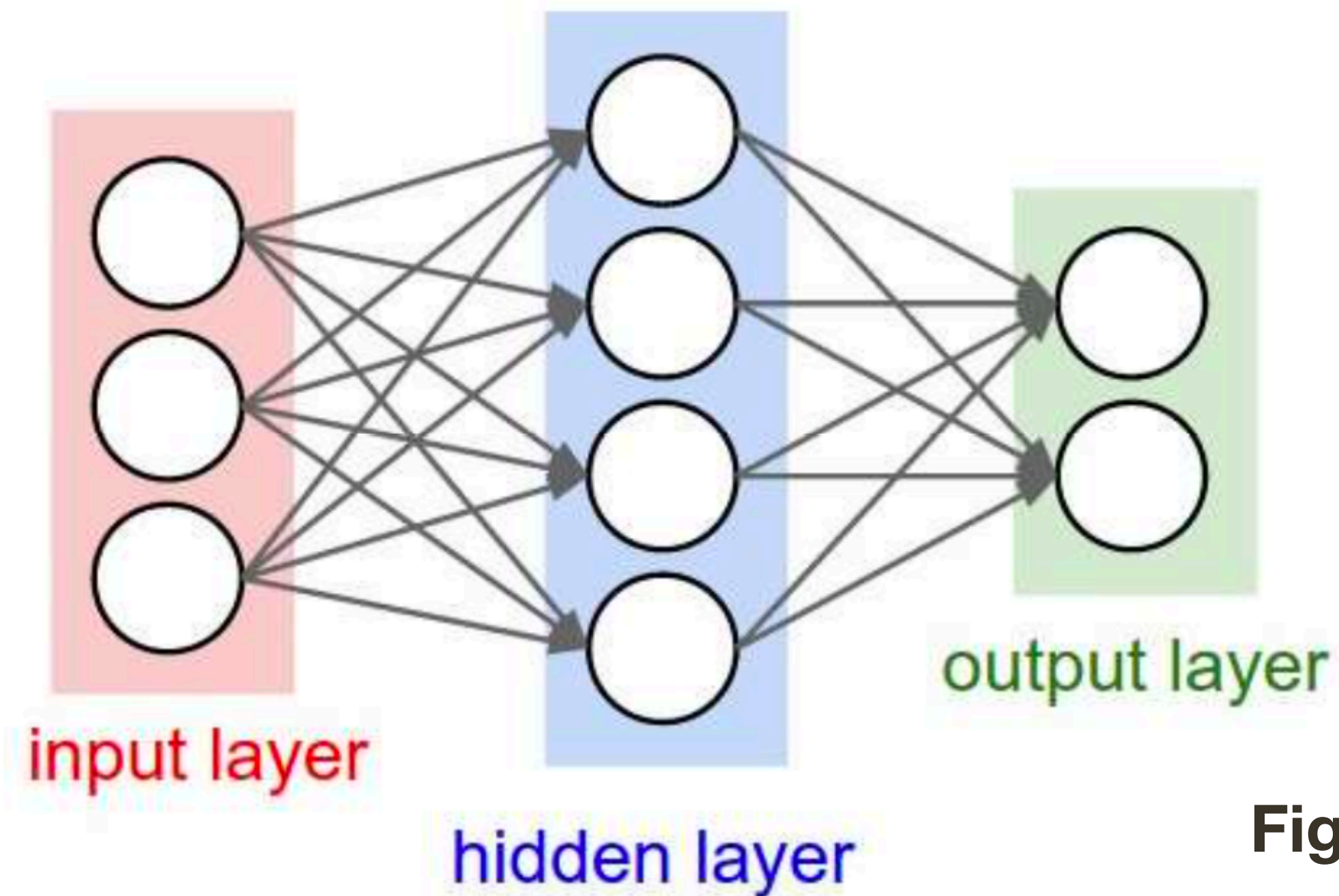


Figure credit: Fei-Fei and Karpathy

$$\hat{\mathbf{y}} = f(\mathbf{x}, \mathbf{W}_1, \mathbf{W}_2, \mathbf{b}_1, \mathbf{b}_2) = \sigma \left(\mathbf{W}_2^{(2 \times 4)} \sigma \left(\mathbf{W}_1^{(4 \times 3)} \mathbf{x} + \mathbf{b}_1^{(4)} \right) + \mathbf{b}_2^{(2)} \right)$$

Gradient Descent

Loss: $\mathcal{L} = \sum_{i=1}^{|\mathcal{D}_{train}|} ||\mathbf{y}_i - \hat{\mathbf{y}}_i|| = \sum_{i=1}^{|\mathcal{D}_{train}|} ||\mathbf{y}_i - f(\mathbf{x}_i, \mathbf{W}_1, \mathbf{W}_2, \mathbf{b}_1, \mathbf{b}_2)||$

Gradient Descent

$$\mathbf{W}_{1,i,j} = \mathbf{W}_{1,i,j} - \lambda \frac{\partial \mathcal{L}(\mathbf{y}, \hat{\mathbf{y}})}{\partial \mathbf{W}_{1,i,j}}$$

$$\mathbf{b}_{1,i} = \mathbf{b}_{1,i} - \lambda \frac{\partial \mathcal{L}(\mathbf{y}, \hat{\mathbf{y}})}{\partial \mathbf{b}_{1,i}}$$

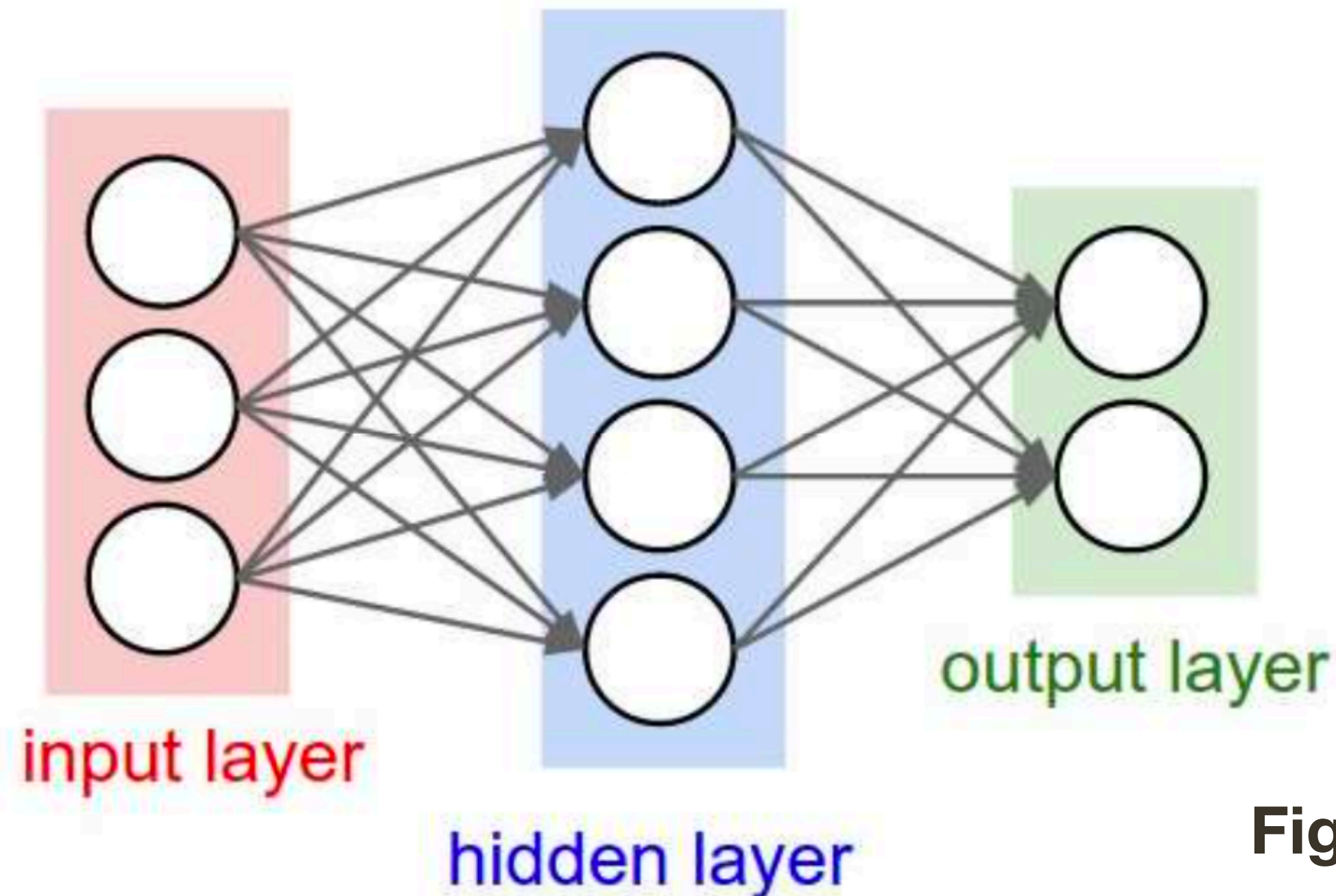


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Stochastic Gradient Descent

$$\frac{\partial \mathcal{L}}{\partial \mathbf{W}_{1,i,j}} = \frac{\partial}{\partial \mathbf{W}_{1,i,j}} \sum_{i=1}^{|\mathcal{D}_{train}|} [y_i - f(\mathbf{x}_i, \mathbf{W}_1, \mathbf{W}_2, \mathbf{b}_1, \mathbf{b}_2)]^2$$

Stochastic Gradient Descent

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Problem: For large datasets computing sum is expensive

Stochastic Gradient Descent

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

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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:

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

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Even better, we can use central differencing:

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

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However, both of these suffer from rounding errors and are not good enough for learning.

$$h = 0.000001$$

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:

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

$$\frac{\partial \mathcal{L}(\mathbf{W}, \mathbf{b})}{\partial b_j} \approx \lim_{h \rightarrow 0} \frac{\mathcal{L}(\mathbf{W}, \mathbf{b} + h\mathbf{1}_j) - \mathcal{L}(\mathbf{W}, \mathbf{b})}{h}$$

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

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

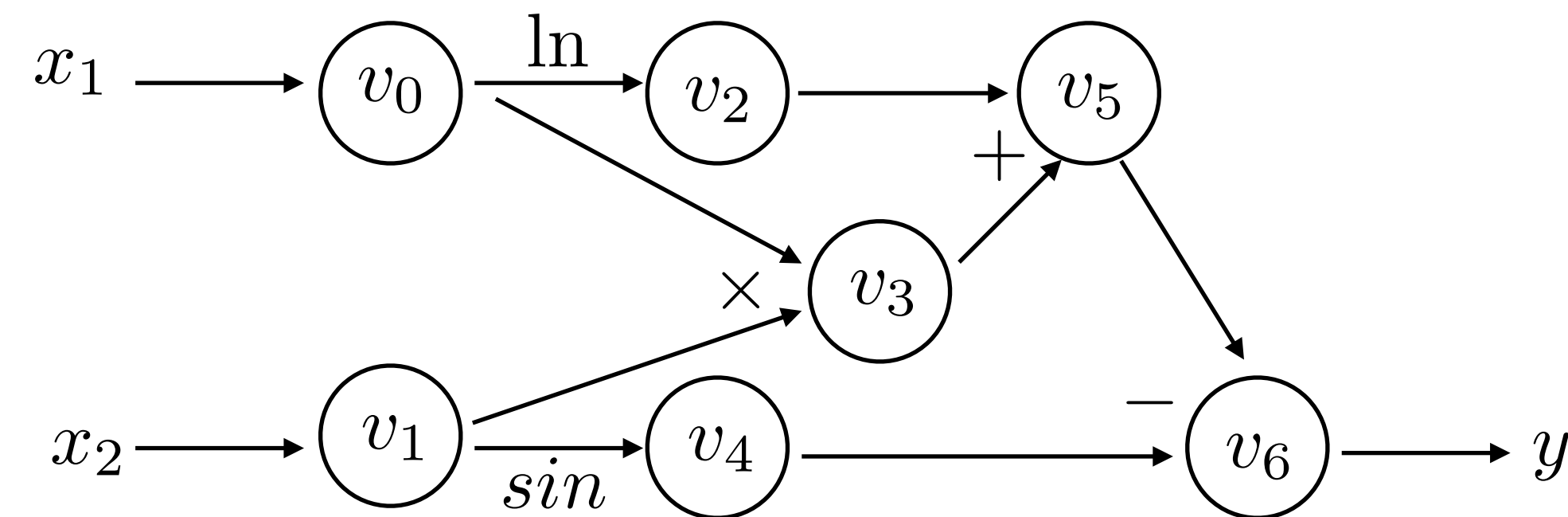
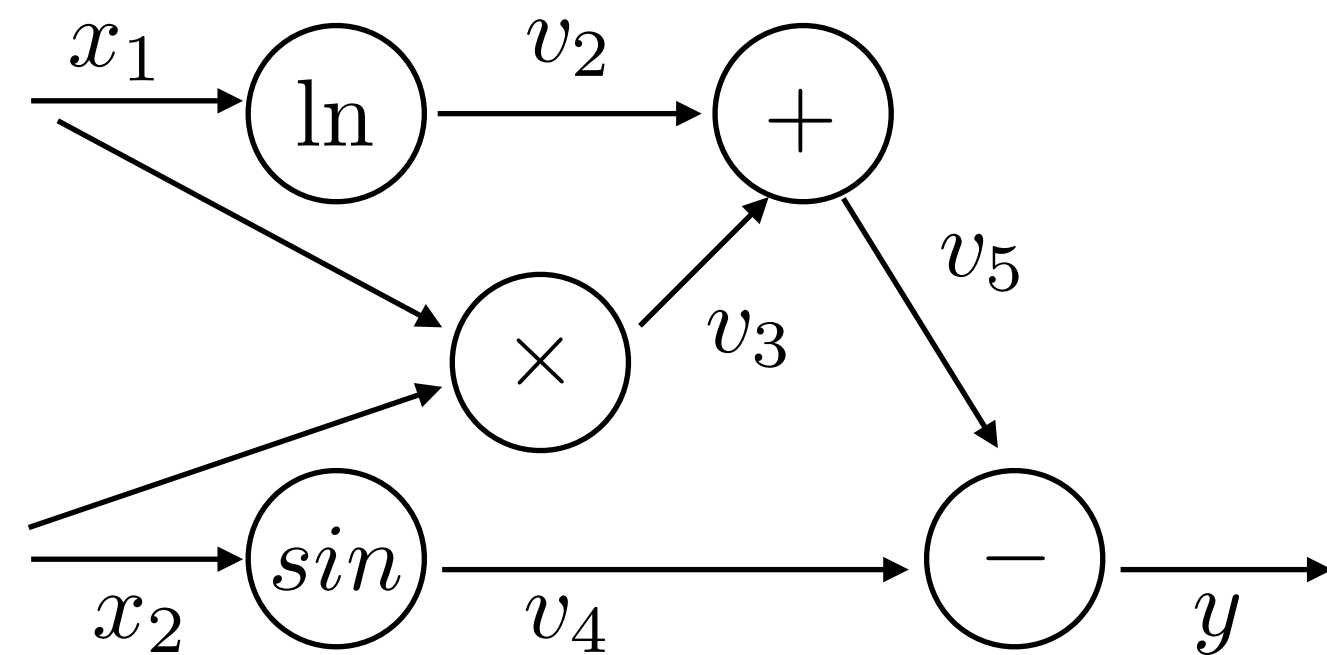
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Symbolic Differentiation

$$y = f(x_1, x_2) = \ln(x_1) + x_1x_2 - \sin(x_2)$$

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



Implements differentiation rules for composite functions:

Sum Rule

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

Product Rule

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

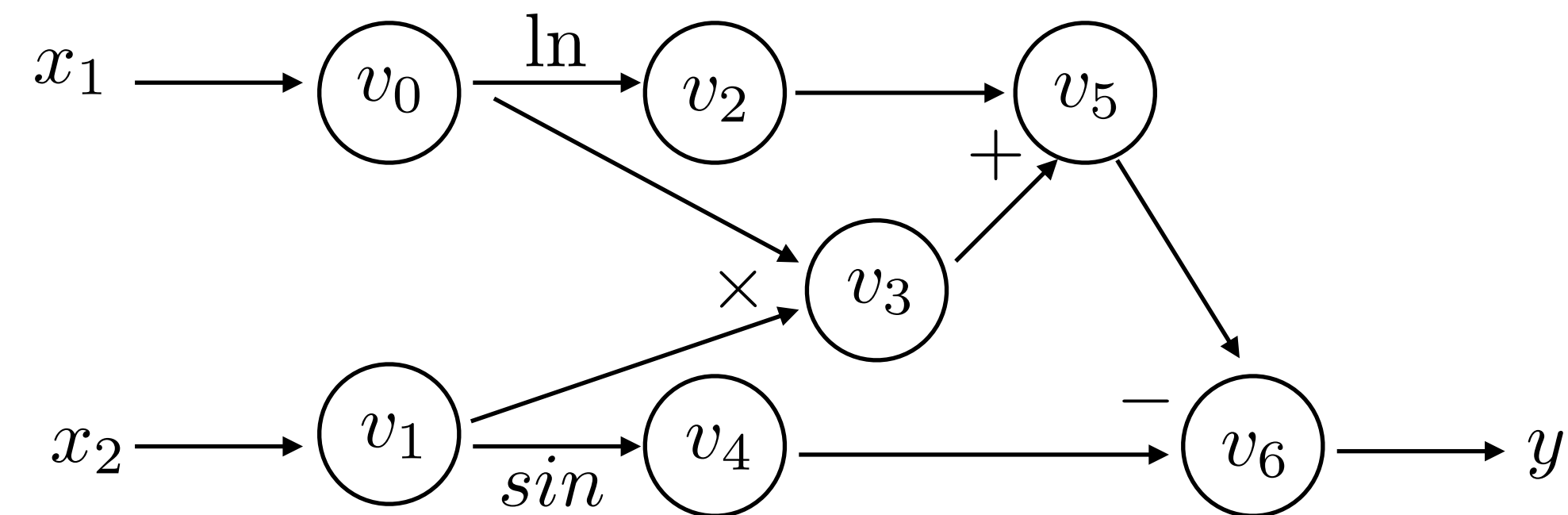
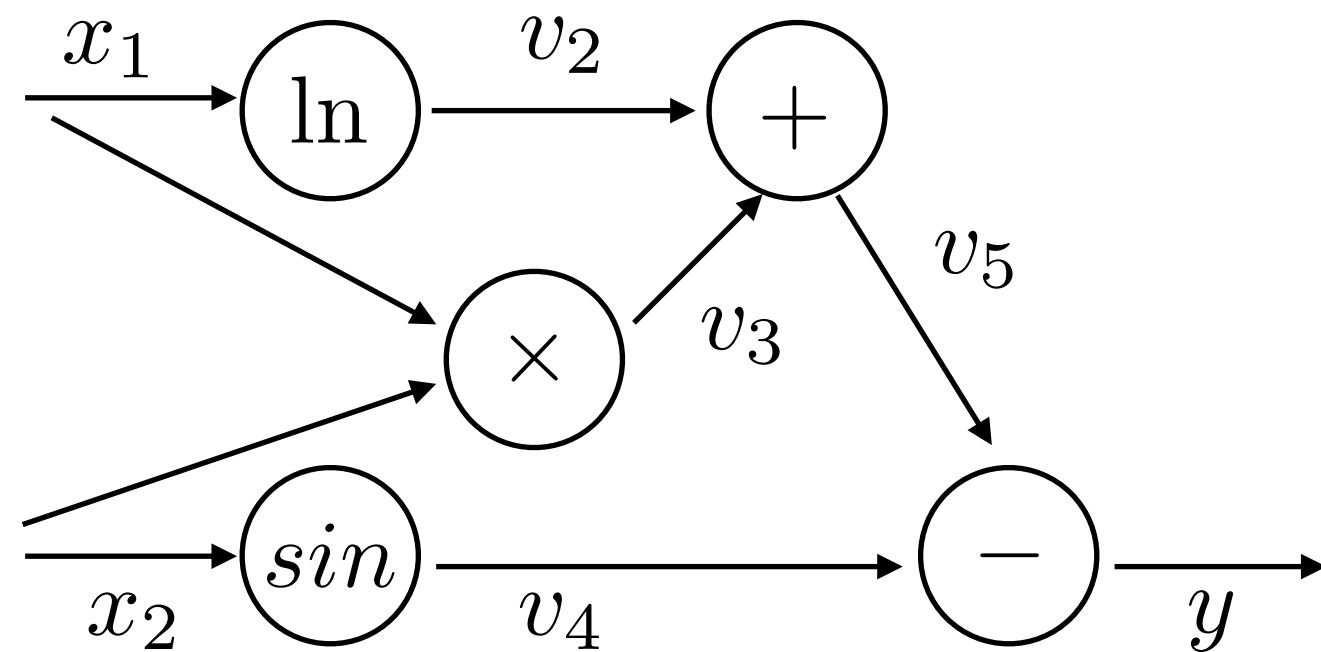
Chain Rule

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

Symbolic Differentiation

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Chain Rule

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

Automatic Differentiation (AutoDiff) $y = f(x_1, x_2) = \ln(x_1) + x_1x_2 - \sin(x_2)$

Intuition: Interleave symbolic differentiation and simplification

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

Automatic Differentiation (AutoDiff) $y = f(x_1, x_2) = \ln(x_1) + x_1x_2 - \sin(x_2)$

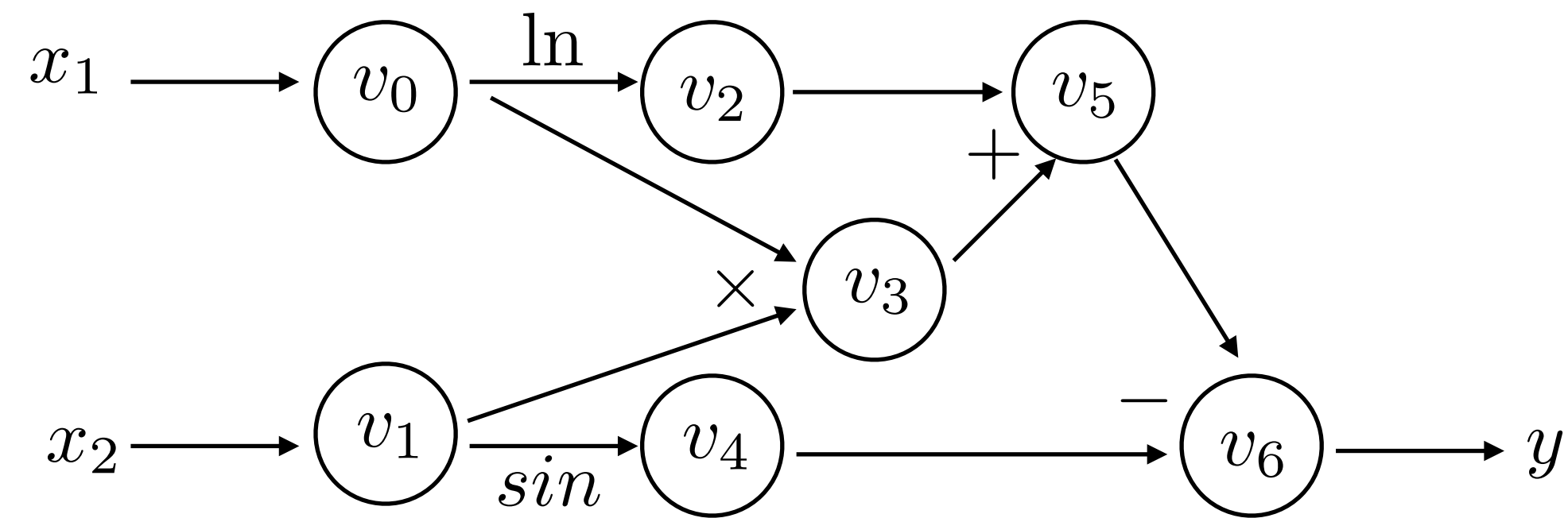
Intuition: Interleave symbolic differentiation and simplification

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, ...)

Automatic Differentiation (AutoDiff)

$$y = f(x_1, x_2) = \ln(x_1) + x_1x_2 - \sin(x_2)$$

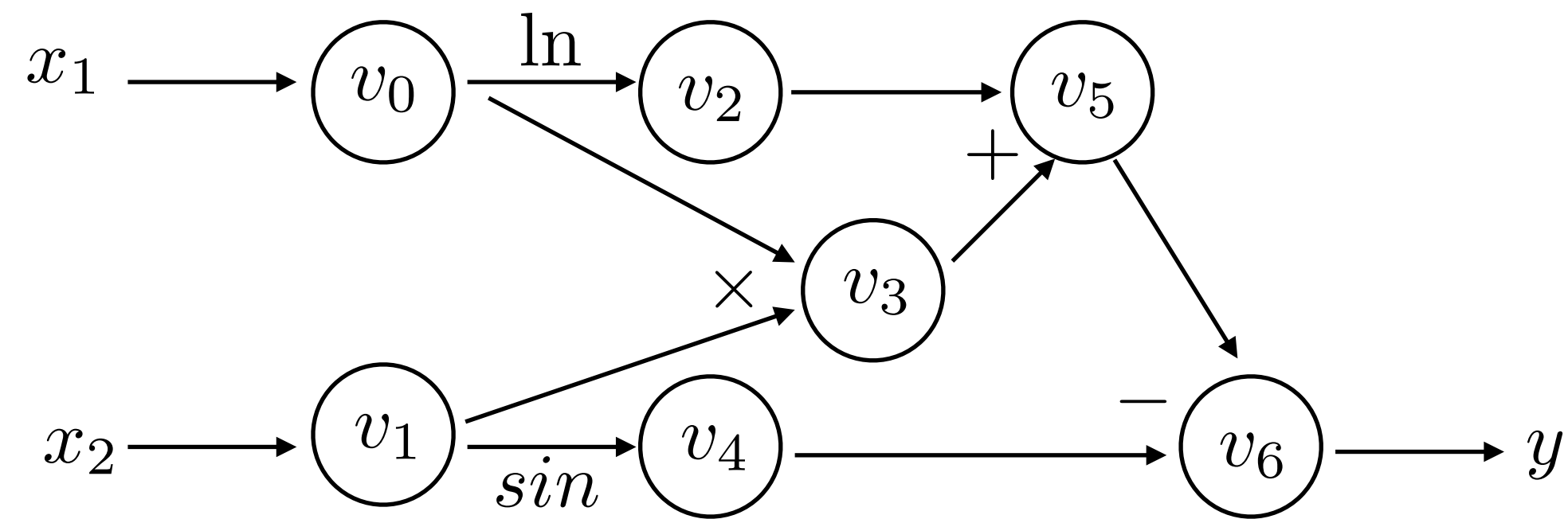


Each **node** is an input, intermediate, or output variable

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

Automatic Differentiation (AutoDiff)

$$y = f(x_1, x_2) = \ln(x_1) + x_1x_2 - \sin(x_2)$$



Computational graph is governed by these equations

$$v_0 = x_1$$

$$v_1 = x_2$$

$$v_2 = \ln(v_0)$$

$$v_3 = v_0 \cdot v_1$$

$$v_4 = \sin(v_1)$$

$$v_5 = v_2 + v_3$$

$$v_6 = v_5 - v_4$$

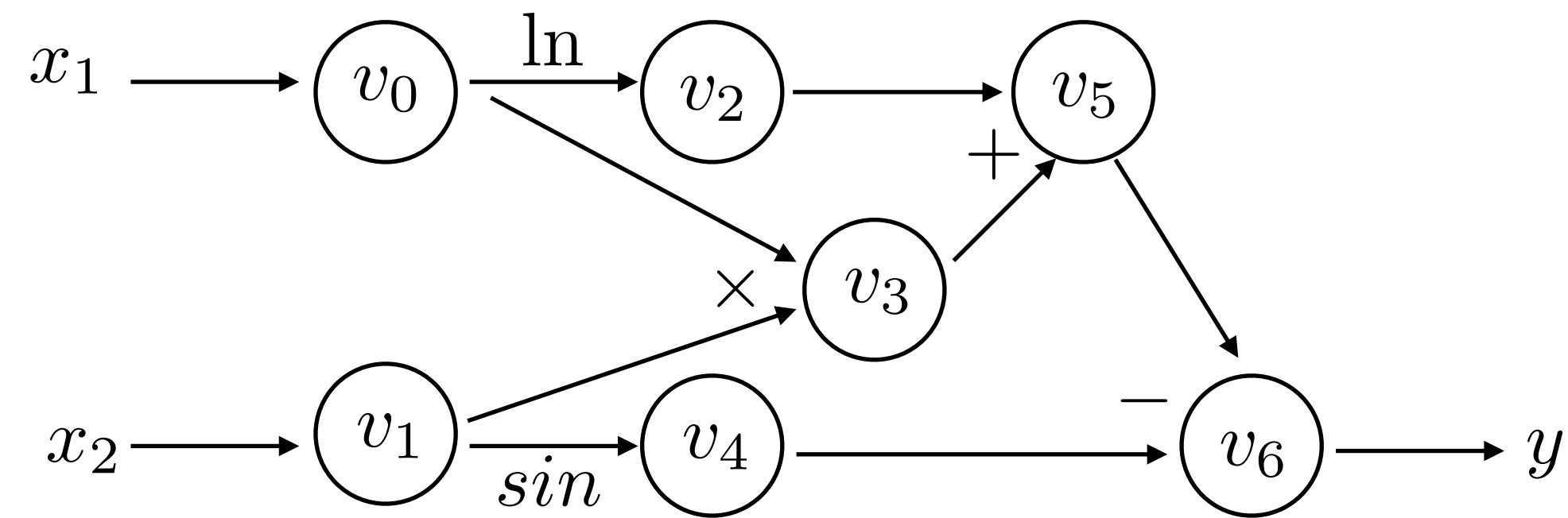
$$y = v_6$$

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

Automatic Differentiation (AutoDiff)

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

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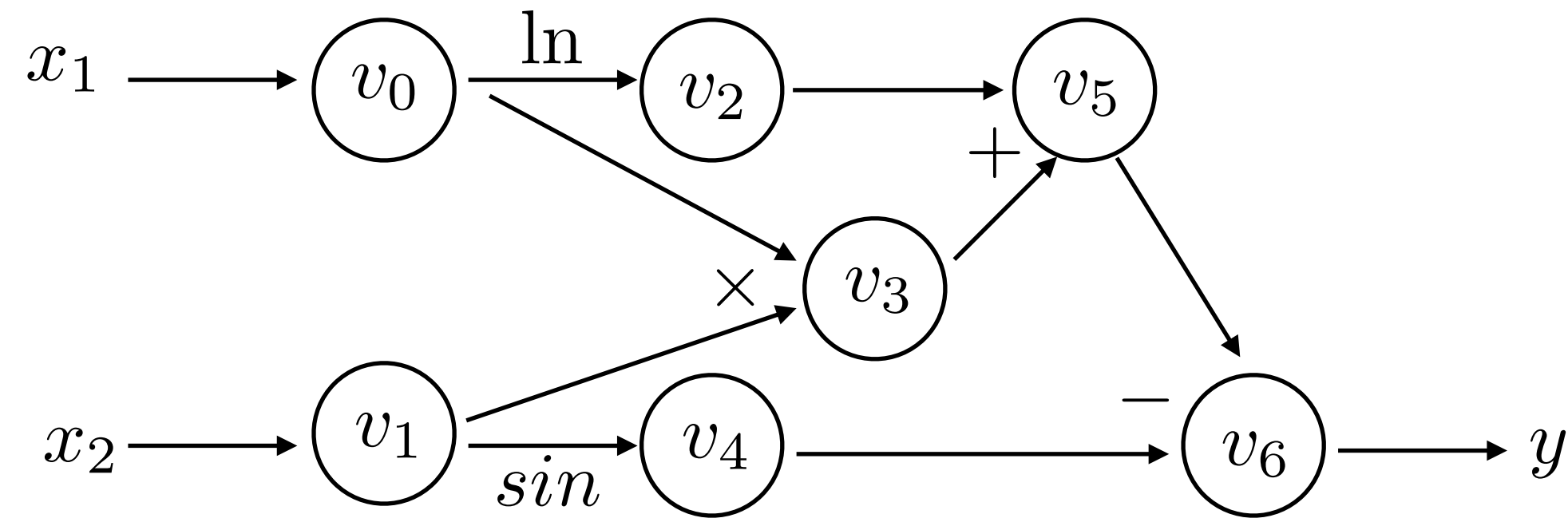
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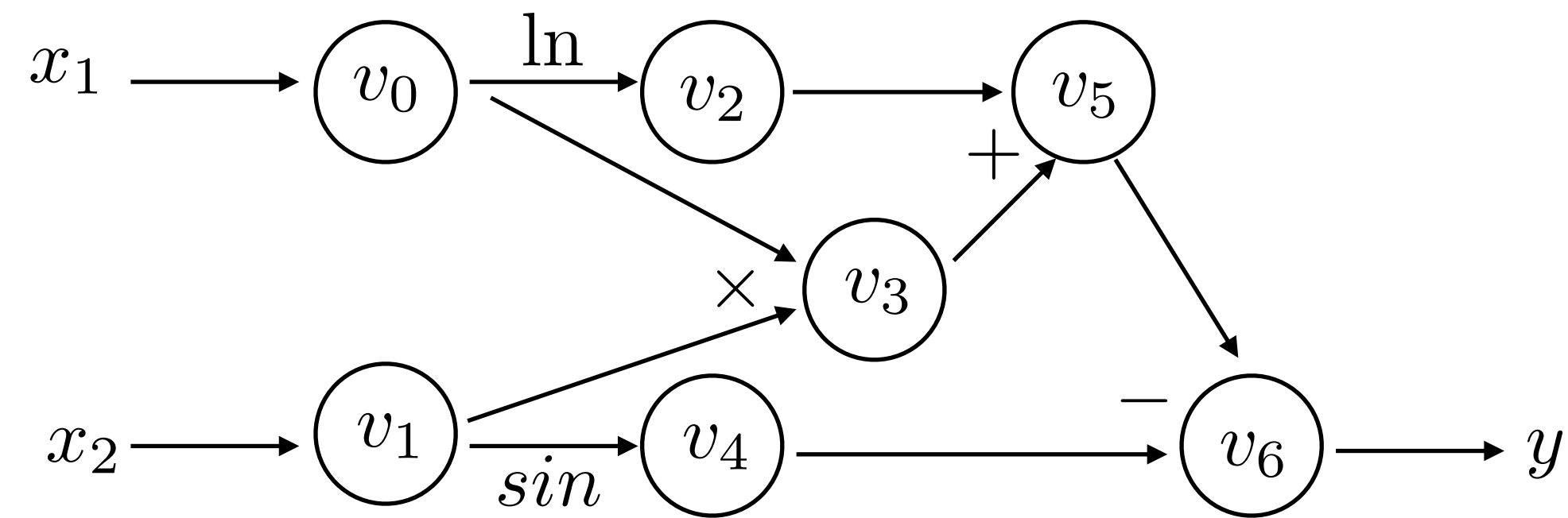
Forward Evaluation Trace:

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

Automatic Differentiation (AutoDiff)

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

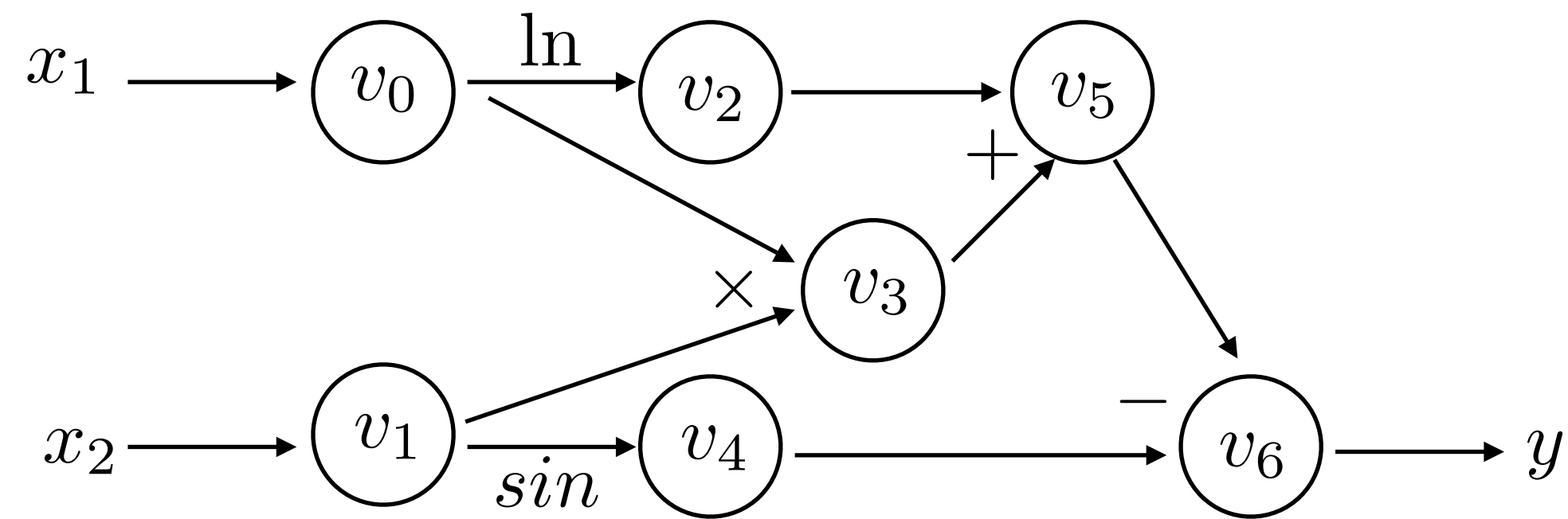
Forward Evaluation Trace:

	$f(2, 5)$
$v_0 = x_1$	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)

$$y = f(x_1, x_2) = \ln(x_1) + x_1x_2 - \sin(x_2)$$

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



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

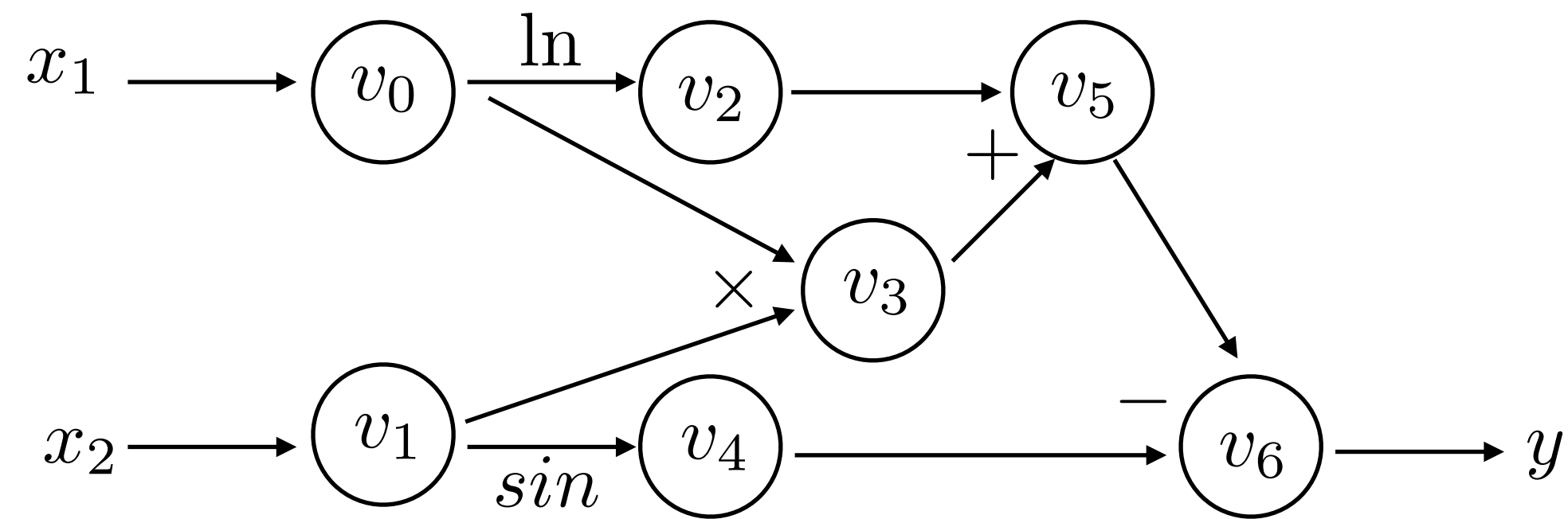
Forward Evaluation Trace:

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

Automatic Differentiation (AutoDiff)

$$y = f(x_1, x_2) = \ln(x_1) + x_1x_2 - \sin(x_2)$$

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.

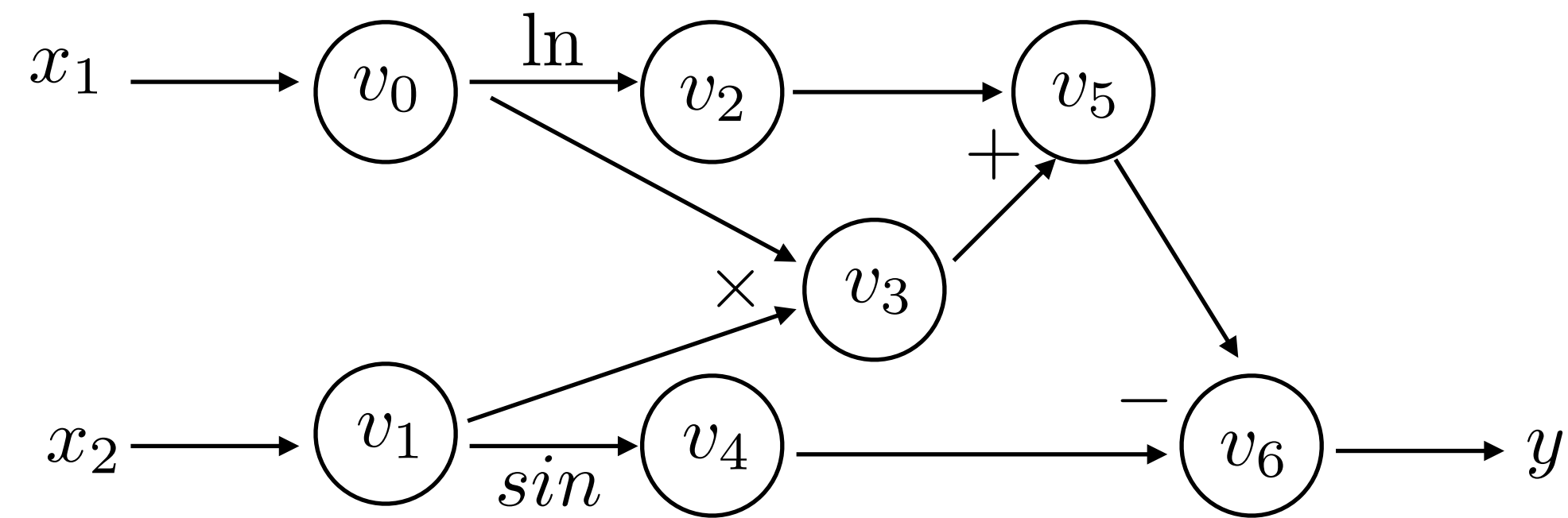
Forward Evaluation Trace:

	$f(2, 5)$
$v_0 = x_1$	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)

$$y = f(x_1, x_2) = \ln(x_1) + x_1x_2 - \sin(x_2)$$

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



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

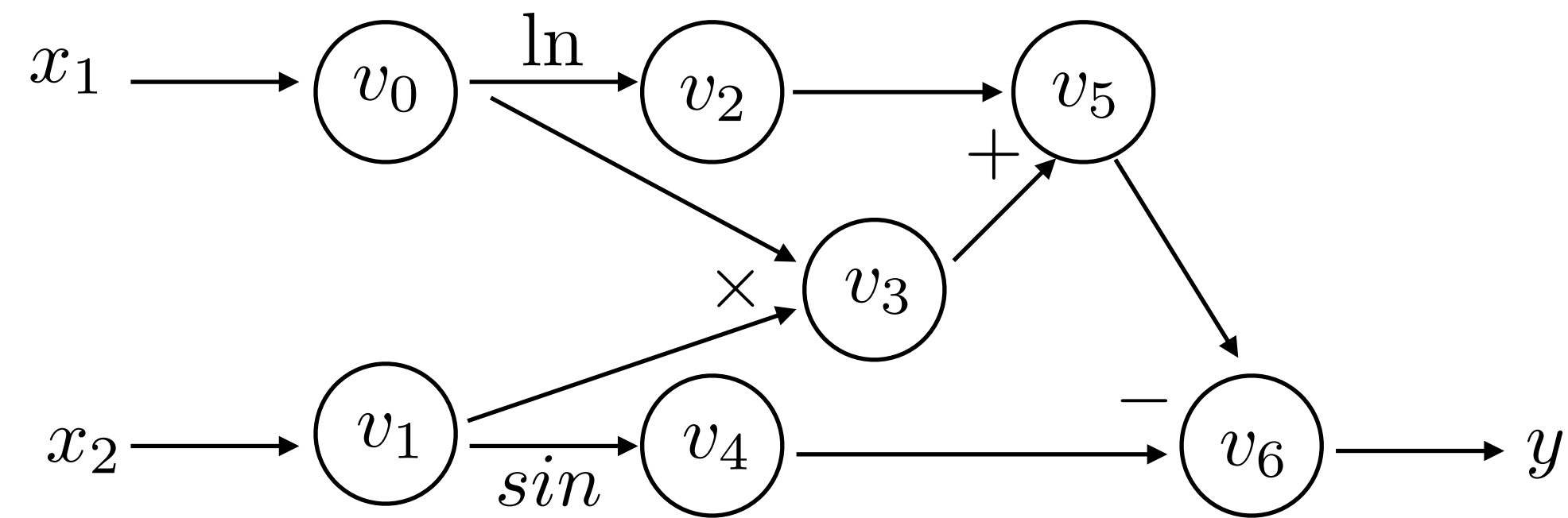
Forward Evaluation Trace:

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

Automatic Differentiation (AutoDiff)

$$y = f(x_1, x_2) = \ln(x_1) + x_1x_2 - \sin(x_2)$$

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



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

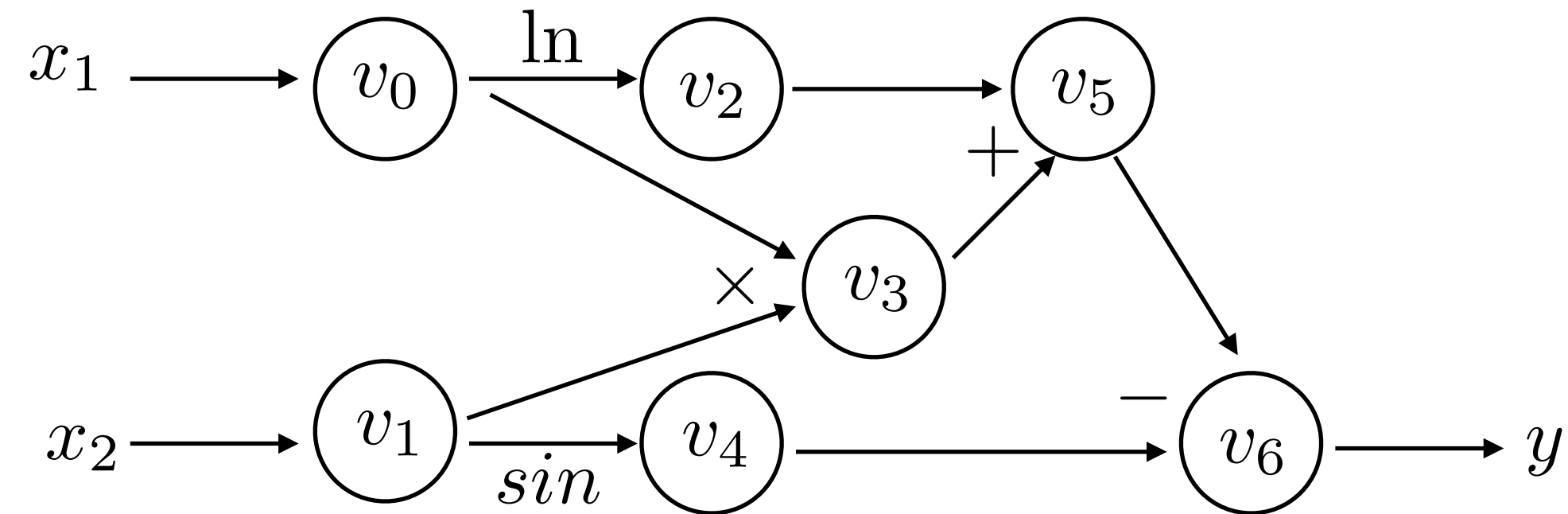
Computational graph (a DAG) with variable ordering from topological sort.

Forward Evaluation Trace:

	$f(2, 5)$
$v_0 = x_1$	2
$v_1 = x_2$	5
$v_2 = \ln(v_0)$	$\ln(2) = 0.693$
$v_3 = v_0 \cdot v_1$	$2 \times 5 = 10$
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Automatic Differentiation (AutoDiff)

$$y = f(x_1, x_2) = \ln(x_1) + x_1x_2 - \sin(x_2)$$

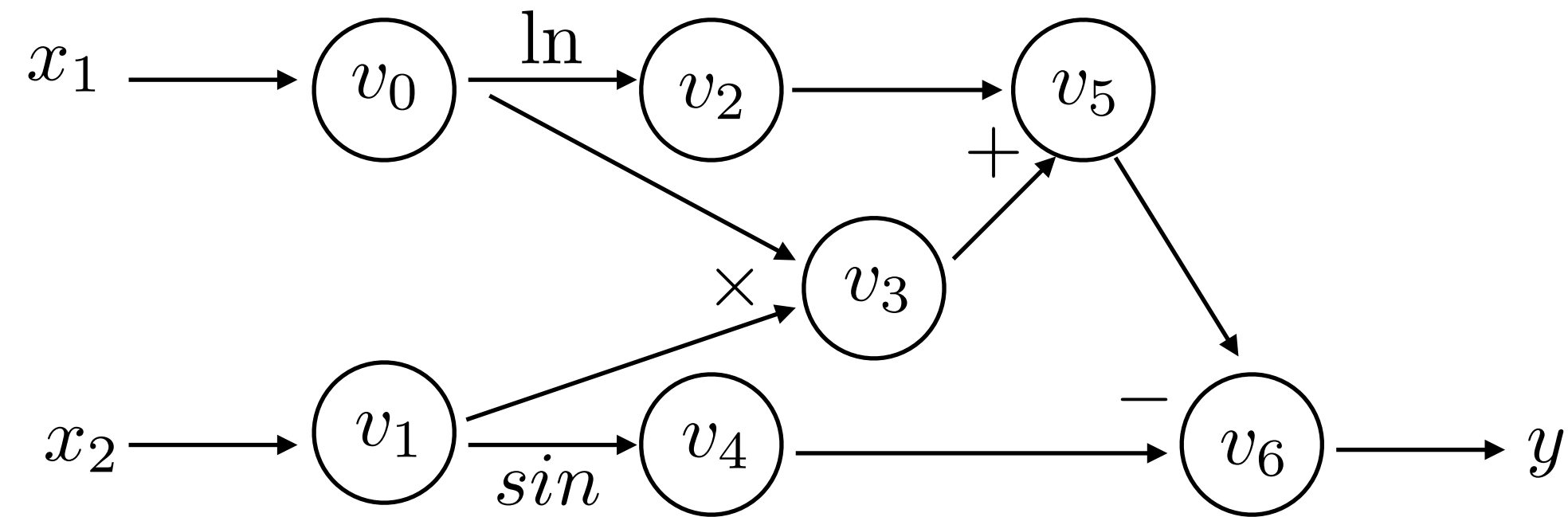


Forward Evaluation Trace:

	$f(2, 5)$
$v_0 = x_1$	2
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$v_2 = \ln(v_0)$	$\ln(2) = 0.693$
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AutoDiff - Forward Mode

$$y = f(x_1, x_2) = \ln(x_1) + x_1x_2 - \sin(x_2)$$



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

Forward Evaluation Trace:

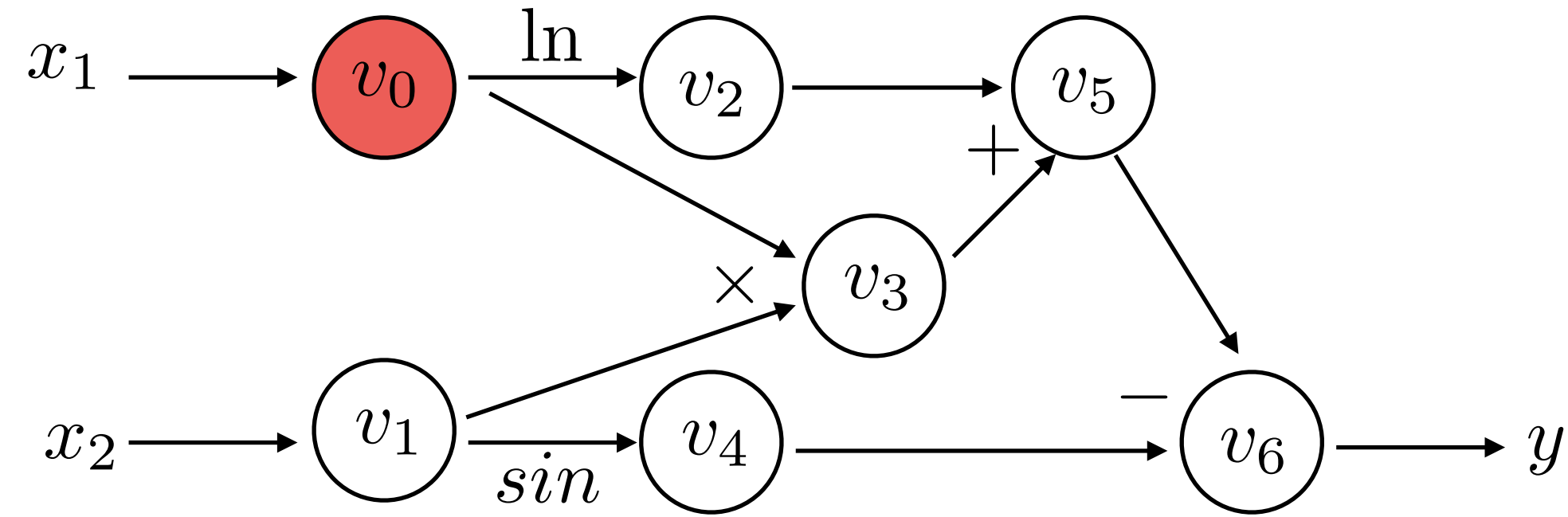
$$\left. \frac{\partial f(x_1, x_2)}{\partial x_1} \right|_{(x_1=2, x_2=5)}$$

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

$$y = f(x_1, x_2) = \ln(x_1) + x_1x_2 - \sin(x_2)$$

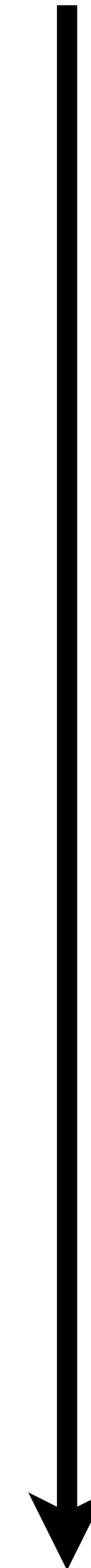


Forward Derivative Trace:

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

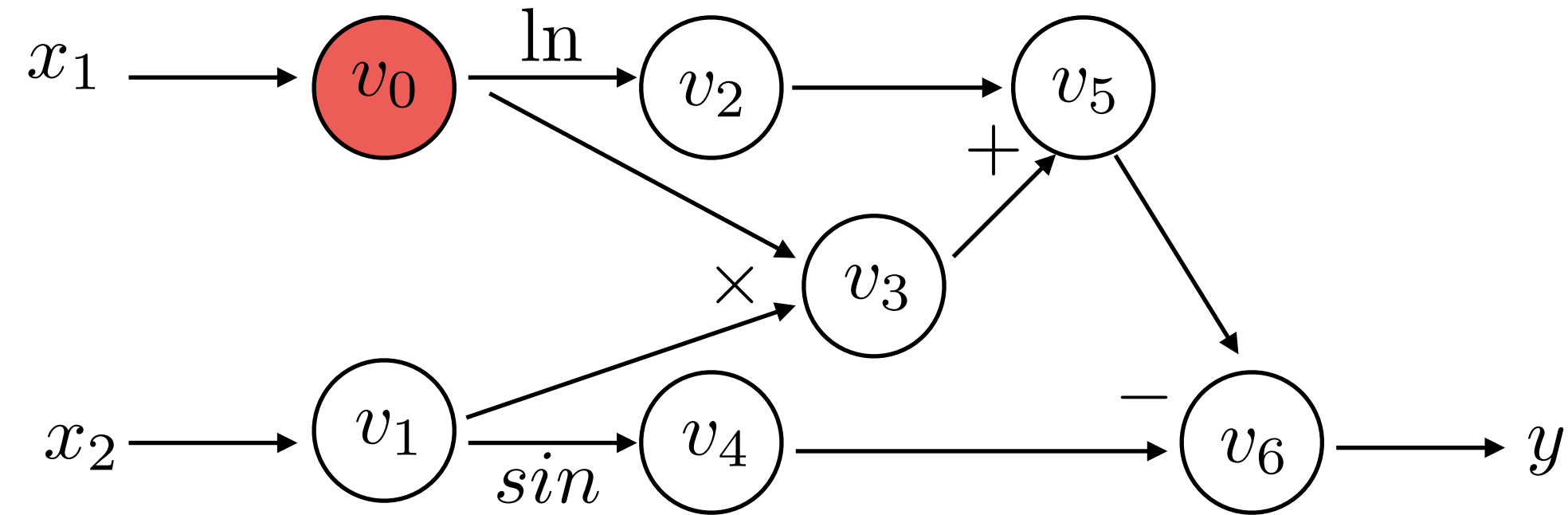
Forward Evaluation Trace:

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

$$y = f(x_1, x_2) = \ln(x_1) + x_1x_2 - \sin(x_2)$$



Forward Derivative Trace:

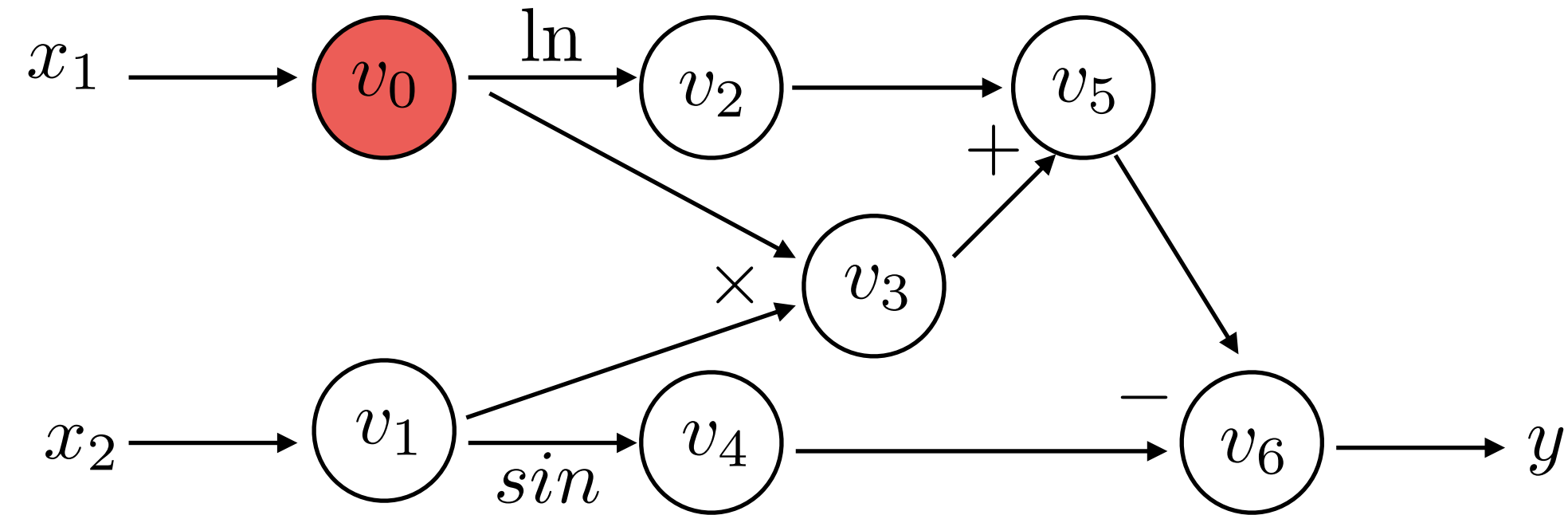
	$\frac{\partial f(x_1, x_2)}{\partial x_1} \Big _{(x_1=2, x_2=5)}$
$\frac{\partial v_0}{\partial x_1}$	

Forward Evaluation Trace:

	$f(2, 5)$
<u>$v_0 = x_1$</u>	2
$v_1 = x_2$	5
$v_2 = \ln(v_0)$	$\ln(2) = 0.693$
$v_3 = v_0 \cdot v_1$	$2 \times 5 = 10$
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AutoDiff - Forward Mode

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Forward Derivative Trace:

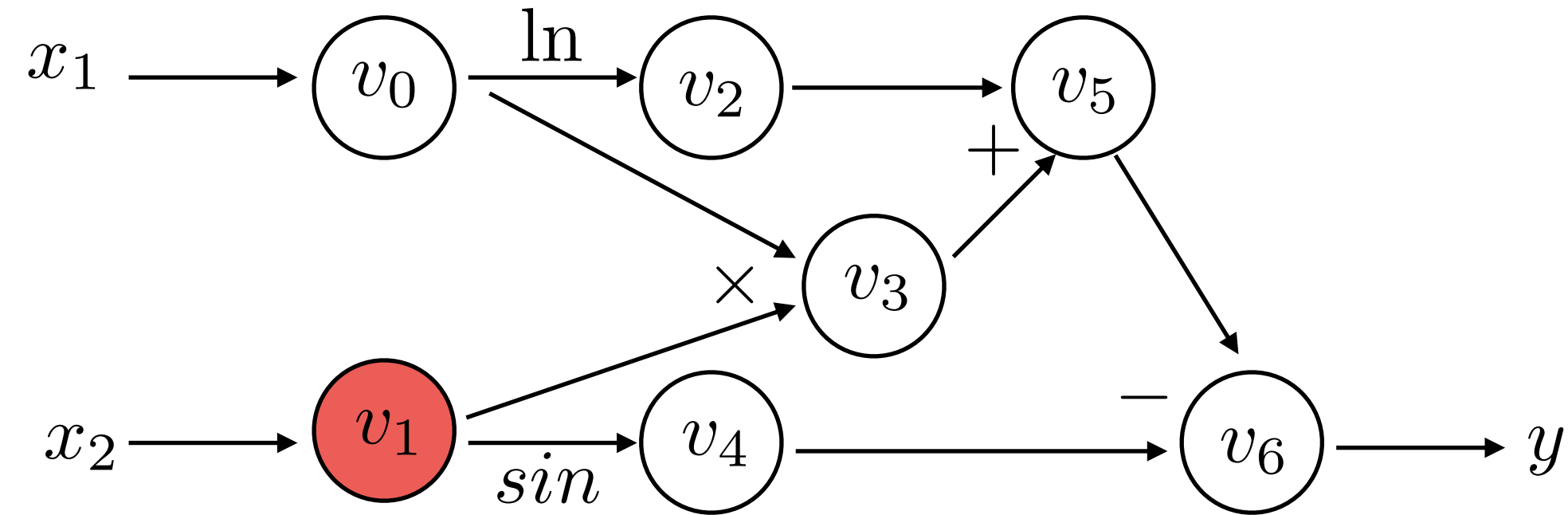
	$\frac{\partial f(x_1, x_2)}{\partial x_1} \Big _{(x_1=2, x_2=5)}$
$\frac{\partial v_0}{\partial x_1}$	1

Forward Evaluation Trace:

	$f(2, 5)$
<u>$v_0 = x_1$</u>	2
$v_1 = x_2$	5
$v_2 = \ln(v_0)$	$\ln(2) = 0.693$
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AutoDiff - Forward Mode

$$y = f(x_1, x_2) = \ln(x_1) + x_1x_2 - \sin(x_2)$$



Forward Derivative Trace:

$$\frac{\partial v_0}{\partial x_1}$$

$$\frac{\partial v_1}{\partial x_1}$$

$$\frac{\partial v_1}{\partial x_1}$$

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

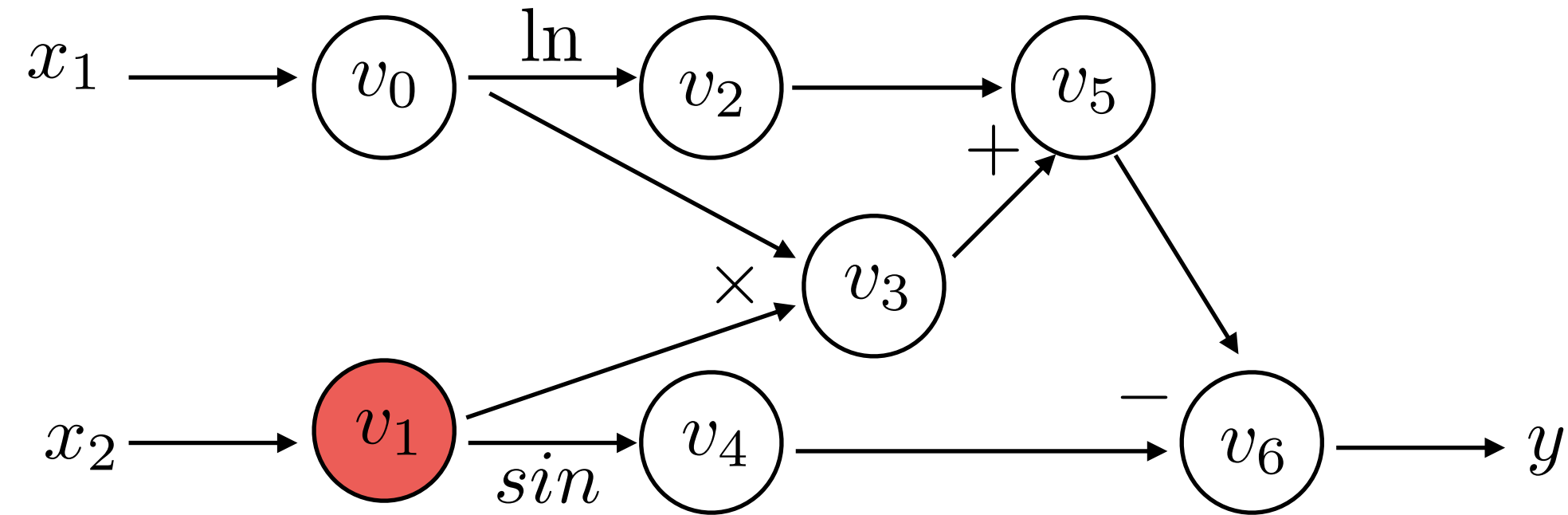
1

Forward Evaluation Trace:

	$f(2, 5)$
$v_0 = x_1$	2
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$v_2 = \ln(v_0)$	$\ln(2) = 0.693$
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Forward Derivative Trace:

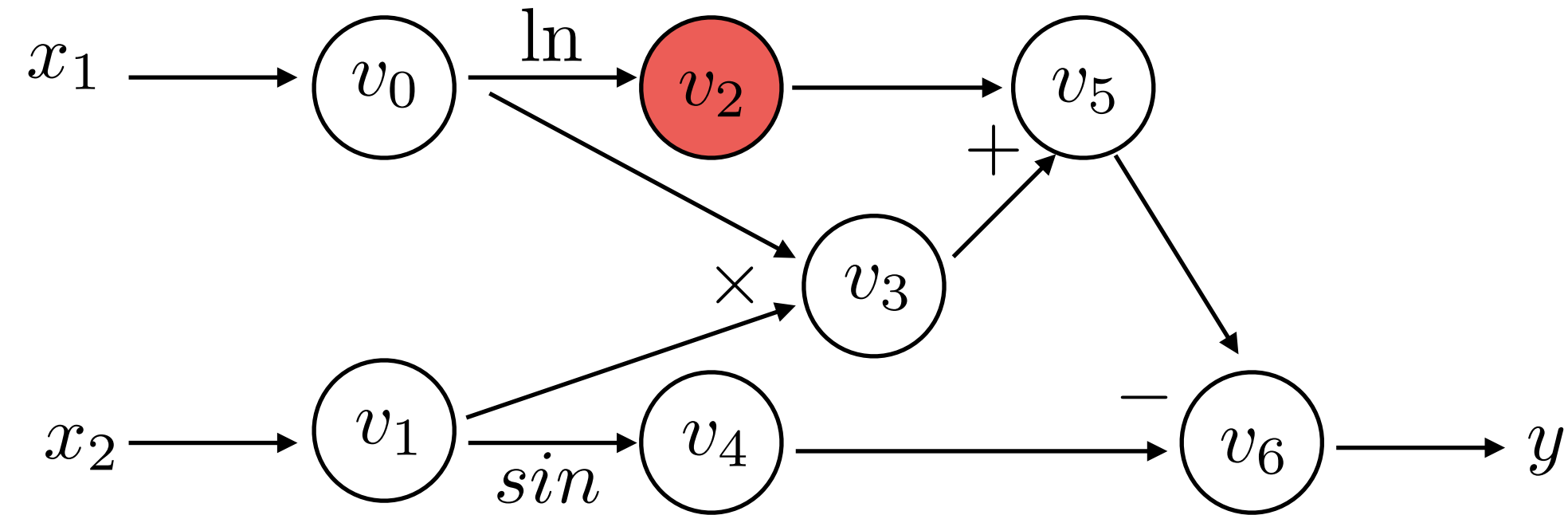
	$\left. \frac{\partial f(x_1, x_2)}{\partial x_1} \right _{(x_1=2, x_2=5)}$
$\frac{\partial v_0}{\partial x_1}$	1
$\frac{\partial v_1}{\partial x_1}$	0

Forward Evaluation Trace:

	$f(2, 5)$
$v_0 = x_1$	2
<u>$v_1 = x_2$</u>	5
$v_2 = \ln(v_0)$	$\ln(2) = 0.693$
$v_3 = v_0 \cdot v_1$	$2 \times 5 = 10$
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AutoDiff - Forward Mode

$$y = f(x_1, x_2) = \ln(x_1) + x_1x_2 - \sin(x_2)$$



Forward Derivative Trace:

$$\frac{\partial v_0}{\partial x_1}$$

$$\frac{\partial v_1}{\partial x_1}$$

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

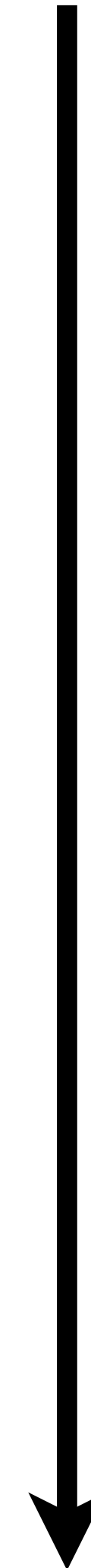
$$\left. \frac{\partial f(x_1, x_2)}{\partial x_1} \right|_{(x_1=2, x_2=5)}$$

1

0

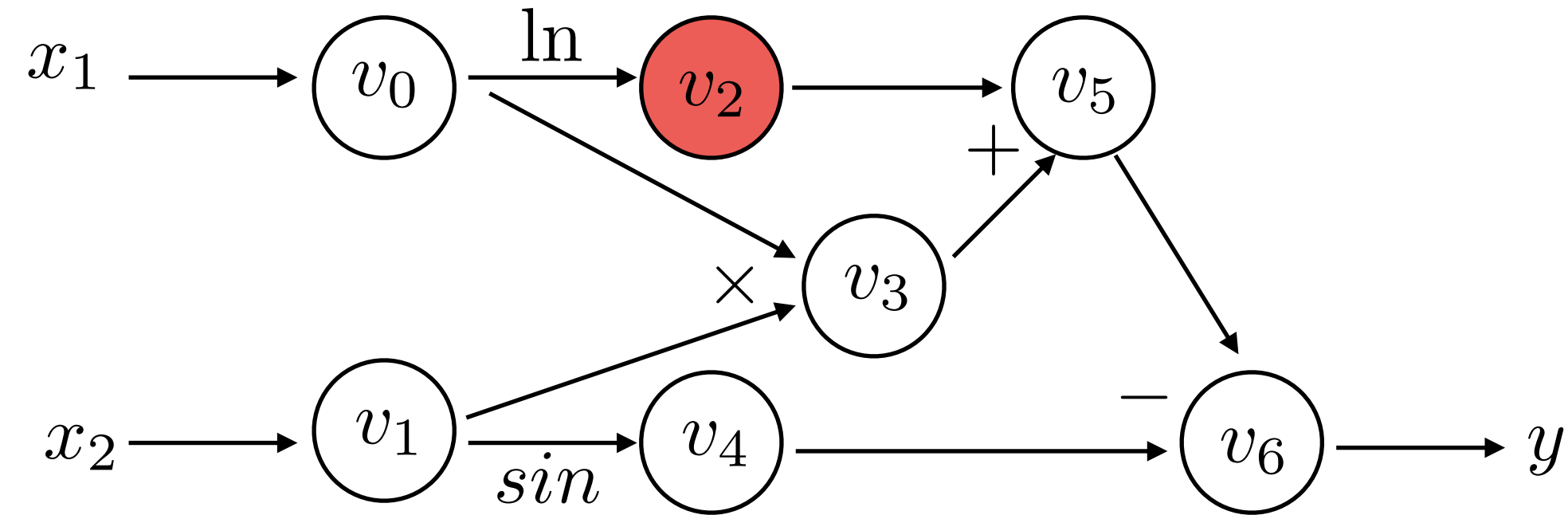
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AutoDiff - Forward Mode

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Forward Derivative Trace:

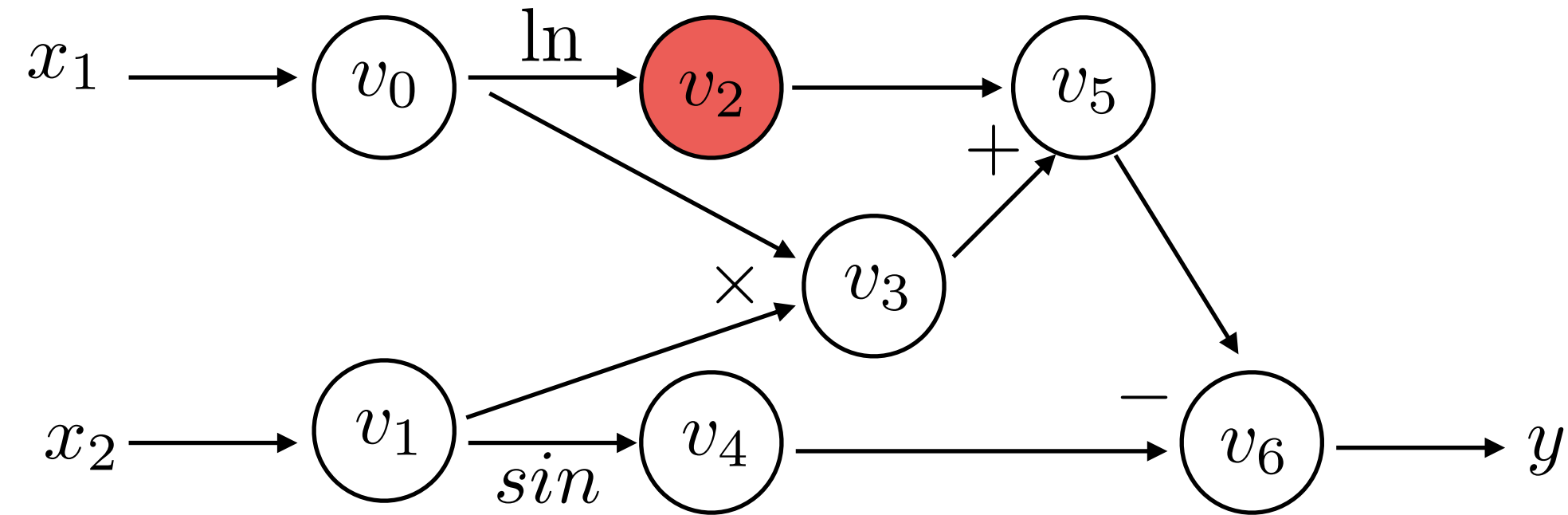
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	$\left. \frac{\partial f(x_1, x_2)}{\partial x_1} \right _{(x_1=2, x_2=5)}$
$\frac{\partial v_0}{\partial x_1}$	1
$\frac{\partial v_1}{\partial x_1}$	0
$\frac{\partial v_2}{\partial x_1}$	
$\frac{\partial v_3}{\partial x_1}$	
$\frac{\partial v_4}{\partial x_1}$	
$\frac{\partial v_5}{\partial x_1}$	
$\frac{\partial v_6}{\partial x_1}$	
	Chain Rule

AutoDiff - Forward Mode

$$y = f(x_1, x_2) = \ln(x_1) + x_1x_2 - \sin(x_2)$$



Forward Evaluation Trace:

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Forward Derivative Trace:

$$\frac{\partial v_0}{\partial x_1} = 1$$

$$\frac{\partial v_1}{\partial x_1} = 0$$

$$\frac{\partial v_2}{\partial x_1} = \frac{1}{v_0} \frac{\partial v_0}{\partial x_1}$$

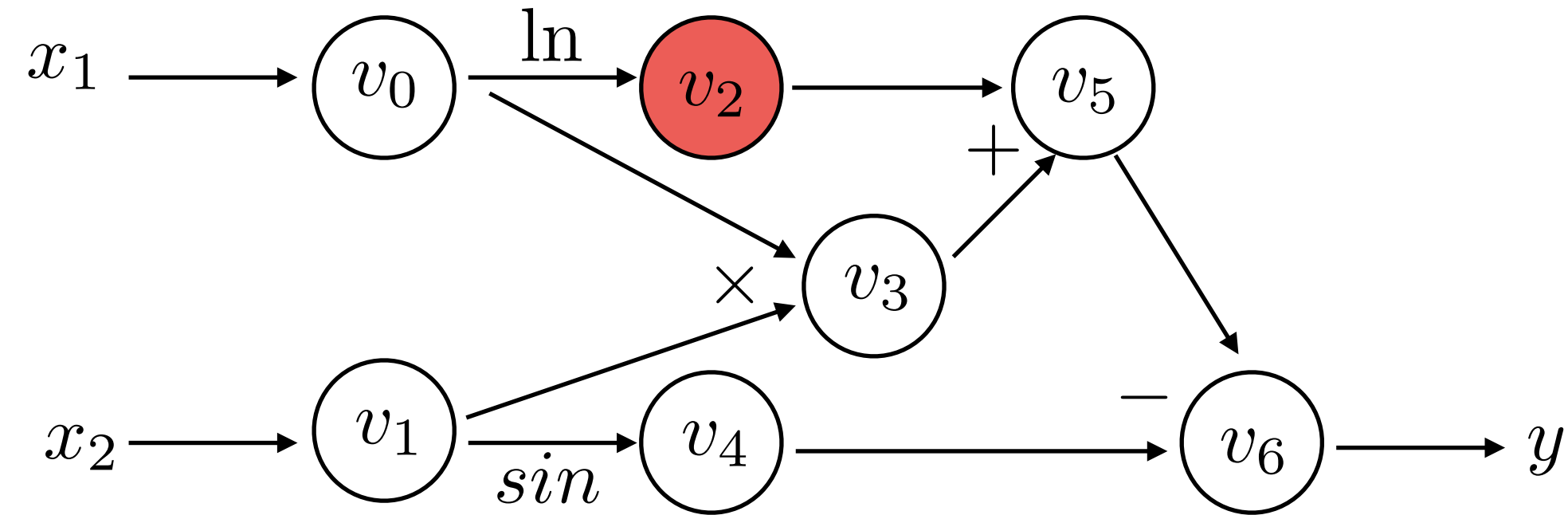
Chain Rule

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

1
0

AutoDiff - Forward Mode

$$y = f(x_1, x_2) = \ln(x_1) + x_1x_2 - \sin(x_2)$$



Forward Evaluation Trace:

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Forward Derivative Trace:

$$\frac{\partial v_0}{\partial x_1}$$

$$\frac{\partial v_1}{\partial x_1}$$

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Chain Rule

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

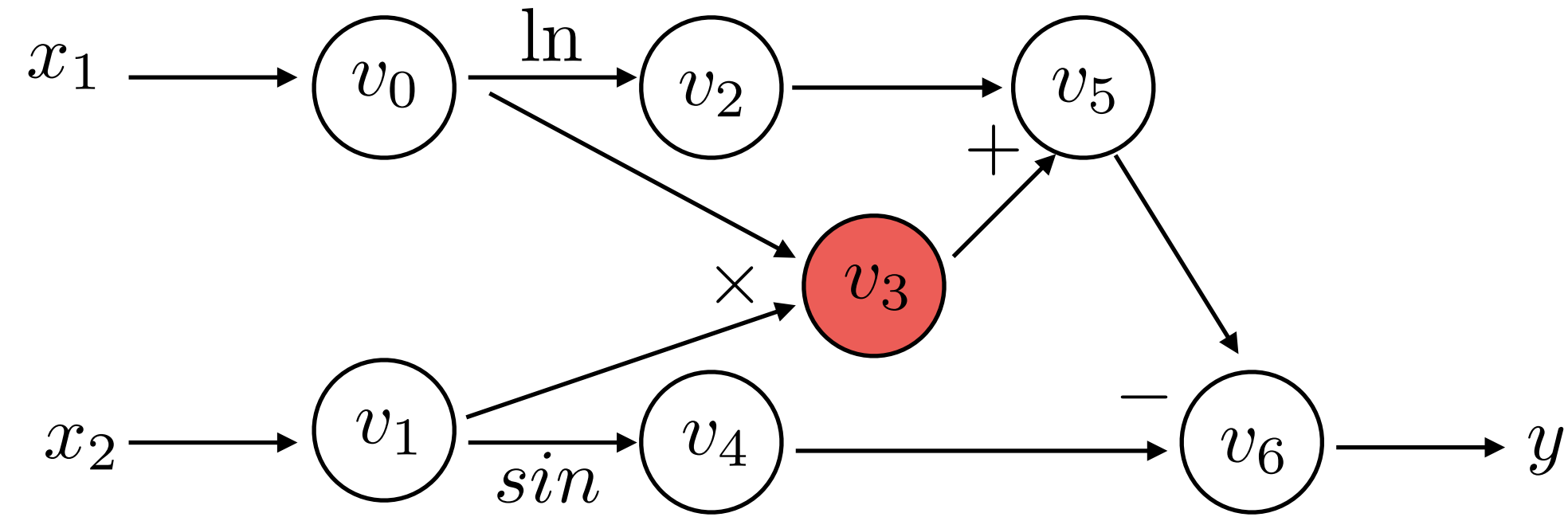
1

0

$$1/2 * 1 = 0.5$$

AutoDiff - Forward Mode

$$y = f(x_1, x_2) = \ln(x_1) + x_1x_2 - \sin(x_2)$$



Forward Evaluation Trace:

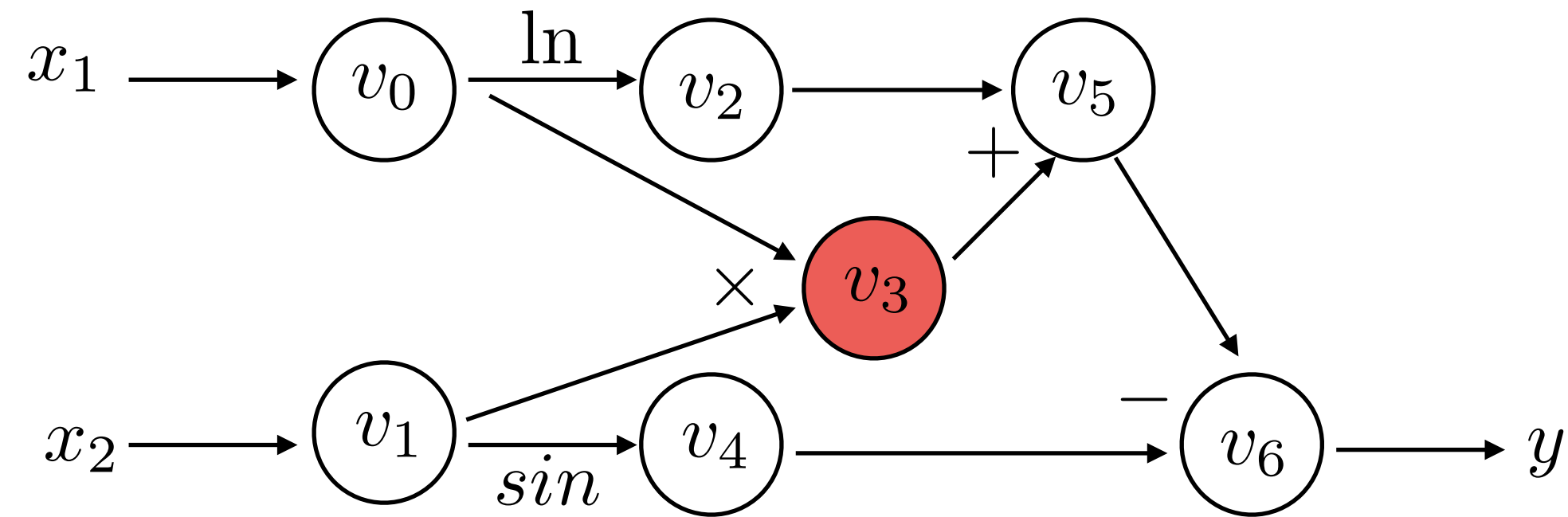
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Forward Derivative Trace:

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

$$y = f(x_1, x_2) = \ln(x_1) + x_1x_2 - \sin(x_2)$$



Forward Evaluation Trace:

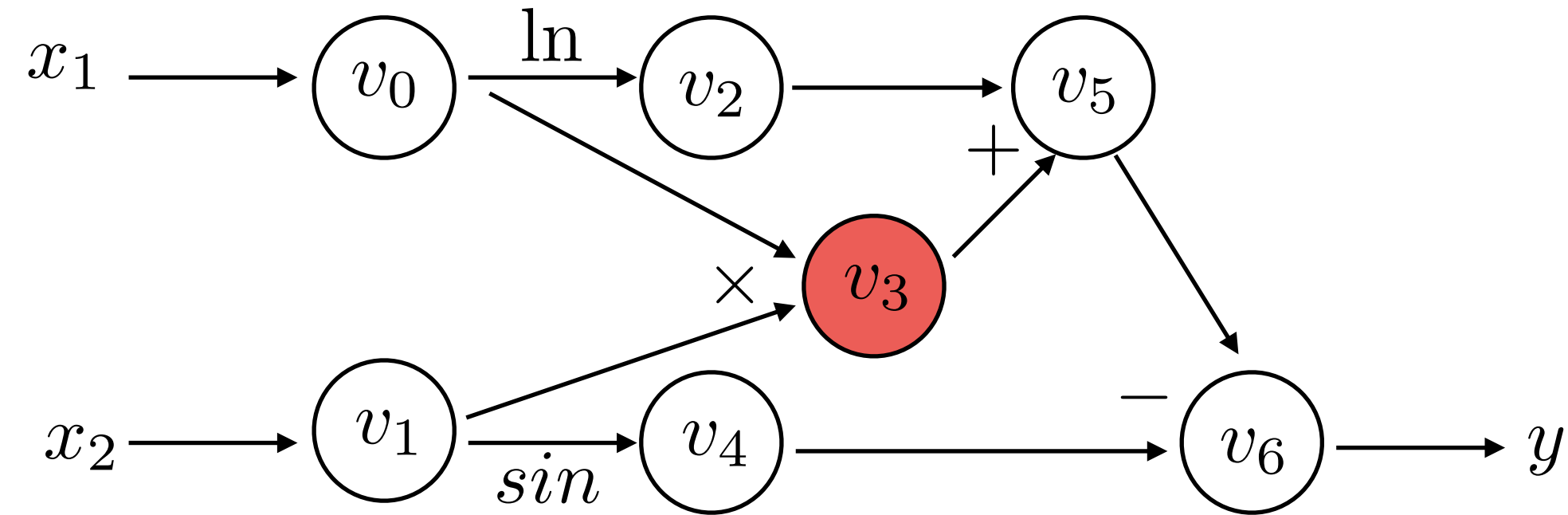
	$f(2, 5)$
$v_0 = x_1$	2
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	$\left. \frac{\partial f(x_1, x_2)}{\partial x_1} \right _{(x_1=2, x_2=5)}$
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Product Rule	

AutoDiff - Forward Mode

$$y = f(x_1, x_2) = \ln(x_1) + x_1x_2 - \sin(x_2)$$



Forward Derivative Trace:

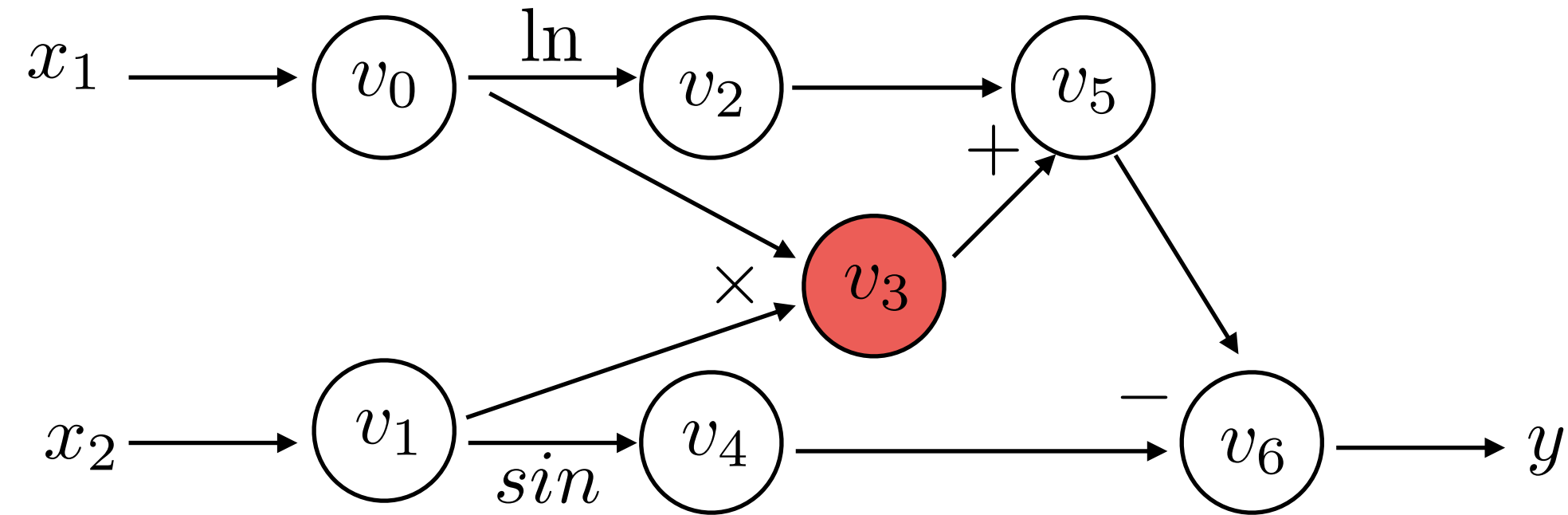
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$\frac{\partial v_2}{\partial x_1} = \frac{1}{v_0} \frac{\partial v_0}{\partial x_1}$	$1/2 * 1 = 0.5$
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Forward Derivative Trace:

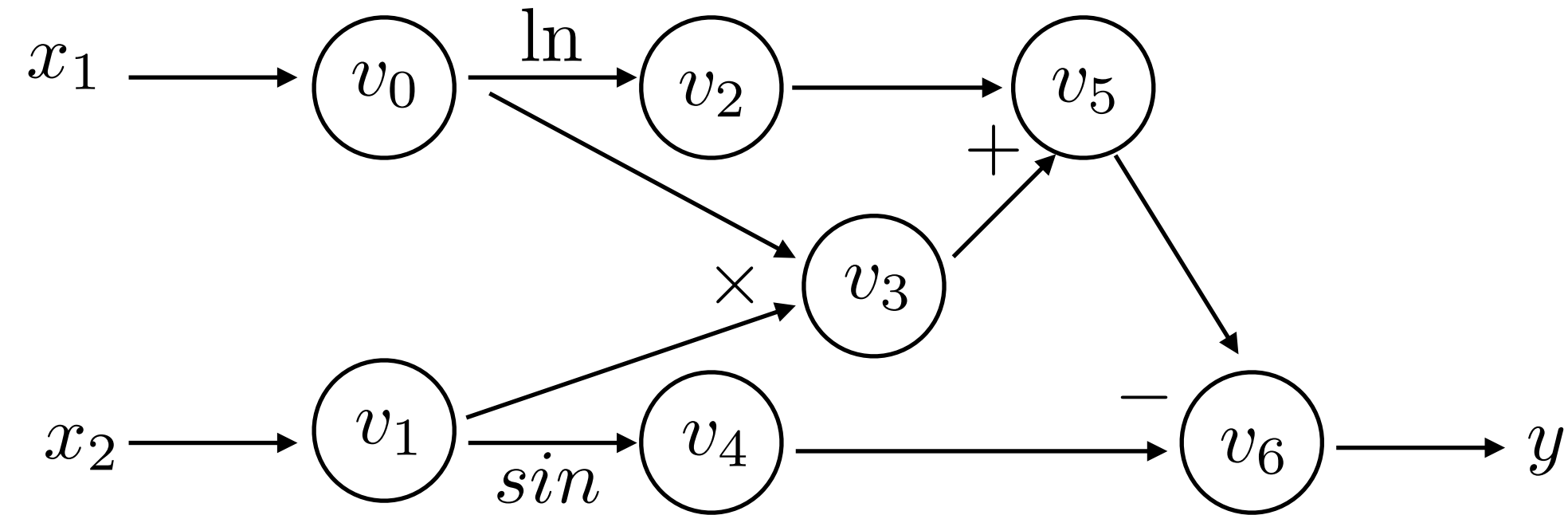
Forward Evaluation Trace:

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

AutoDiff - Forward Mode

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Forward Evaluation Trace:

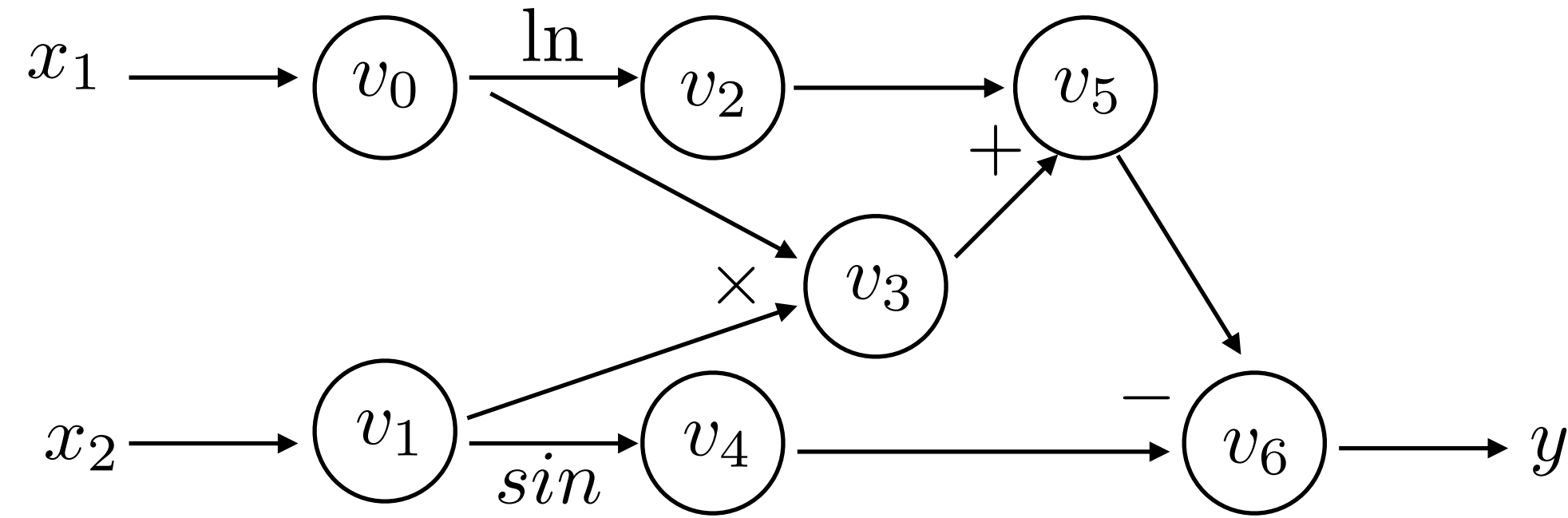
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$\frac{\partial v_2}{\partial x_1} = \frac{1}{v_0} \frac{\partial v_0}{\partial x_1}$	$1/2 * 1 = 0.5$
$\frac{\partial v_3}{\partial x_1} = \frac{\partial v_0}{\partial x_1} \cdot v_1 + v_0 \cdot \frac{\partial v_1}{\partial x_1}$	$1 * 5 + 2 * 0 = 5$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

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Forward Derivative Trace:

We now have:

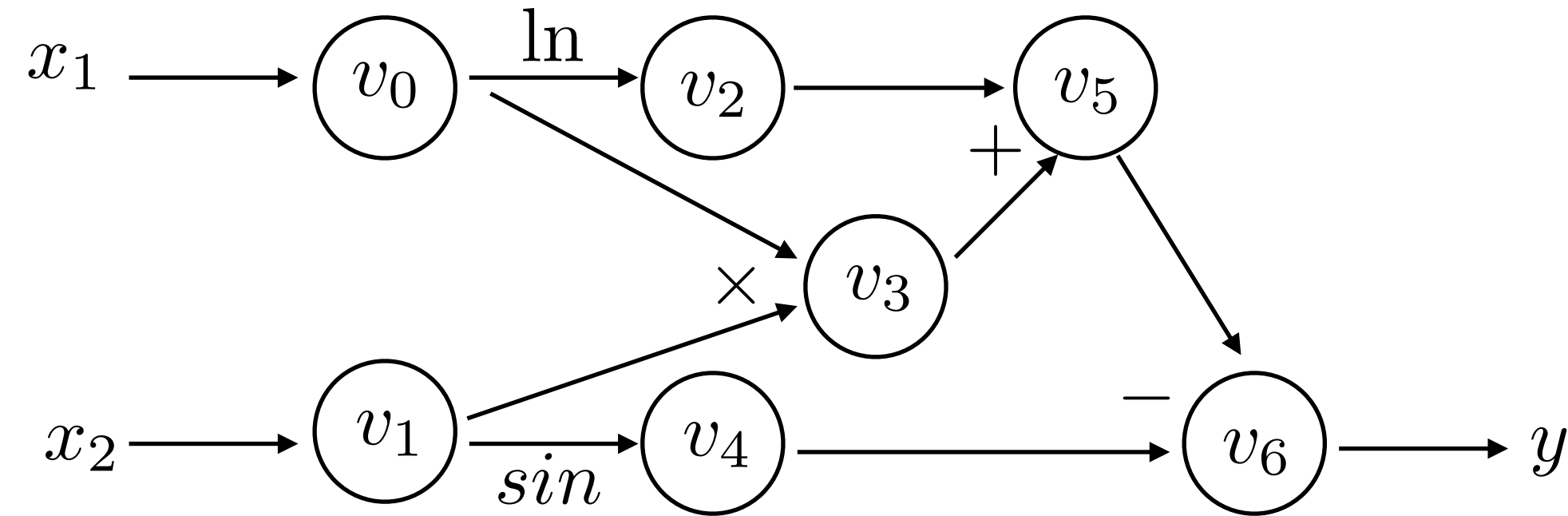
$$\left. \frac{\partial f(x_1, x_2)}{\partial x_1} \right|_{(x_1=2, x_2=5)} = 5.5$$

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Forward Derivative Trace:

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:

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

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

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

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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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Why?

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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

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

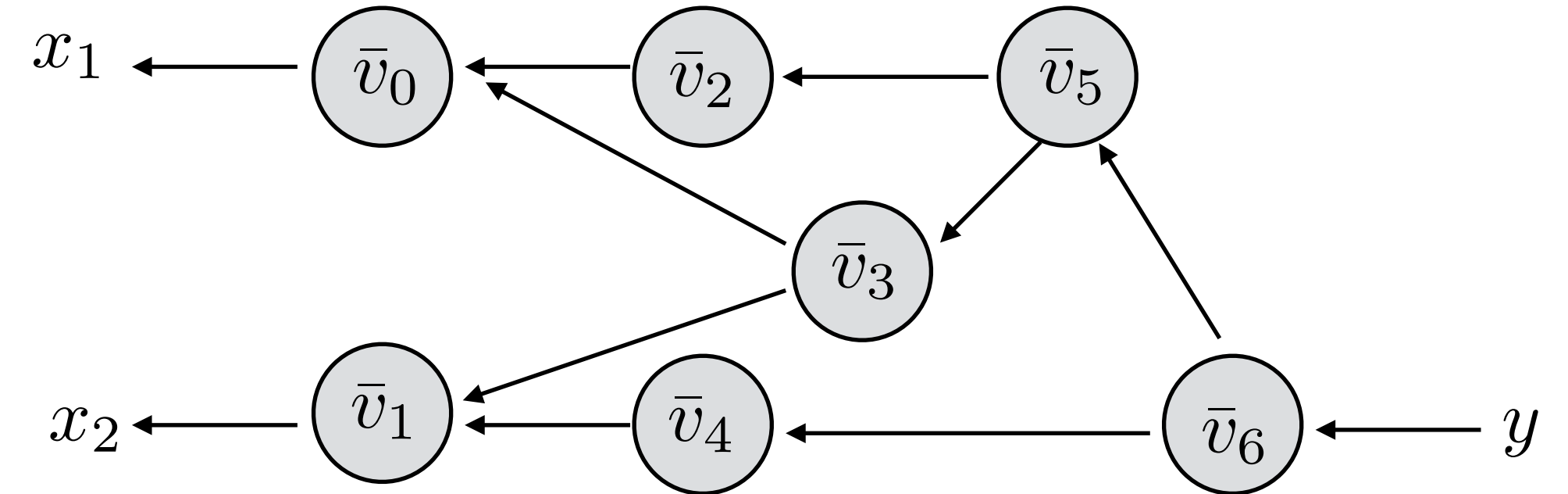
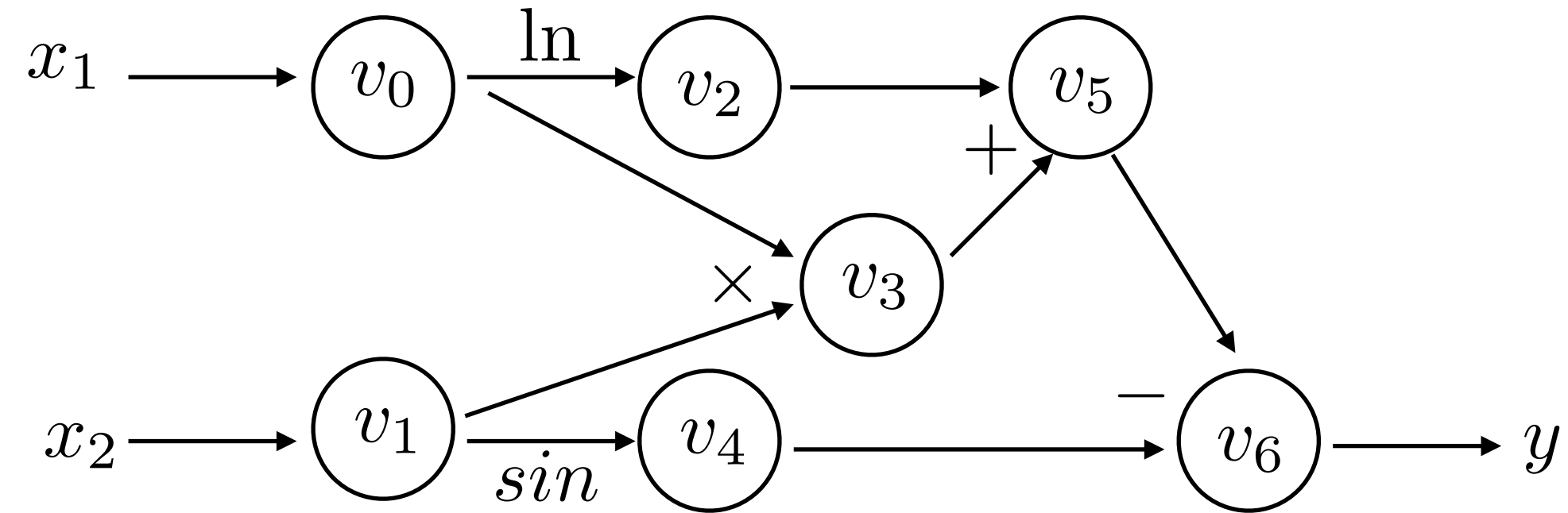
Problem: DNN typically has large number of inputs:

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**)

AutoDiff - Reverse Mode



Forward Evaluation Trace:

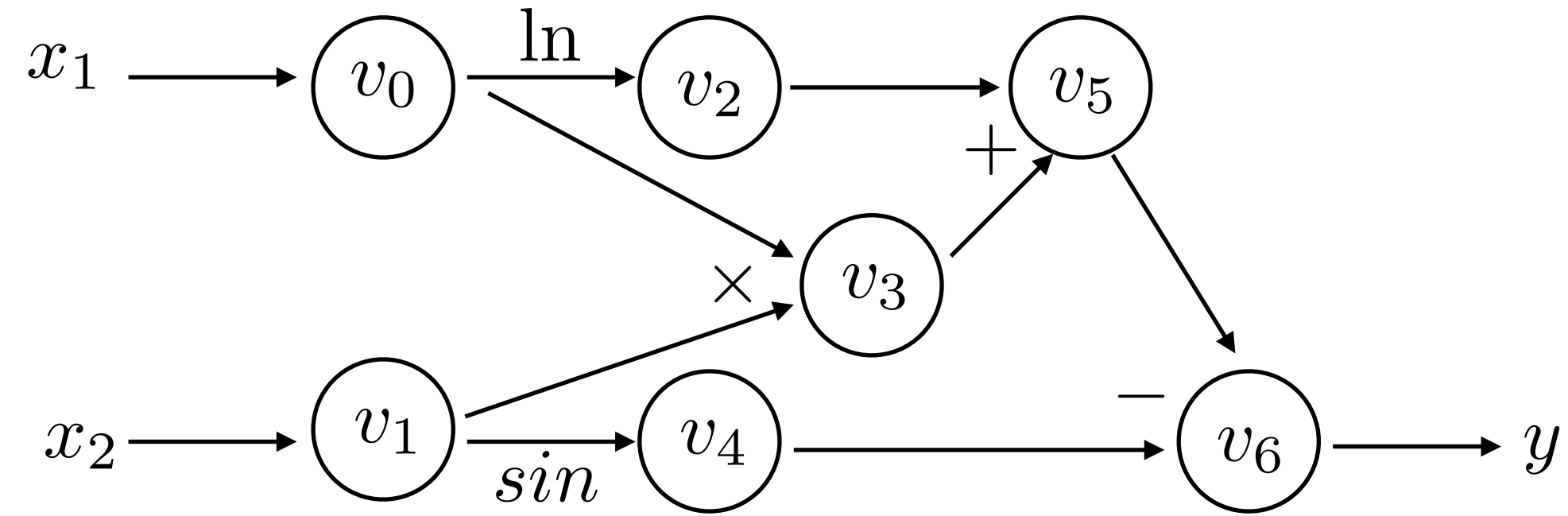
	$f(2, 5)$
$v_0 = x_1$	2
$v_1 = x_2$	5
$v_2 = \ln(v_0)$	$\ln(2) = 0.693$
$v_3 = v_0 \cdot v_1$	$2 \times 5 = 10$
$v_4 = \sin(v_1)$	$\sin(5) = 0.959$
$v_5 = v_2 + v_3$	$0.693 + 10 = 10.693$
$v_6 = v_5 - v_4$	$10.693 + 0.959 = 11.652$
$y = v_6$	11.652

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):

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

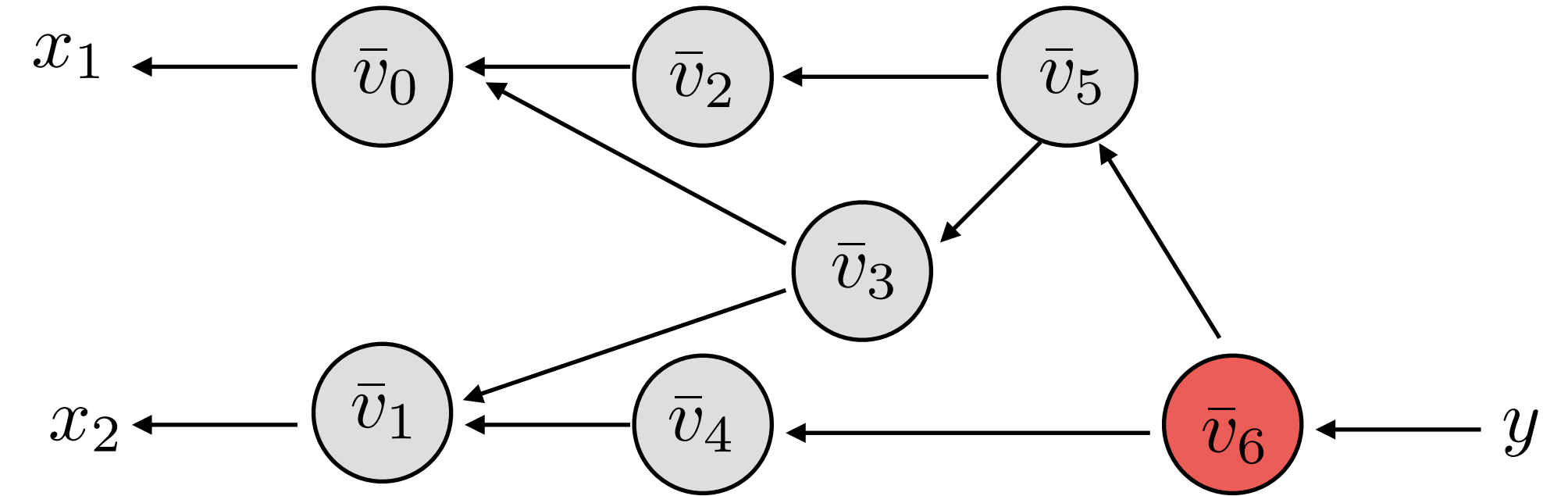
“local” derivative

AutoDiff - Reverse Mode



Forward Evaluation Trace:

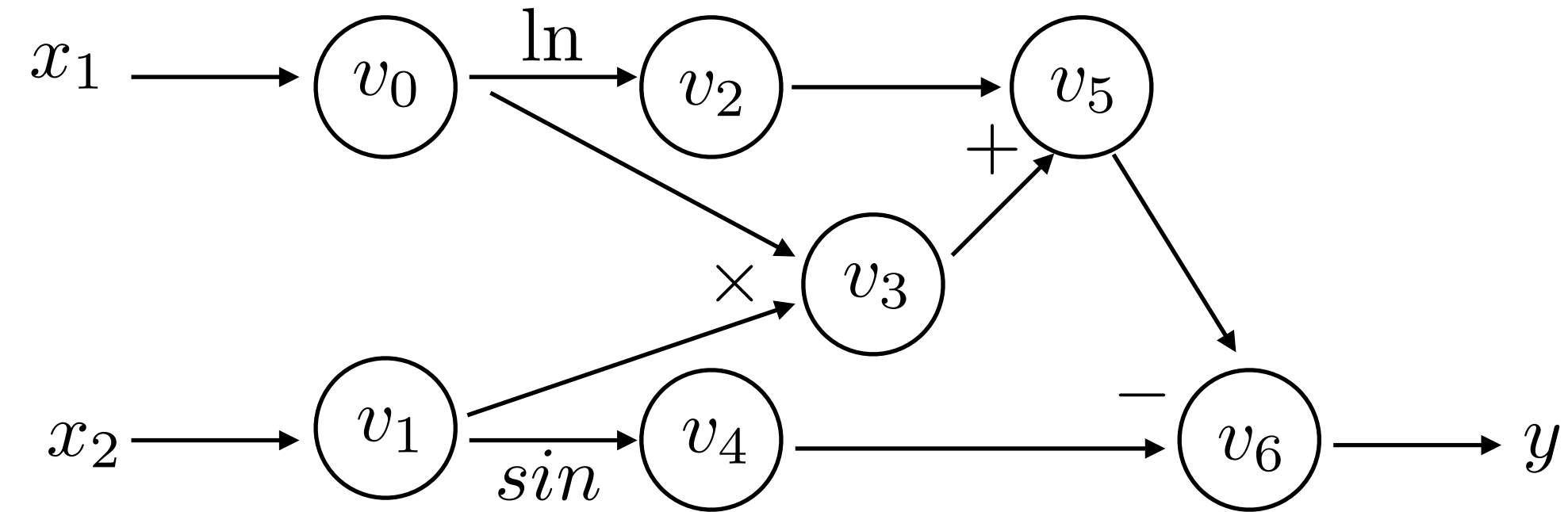
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Backwards Derivative Trace:

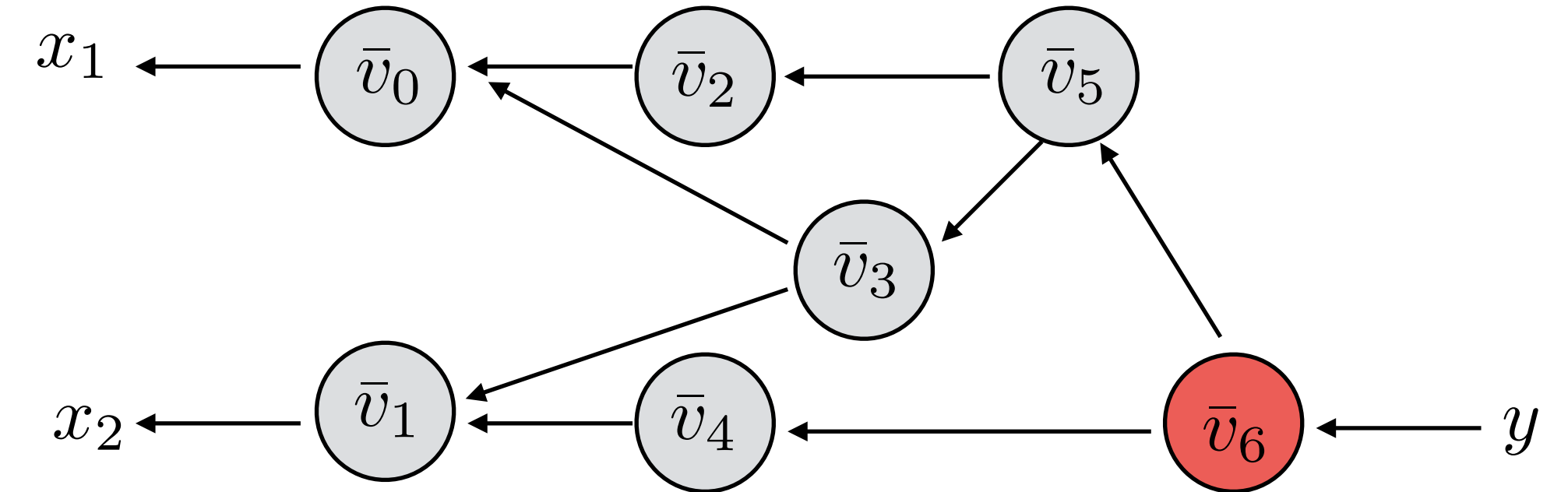
$$\bar{v}_6 = \frac{\partial y}{\partial v_6}$$

AutoDiff - Reverse Mode



Forward Evaluation Trace:

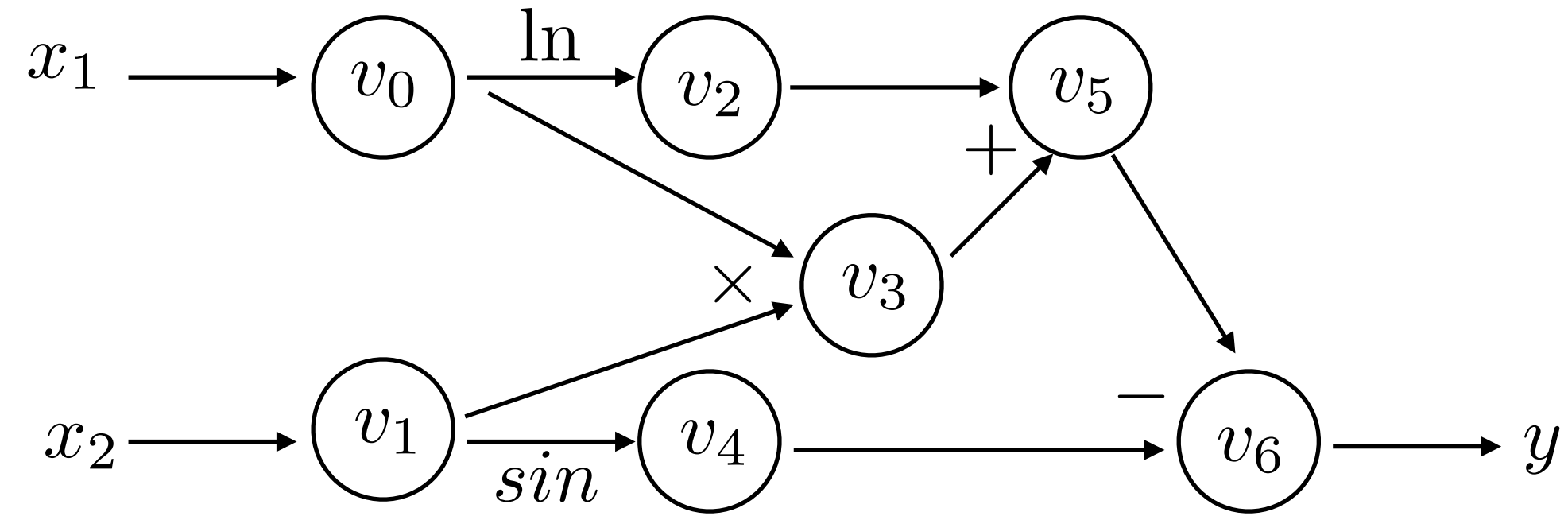
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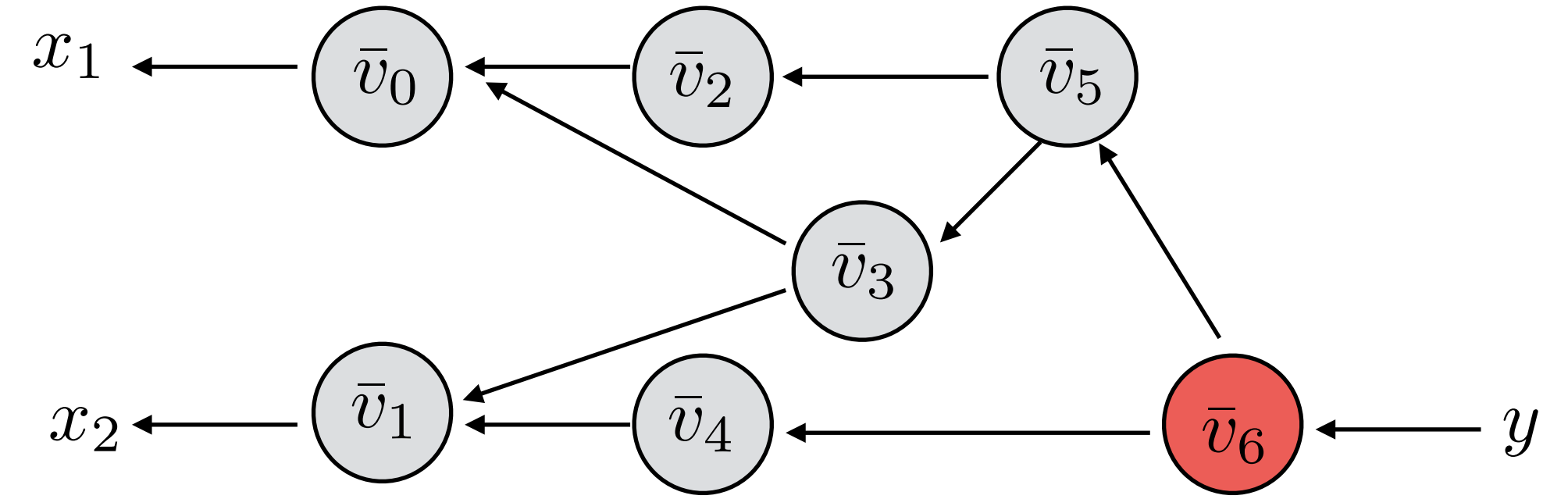
$$\bar{v}_6 = \frac{\partial y}{\partial v_6}$$

AutoDiff - Reverse Mode



Forward Evaluation Trace:

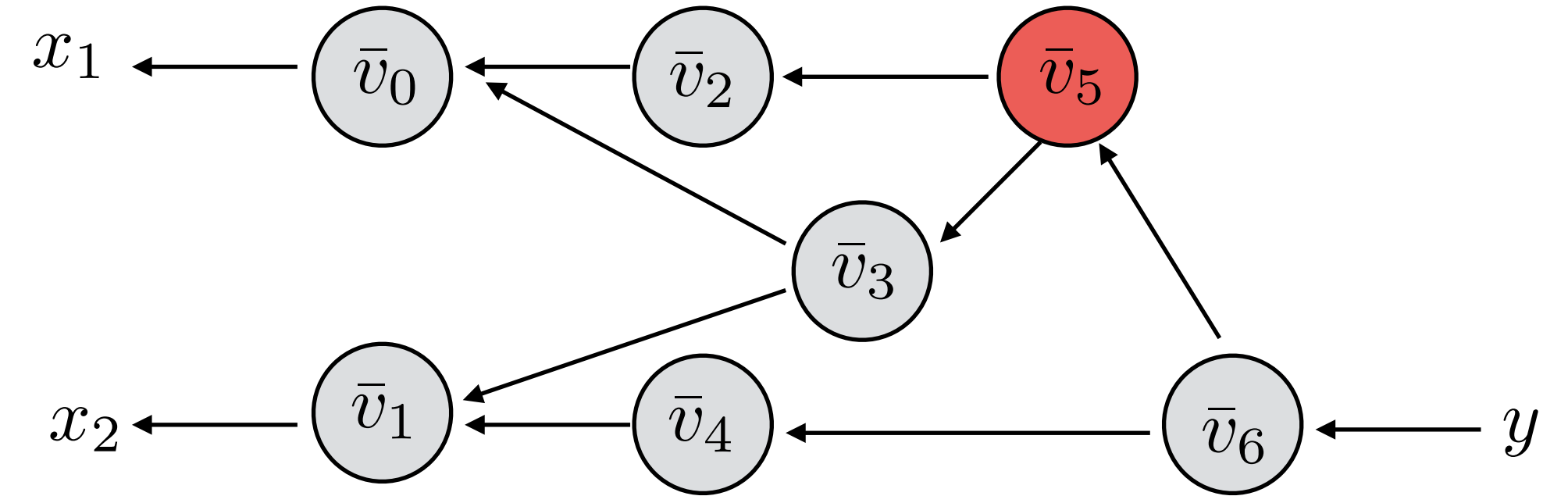
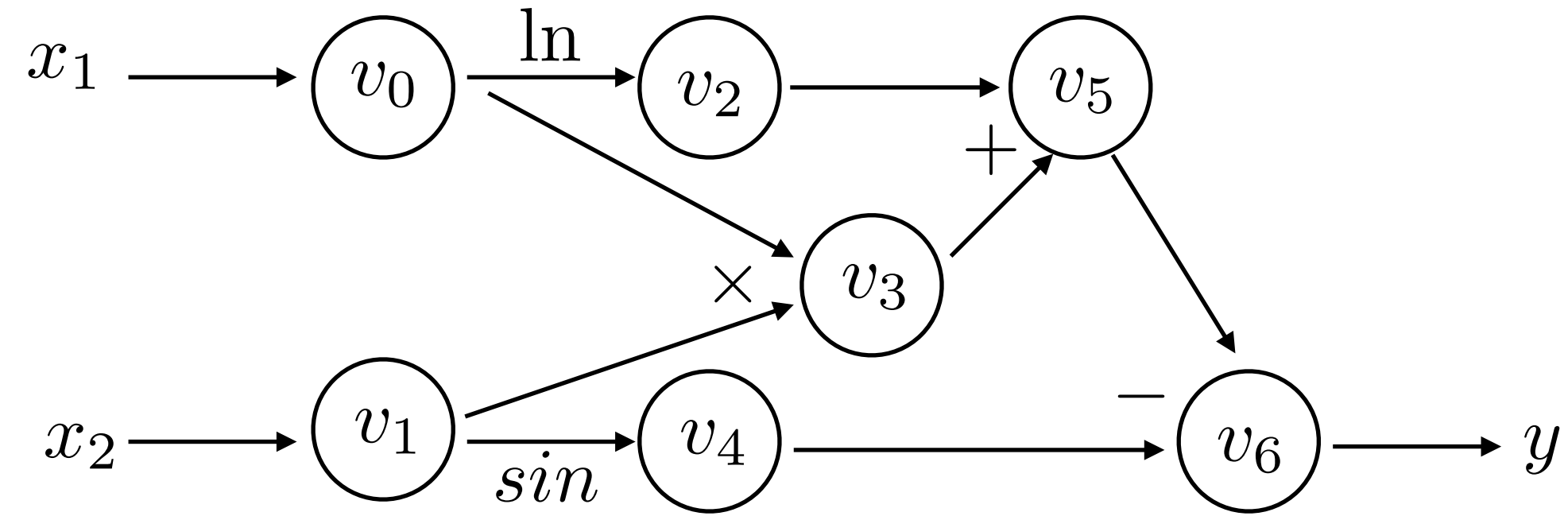
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Backwards Derivative Trace:

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

AutoDiff - Reverse Mode



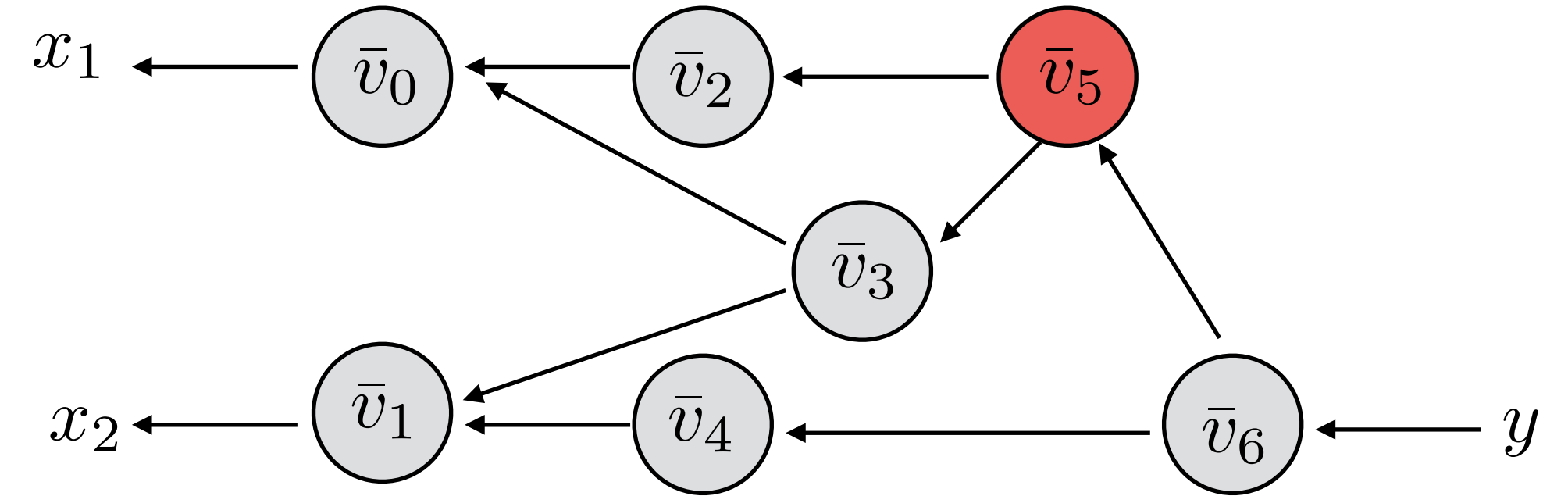
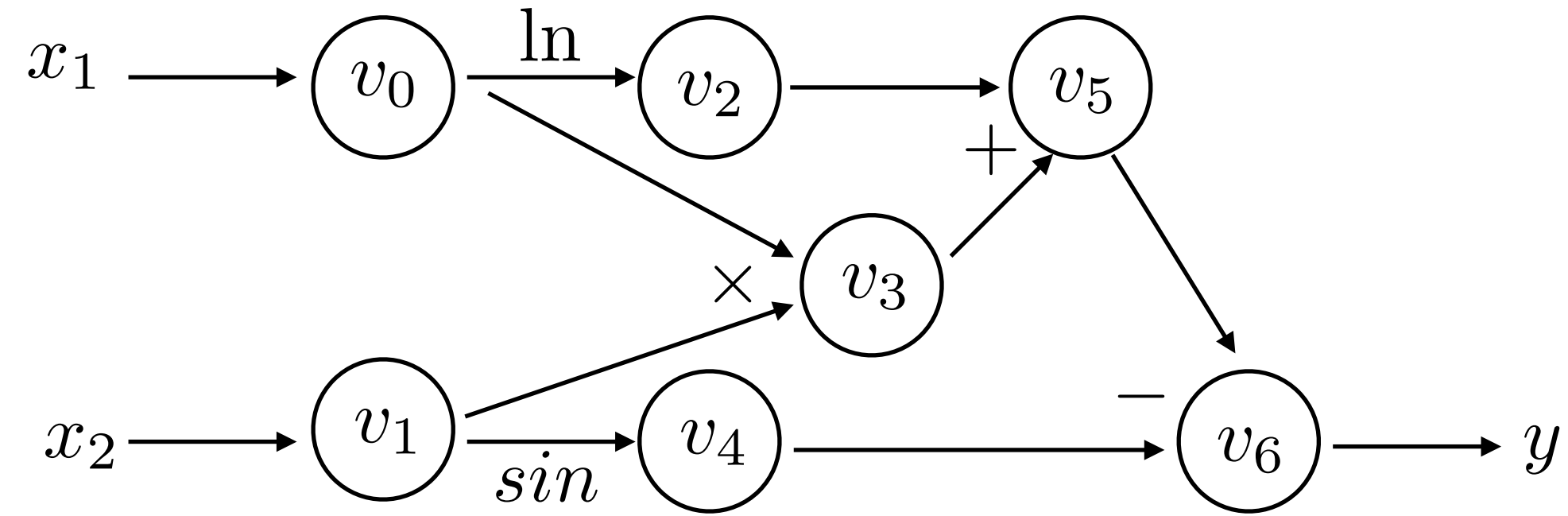
Backwards Derivative Trace:

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AutoDiff - Reverse Mode



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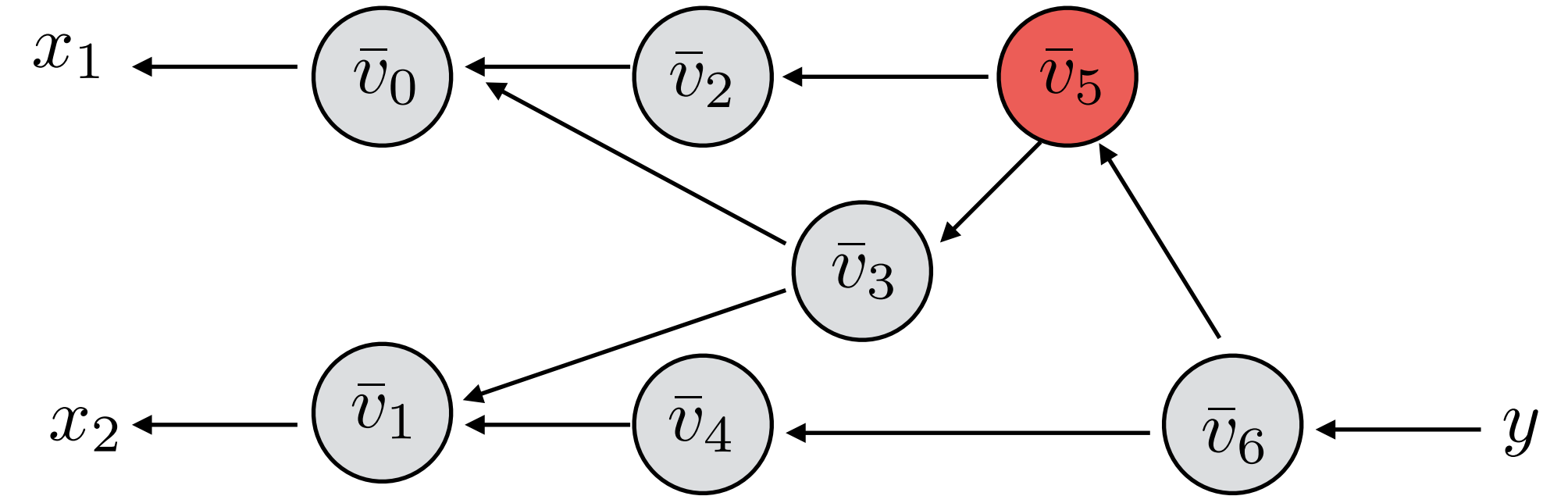
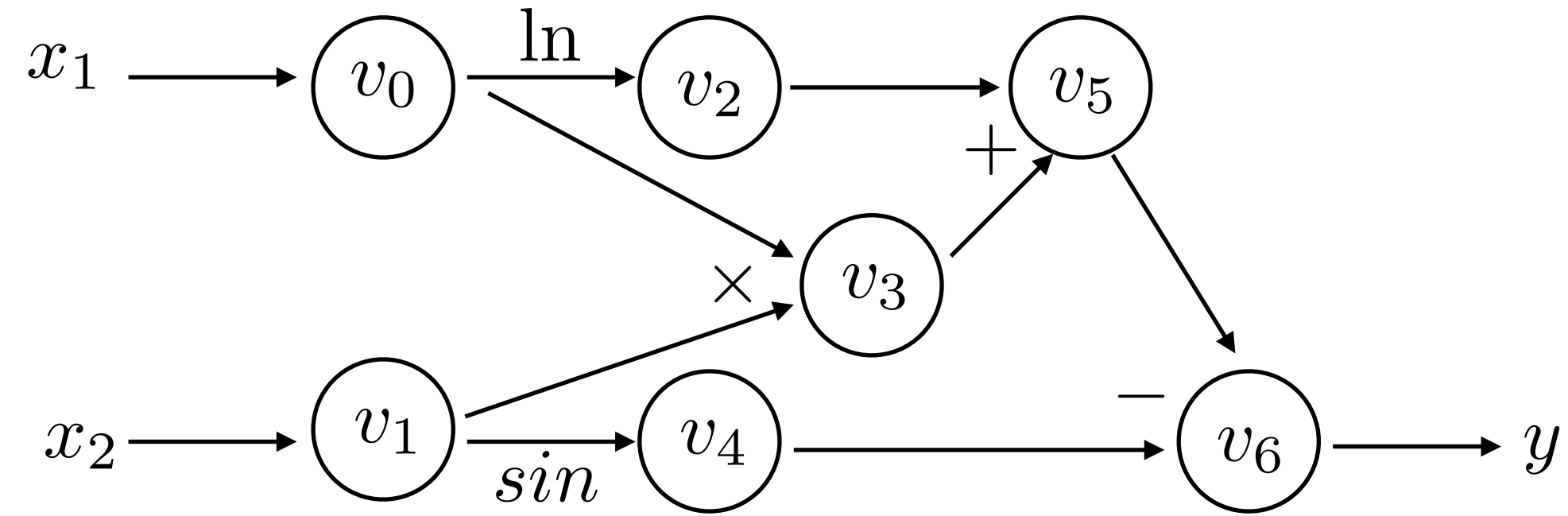
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$$\bar{v}_5 = \bar{v}_6 \frac{\partial v_6}{\partial v_5}$$

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

AutoDiff - Reverse Mode



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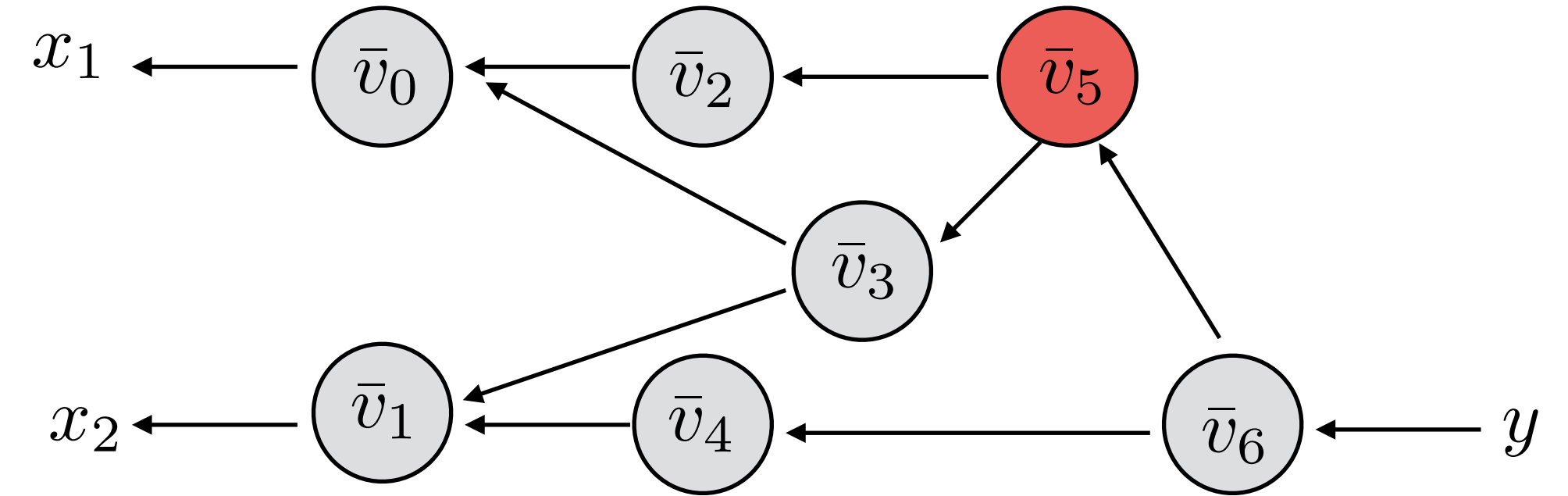
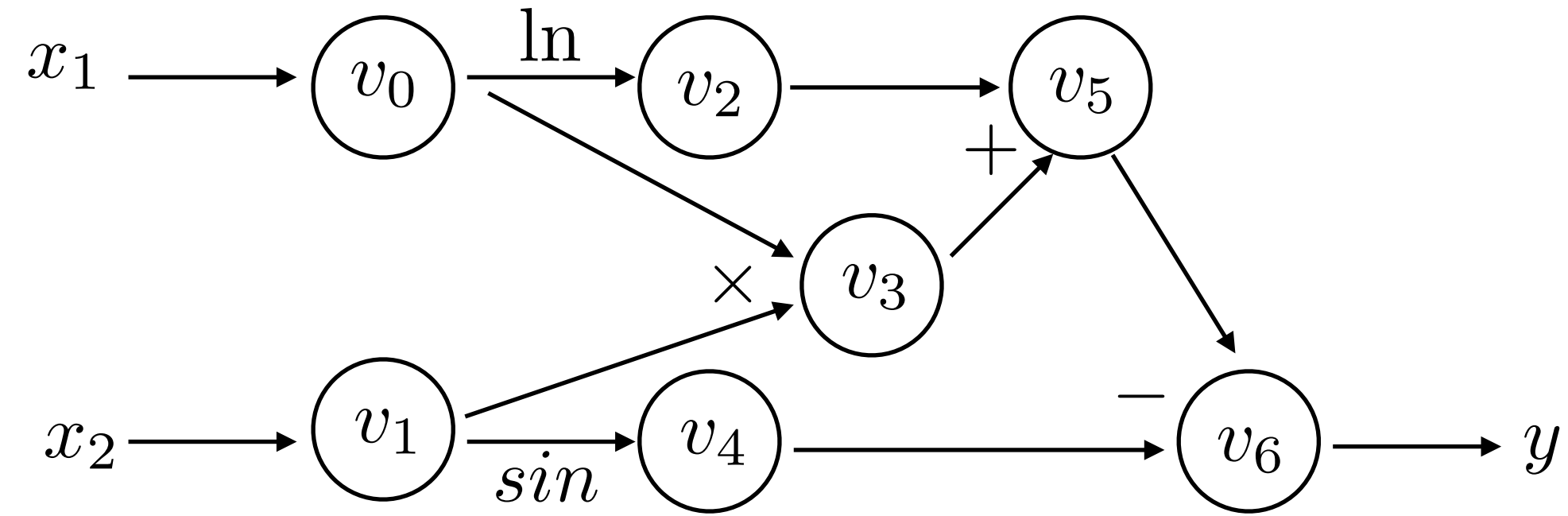
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$$\bar{v}_5 = \bar{v}_6 \frac{\partial v_6}{\partial v_5} = \bar{v}_6 \cdot 1$$

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AutoDiff - Reverse Mode



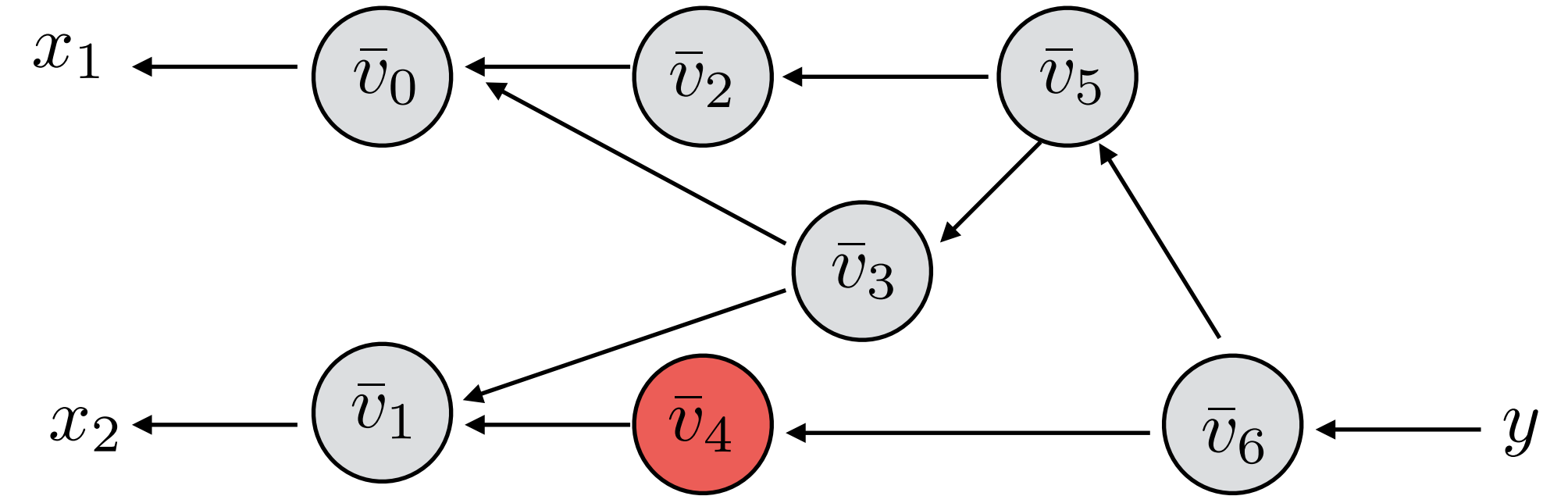
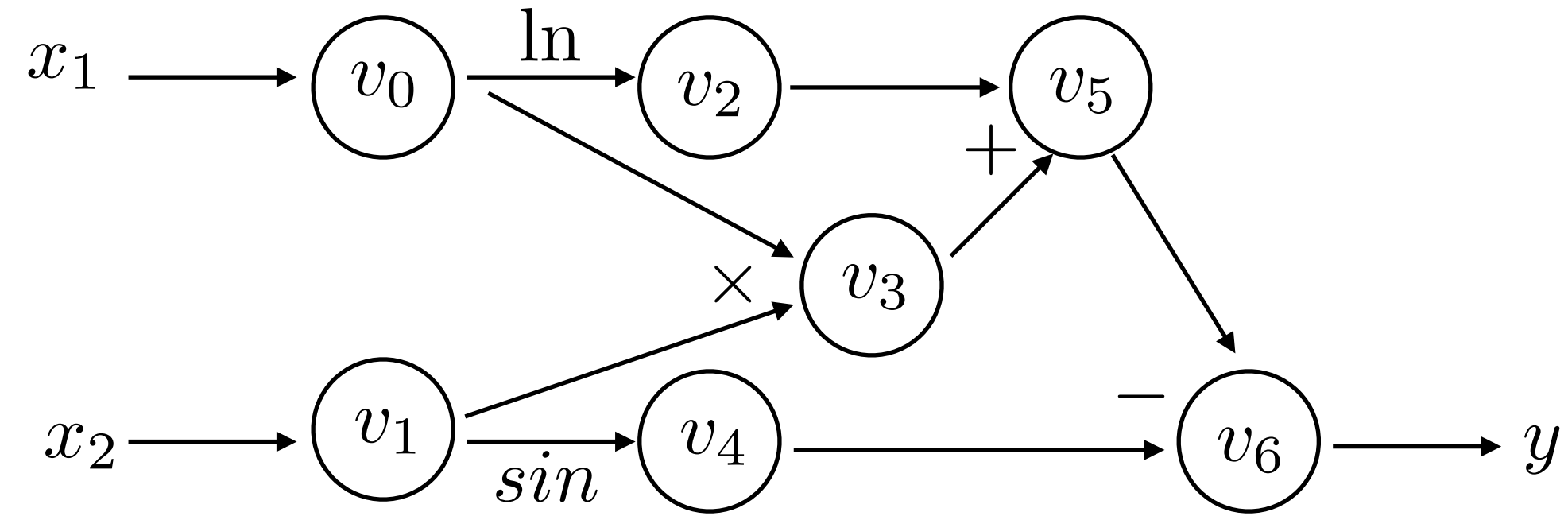
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AutoDiff - Reverse Mode



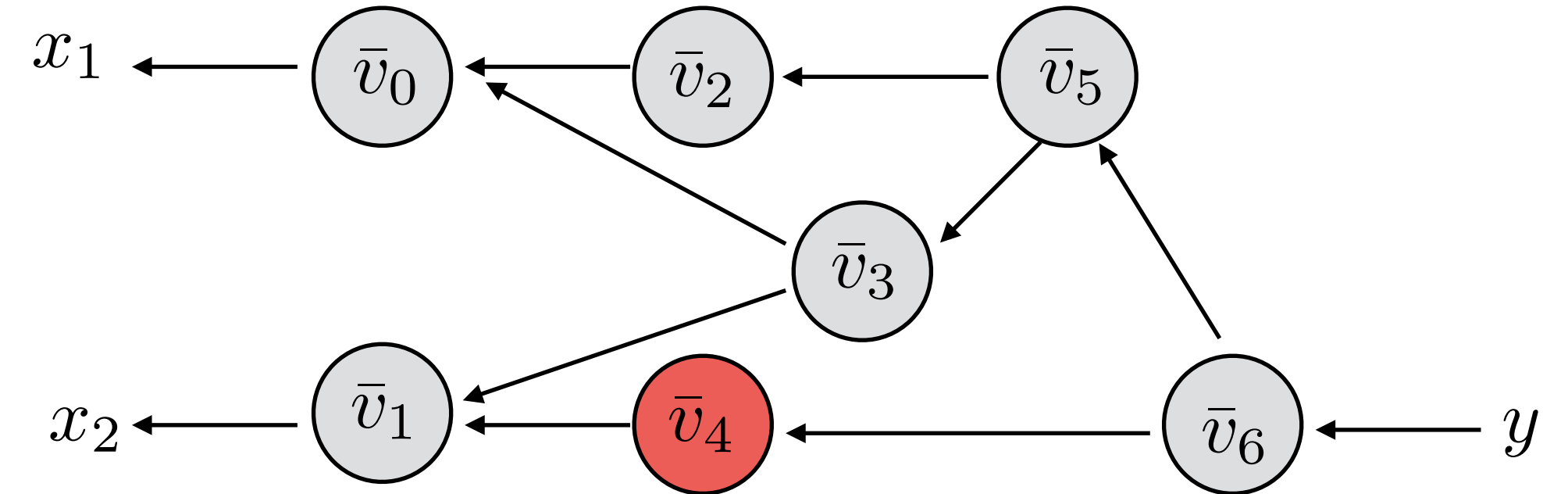
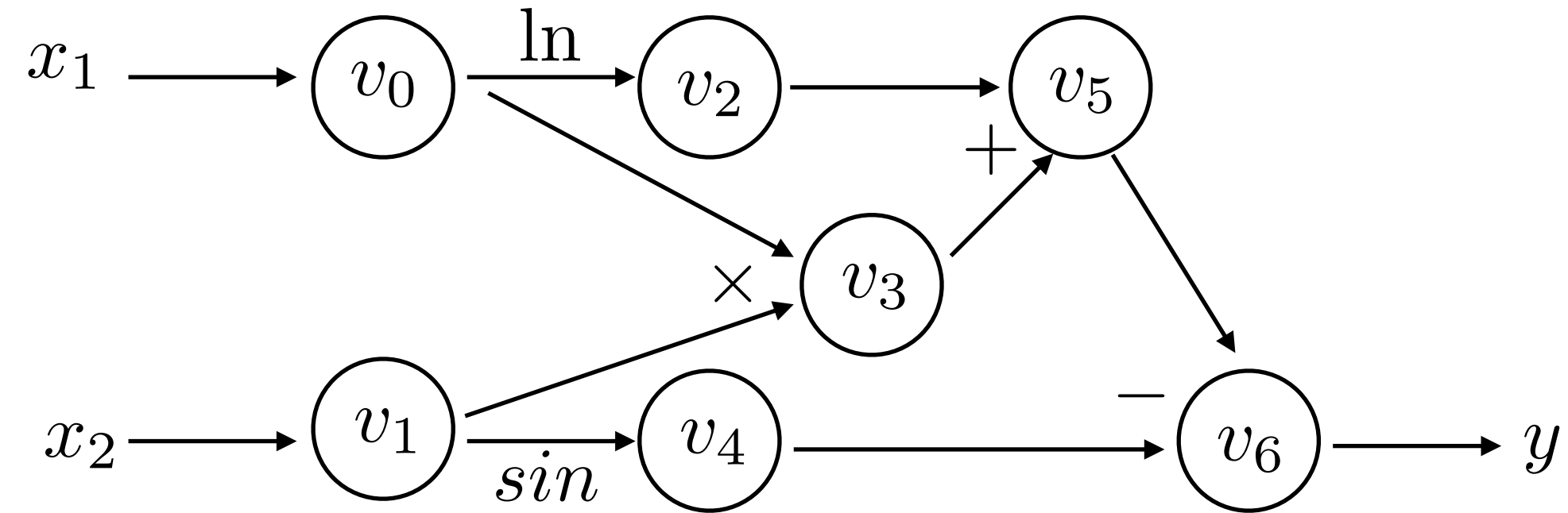
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AutoDiff - Reverse Mode



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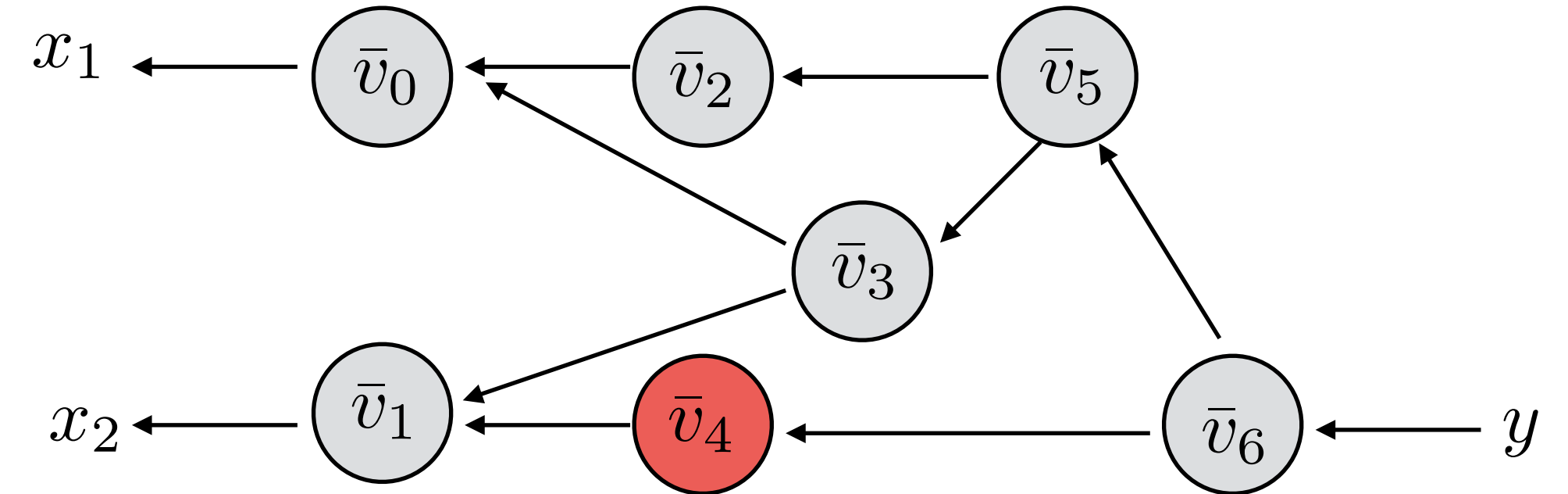
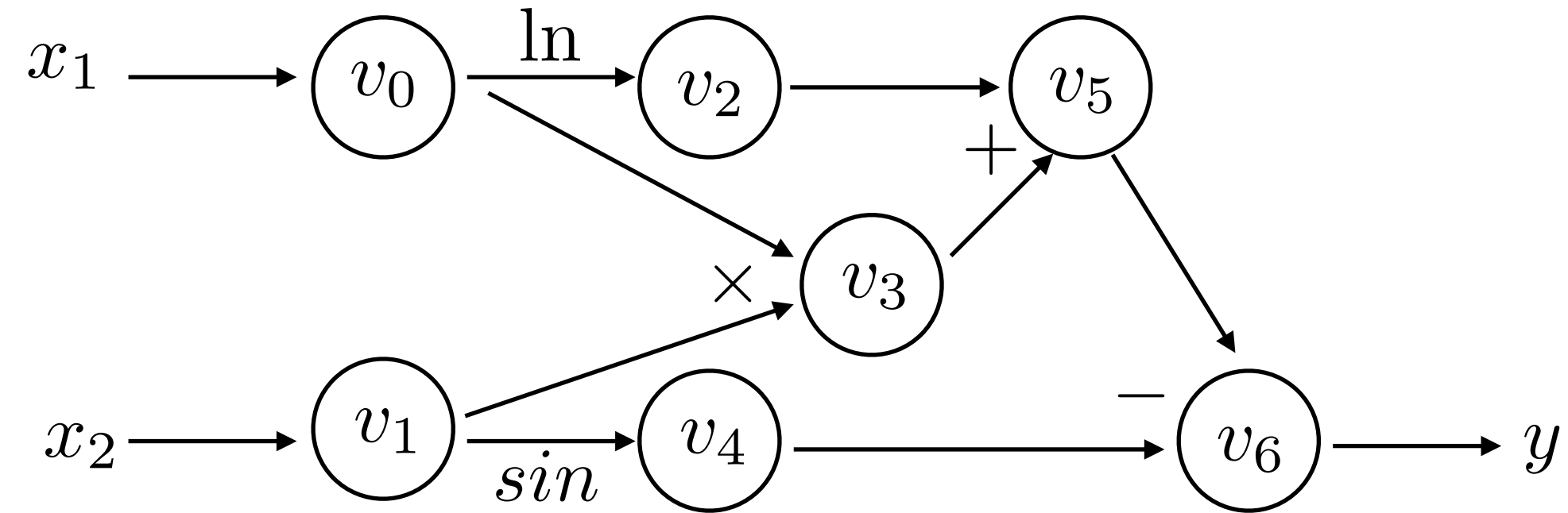
Backwards Derivative Trace:

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AutoDiff - Reverse Mode



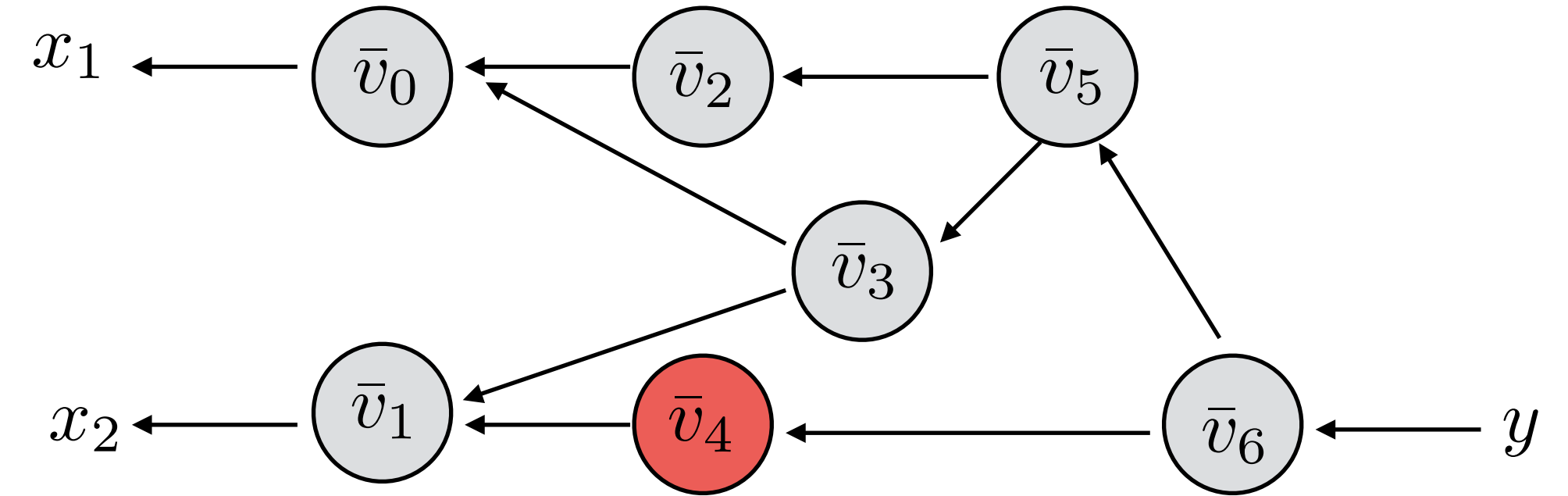
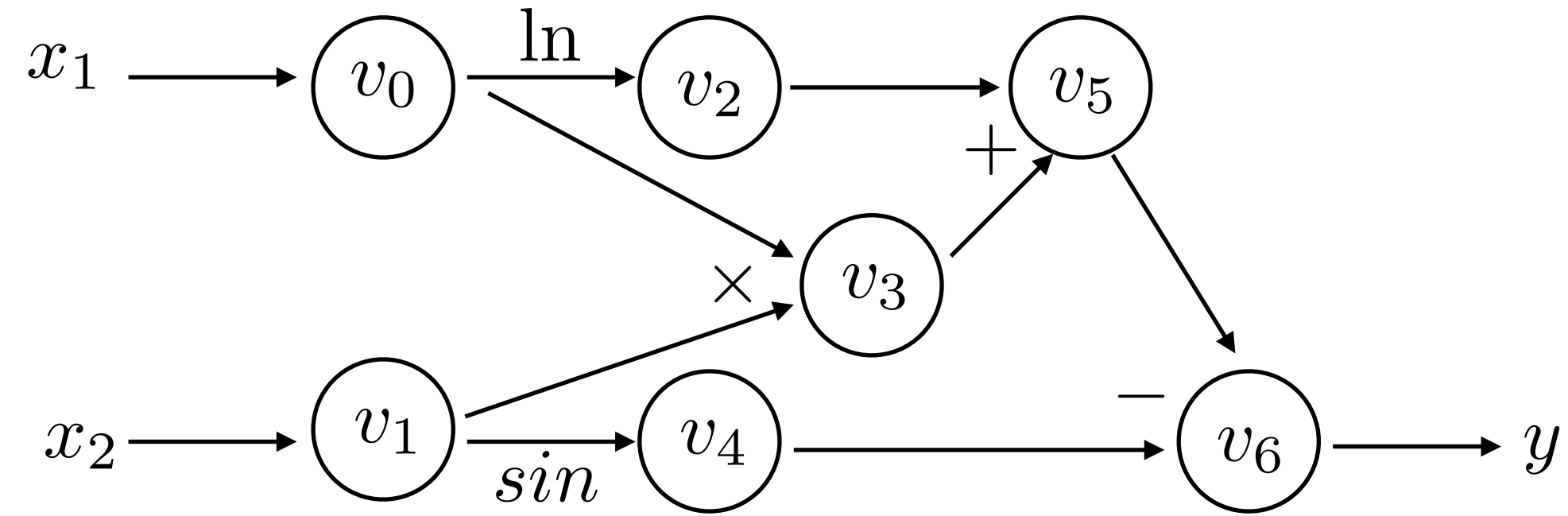
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$\bar{v}_5 = \bar{v}_6 \frac{\partial v_6}{\partial v_5} = \bar{v}_6 \cdot 1$	
$\bar{v}_6 = \frac{\partial y}{\partial v_6}$	$1 \times 1 = 1$
	1

AutoDiff - Reverse Mode



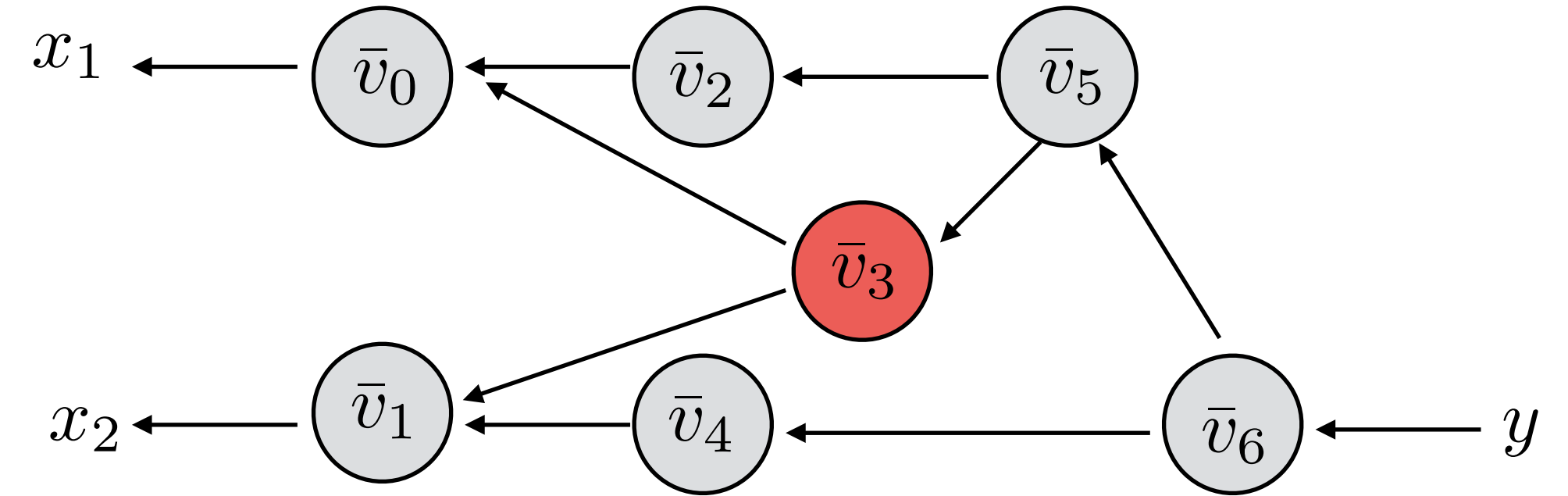
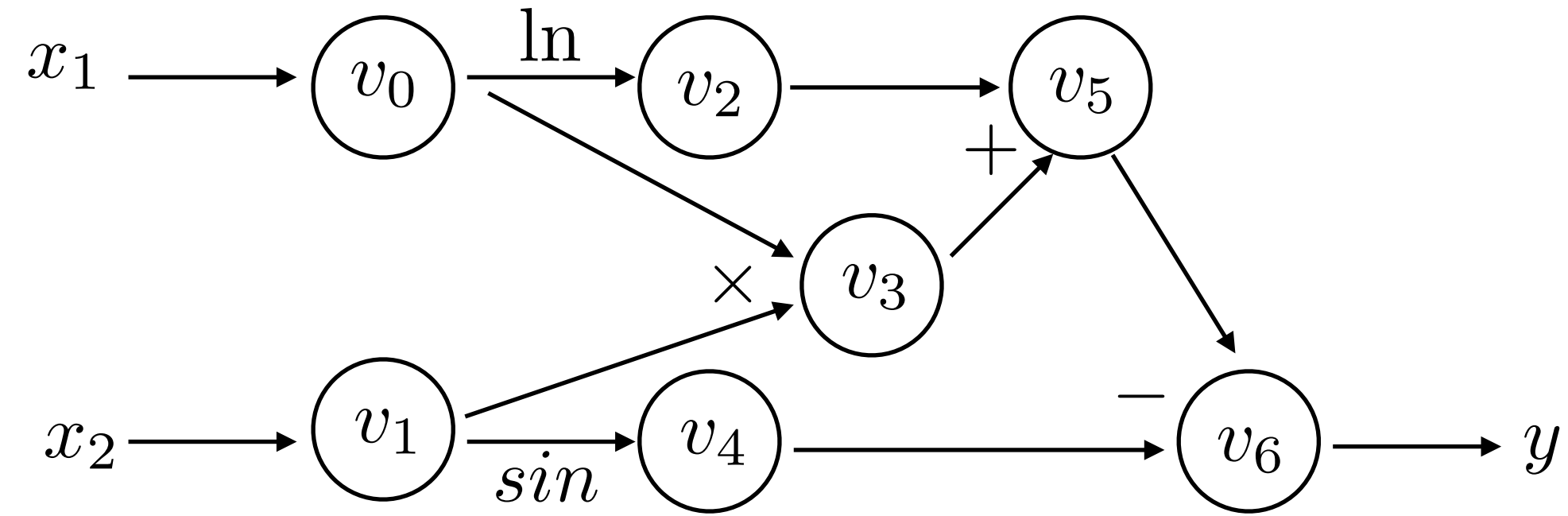
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AutoDiff - Reverse Mode



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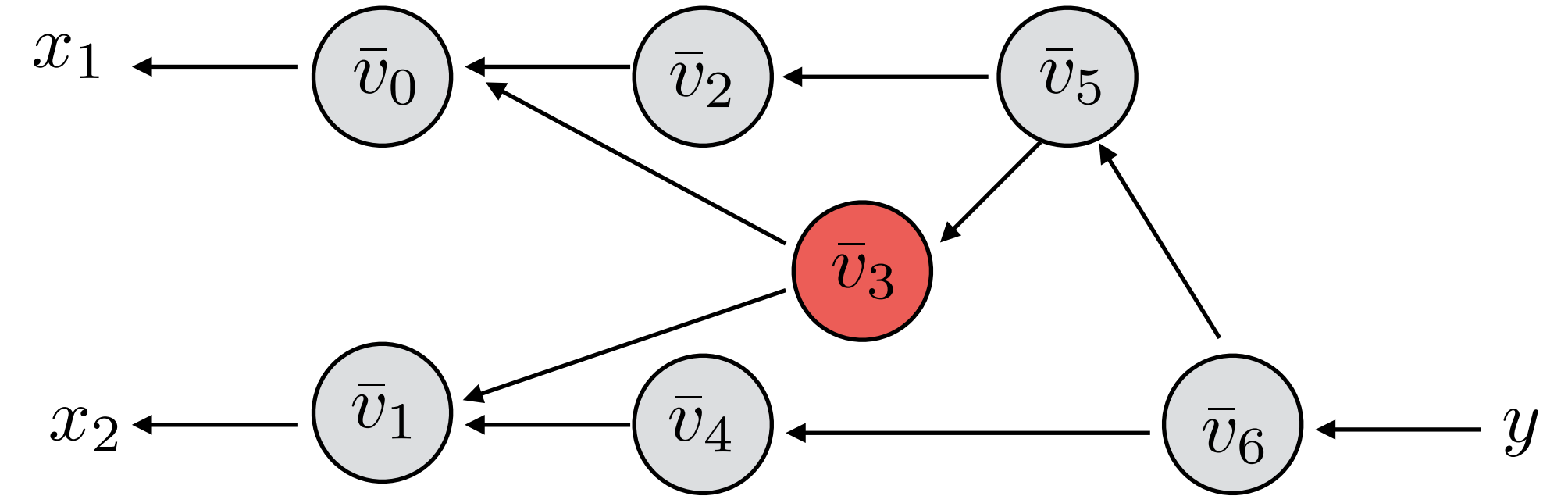
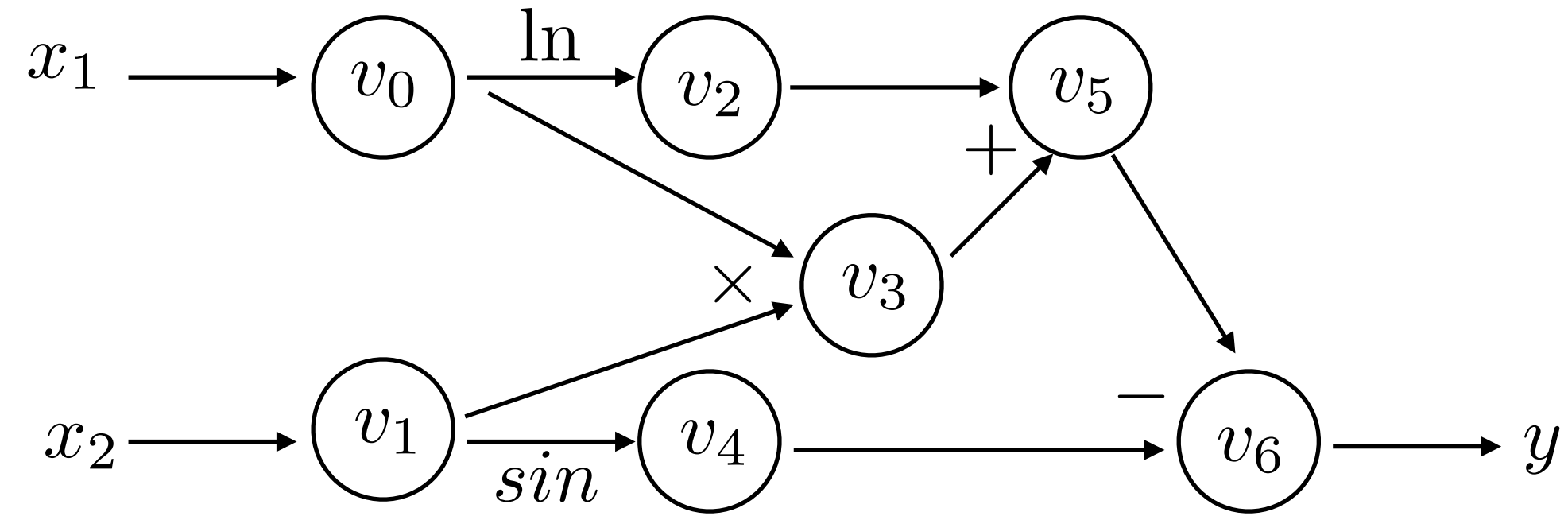
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AutoDiff - Reverse Mode



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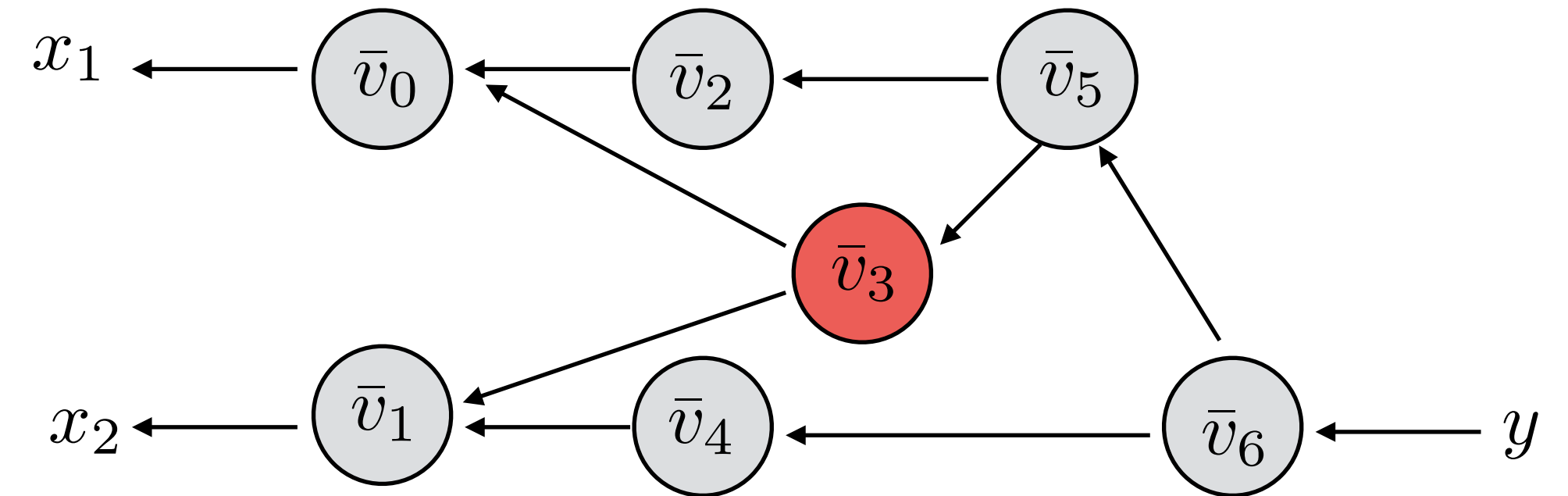
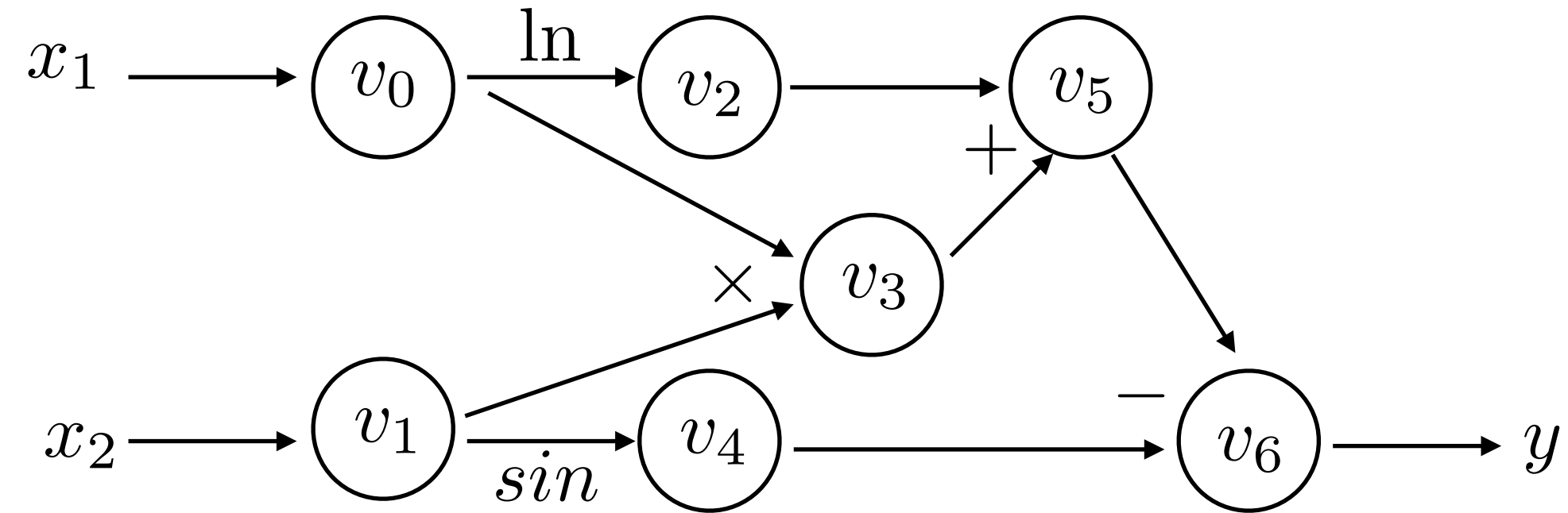
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AutoDiff - Reverse Mode



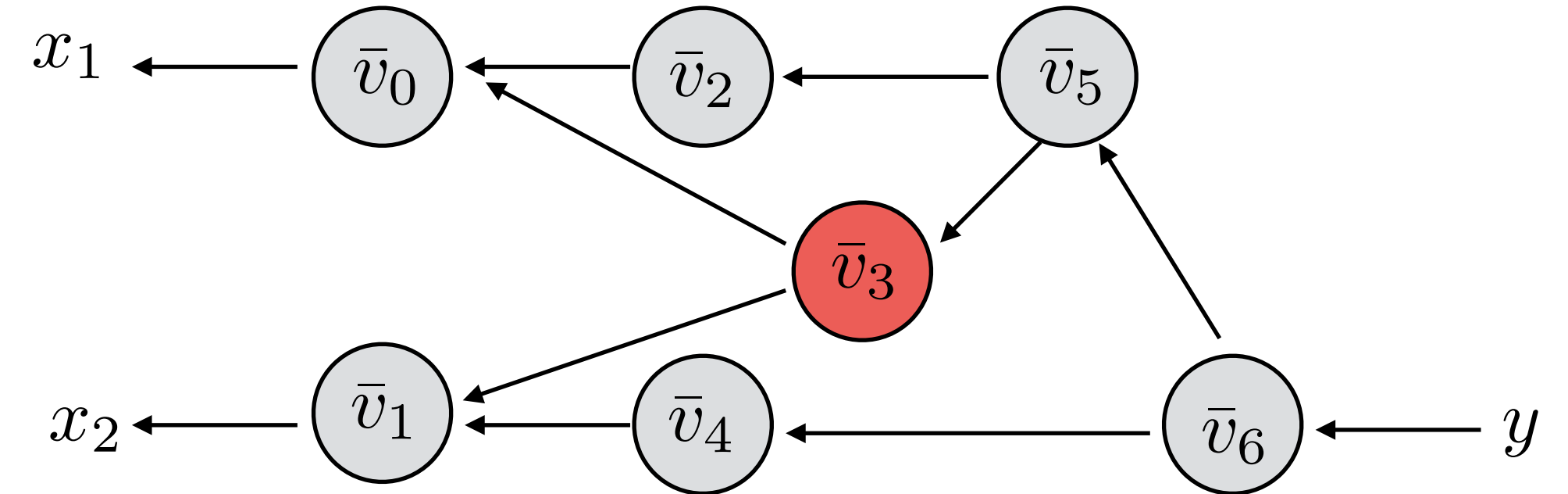
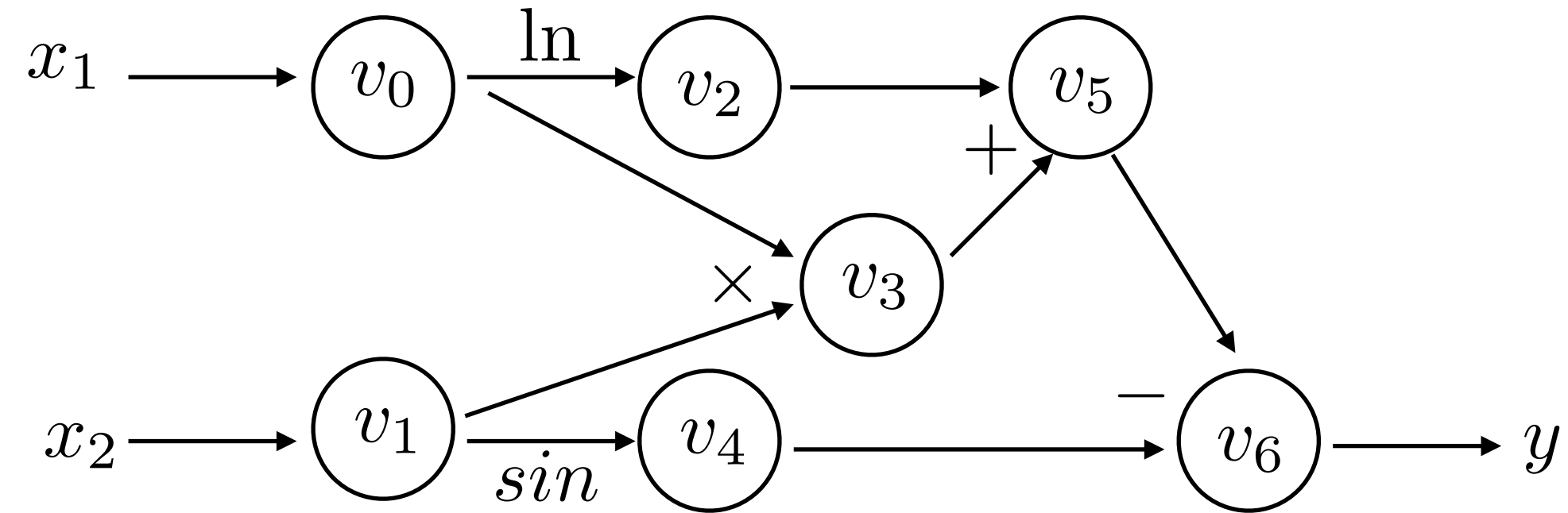
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AutoDiff - Reverse Mode



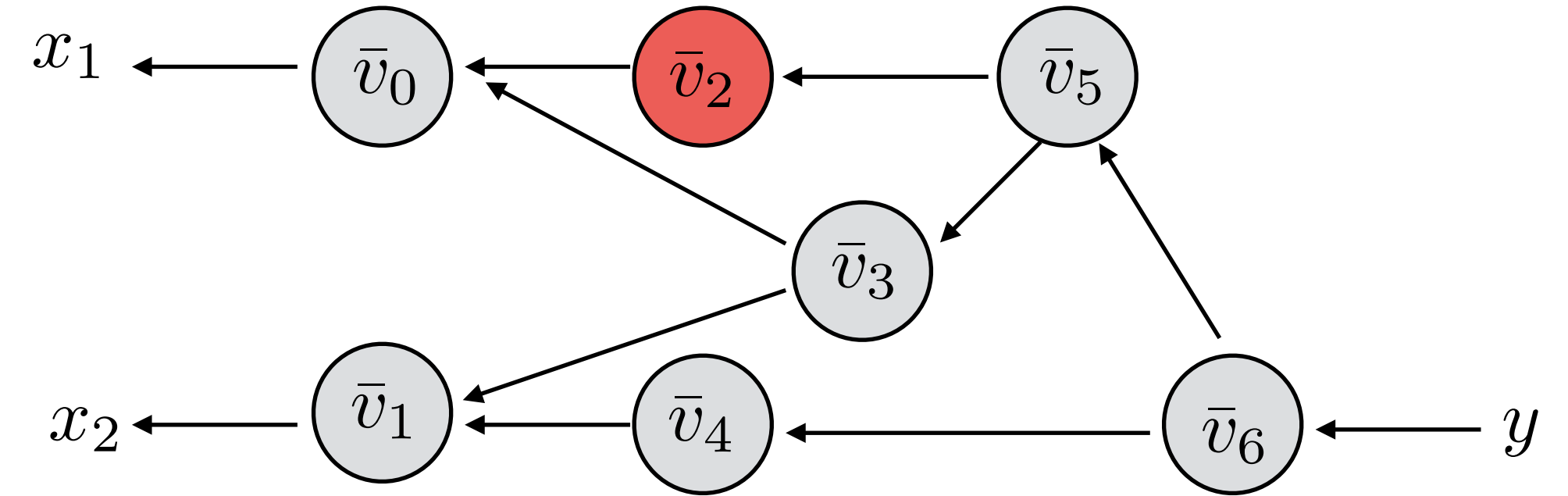
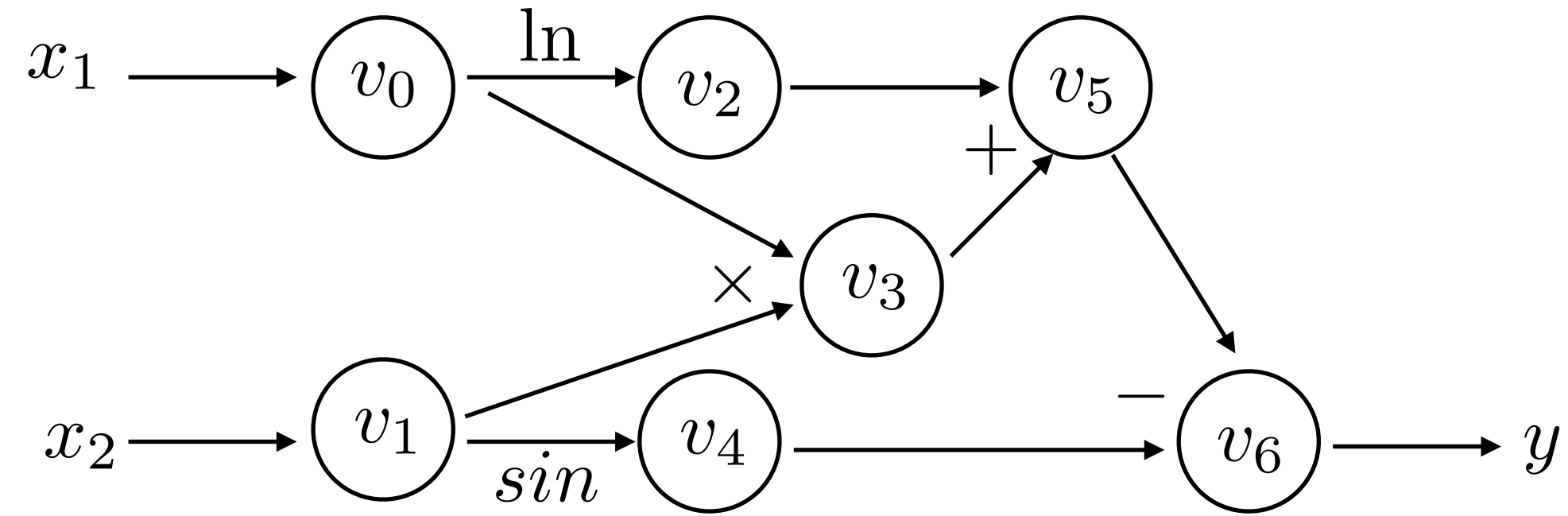
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AutoDiff - Reverse Mode



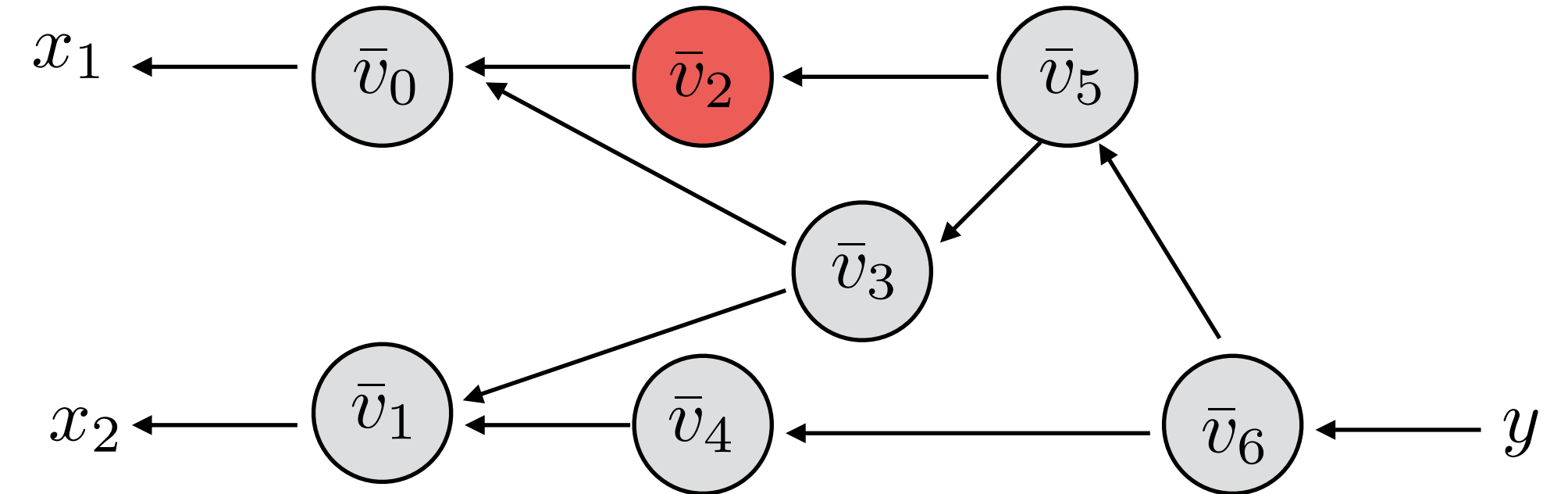
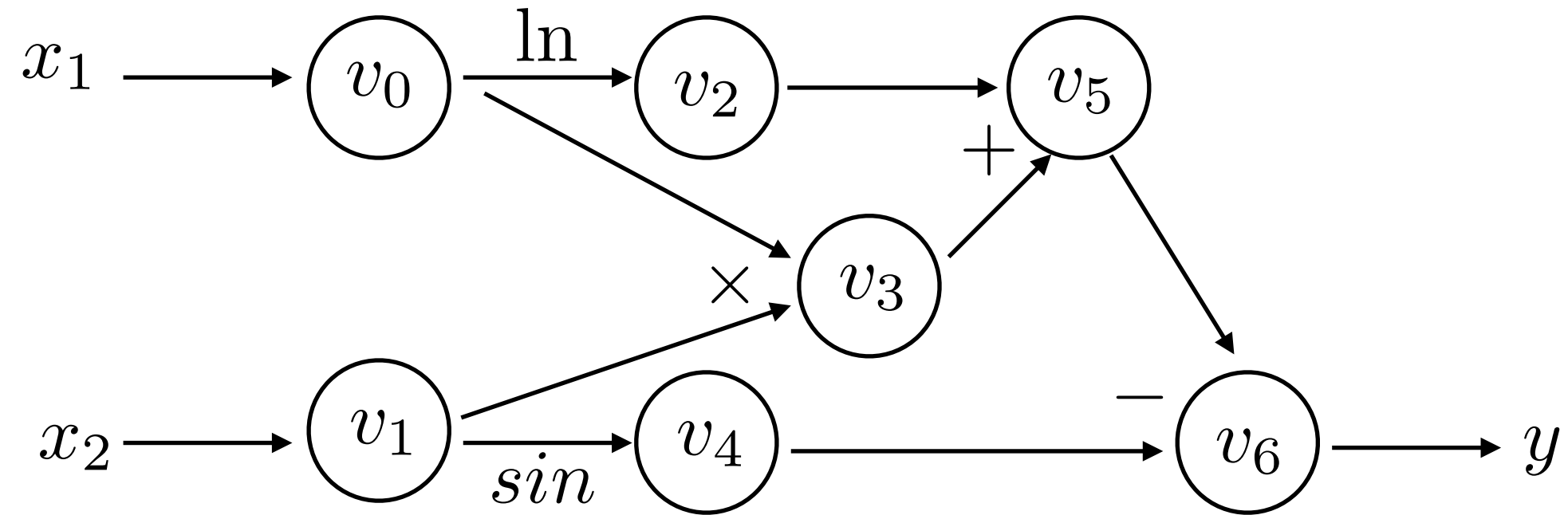
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$v_3 = v_0 \cdot v_1$	$2 \times 5 = 10$
$v_4 = \sin(v_1)$	$\sin(5) = 0.959$
$v_5 = v_2 + v_3$	$0.693 + 10 = 10.693$
$v_6 = v_5 - v_4$	$10.693 + 0.959 = 11.652$
$y = v_6$	11.652

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

AutoDiff - Reverse Mode



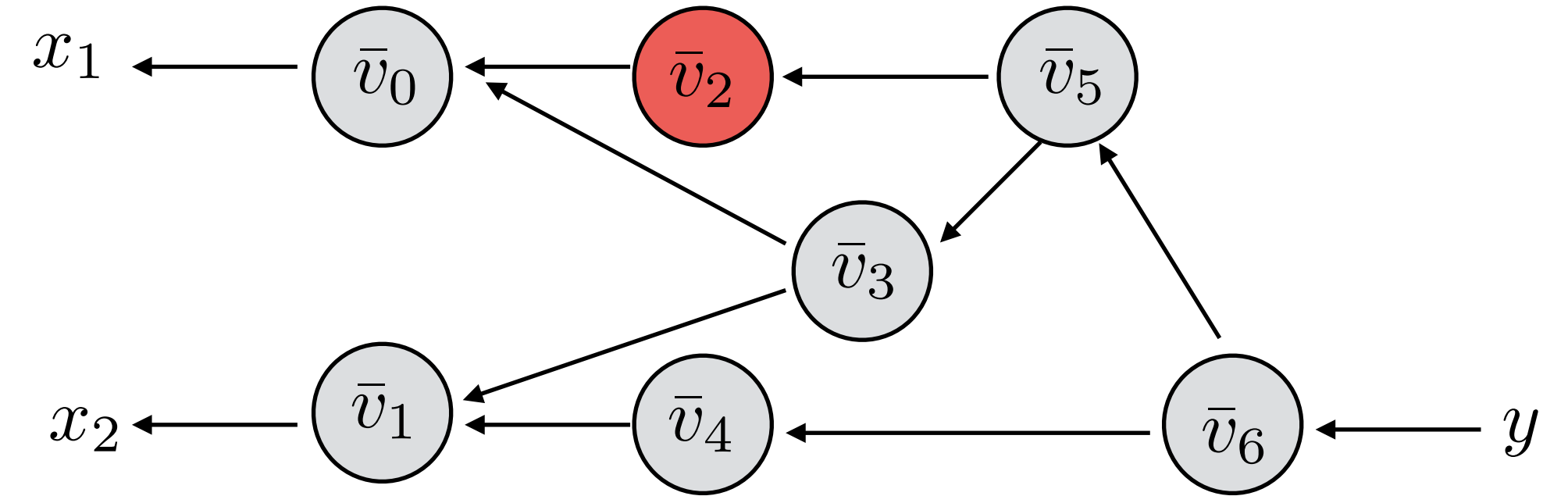
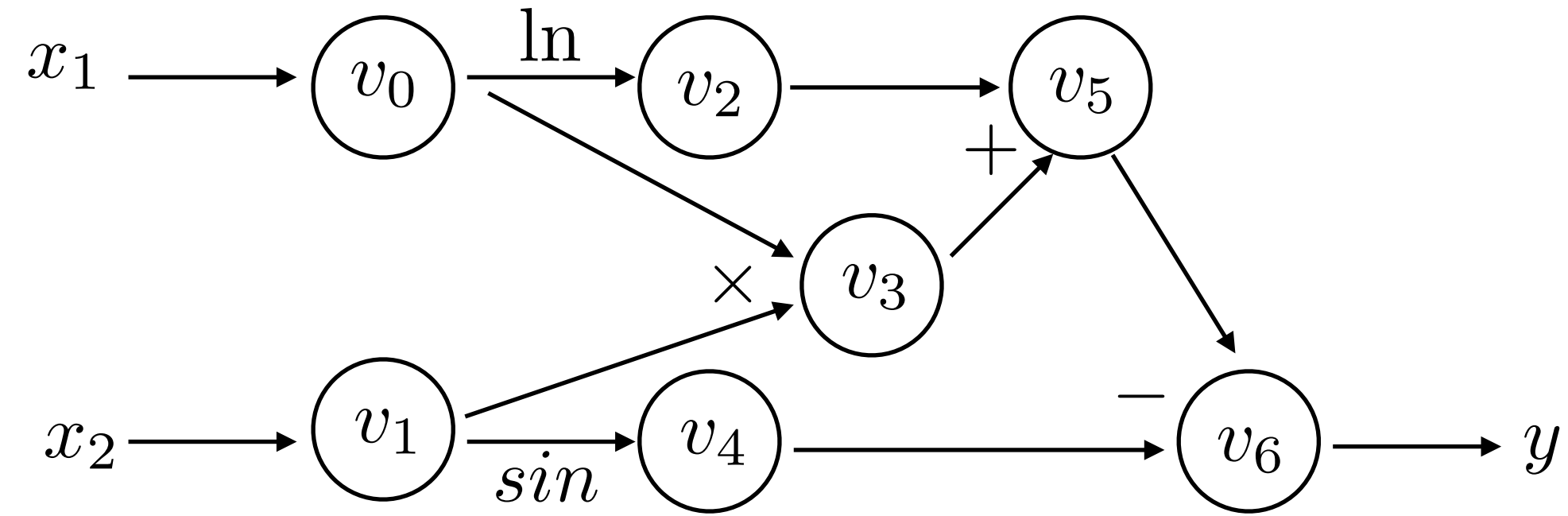
Backwards Derivative Trace:

Forward Evaluation Trace:

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

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

AutoDiff - Reverse Mode



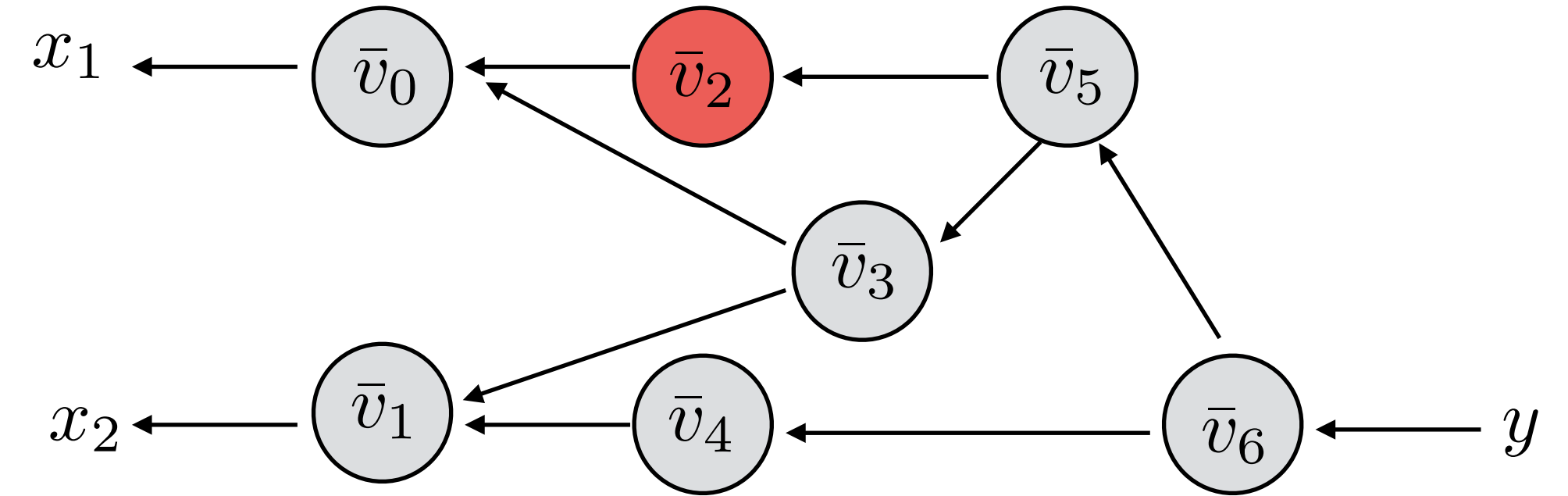
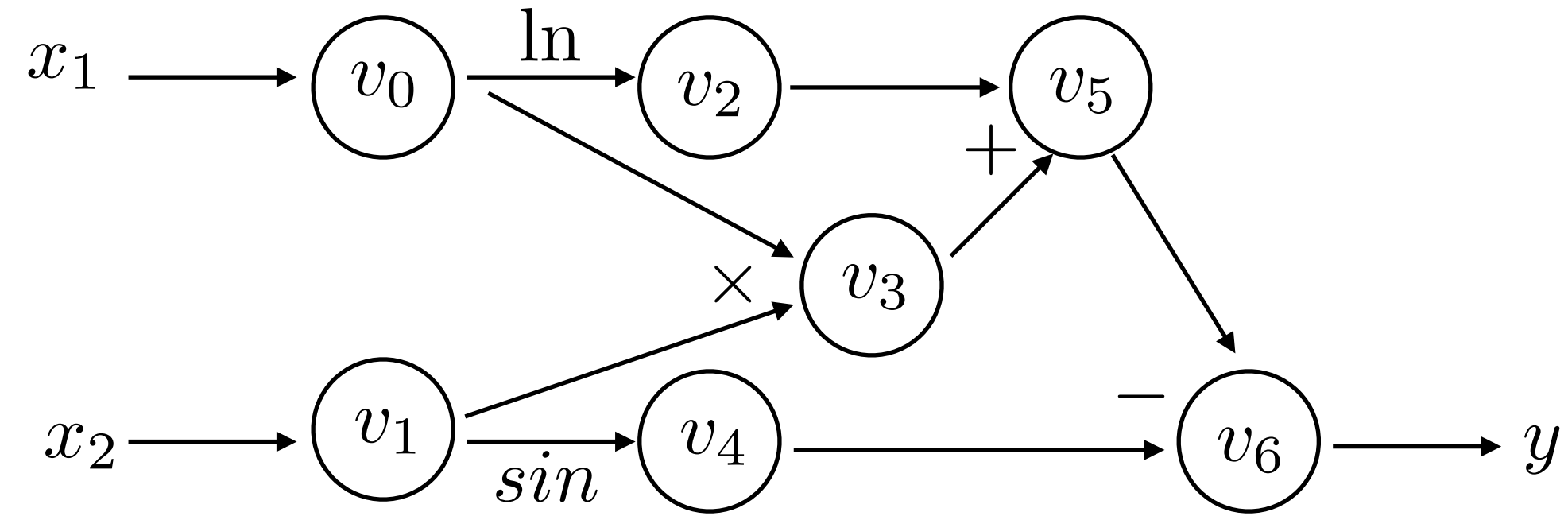
Backwards Derivative Trace:

Forward Evaluation Trace:

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

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

AutoDiff - Reverse Mode



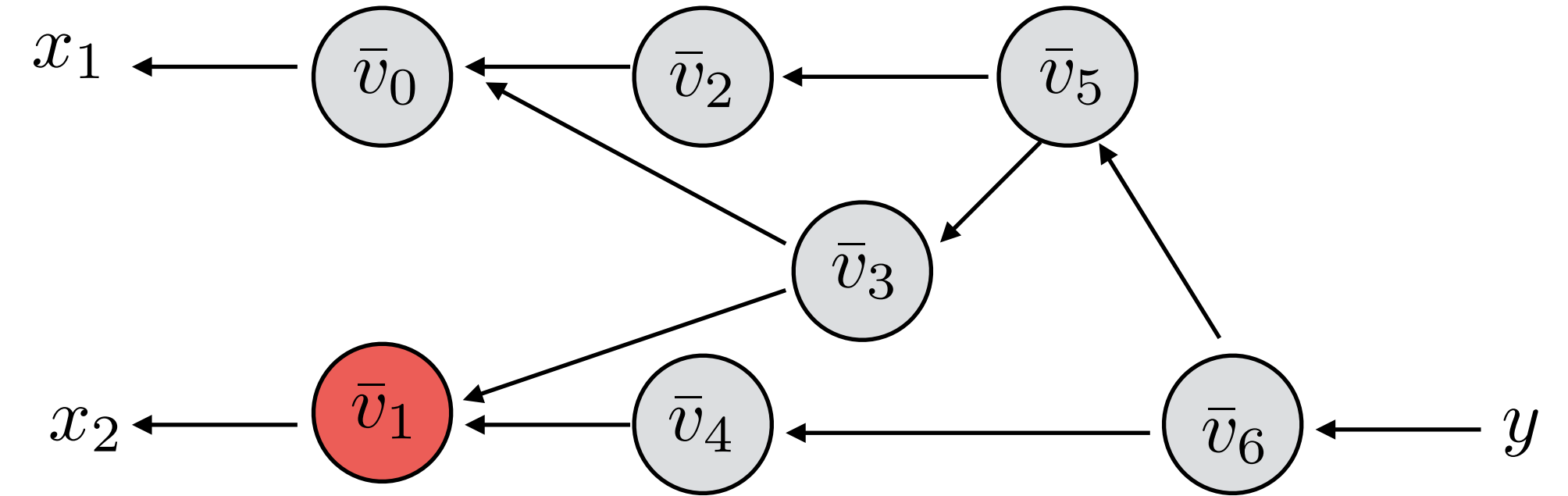
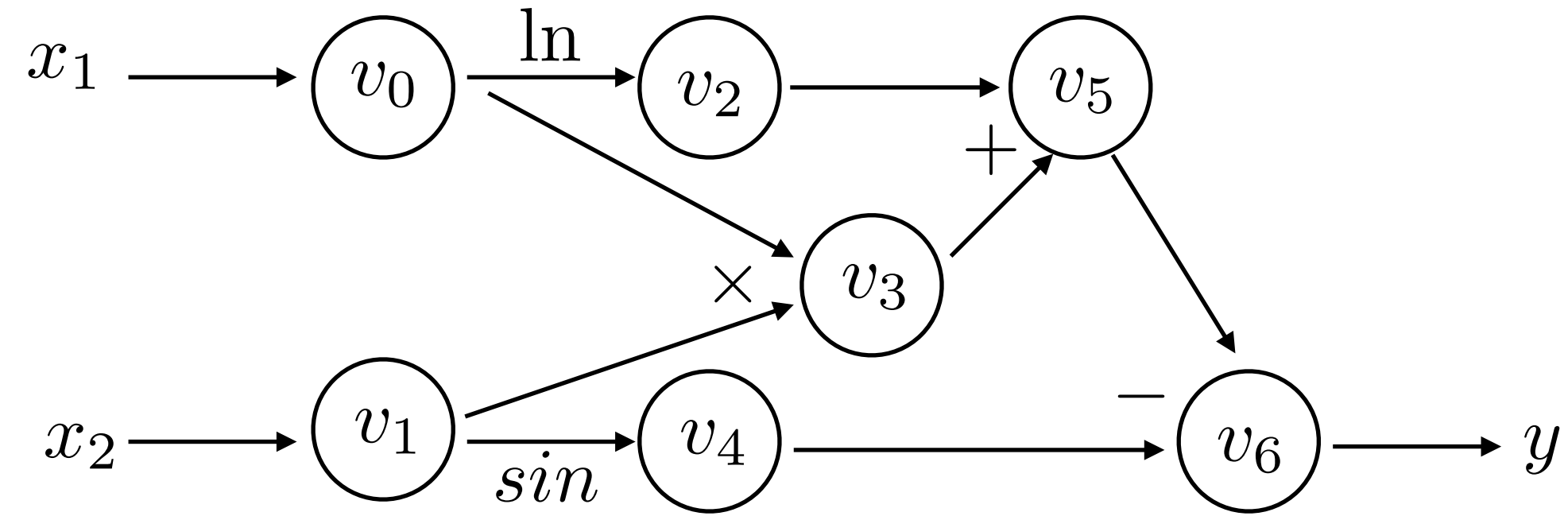
Backwards Derivative Trace:

Forward Evaluation Trace:

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

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

AutoDiff - Reverse Mode



Backwards Derivative Trace:

Forward Evaluation Trace:

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

\bar{v}_1 :

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

$$1 \times 1 = 1$$

$$\bar{v}_3 = \bar{v}_5 \frac{\partial v_5}{\partial v_3} = \bar{v}_5 \cdot (1)$$

$$1 \times 1 = 1$$

$$\bar{v}_4 = \bar{v}_6 \frac{\partial v_6}{\partial v_4} = \bar{v}_6 \cdot (-1)$$

$$1 \times -1 = -1$$

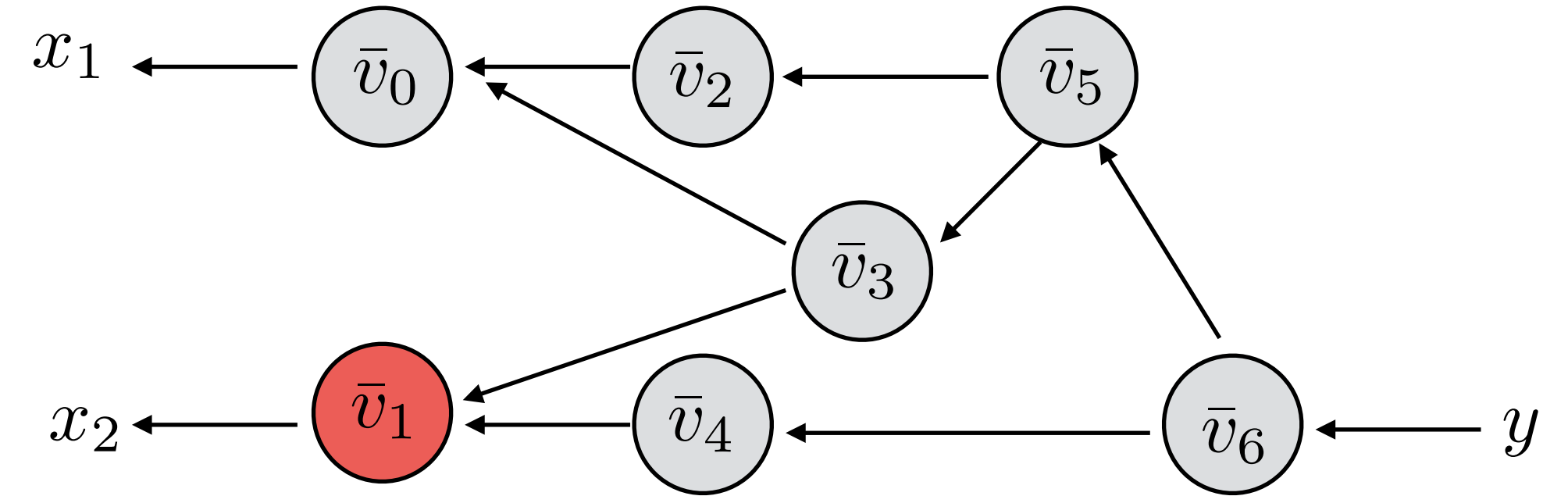
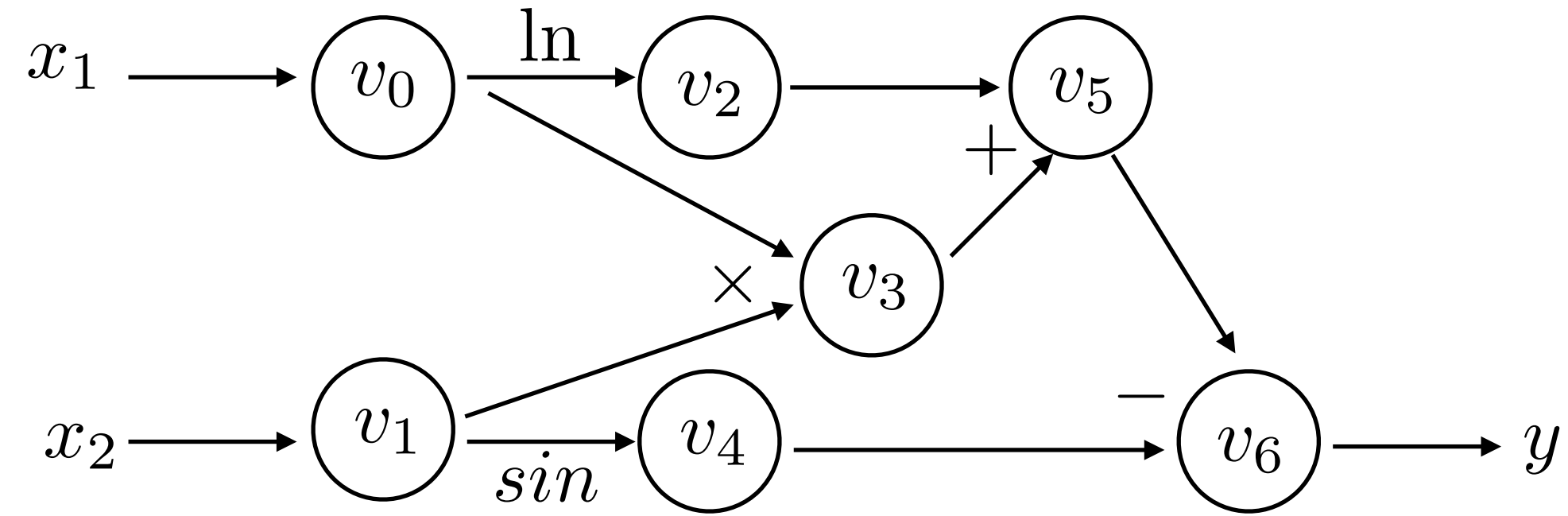
$$\bar{v}_5 = \bar{v}_6 \frac{\partial v_6}{\partial v_5} = \bar{v}_6 \cdot 1$$

$$1 \times 1 = 1$$

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

$$1$$

AutoDiff - Reverse Mode



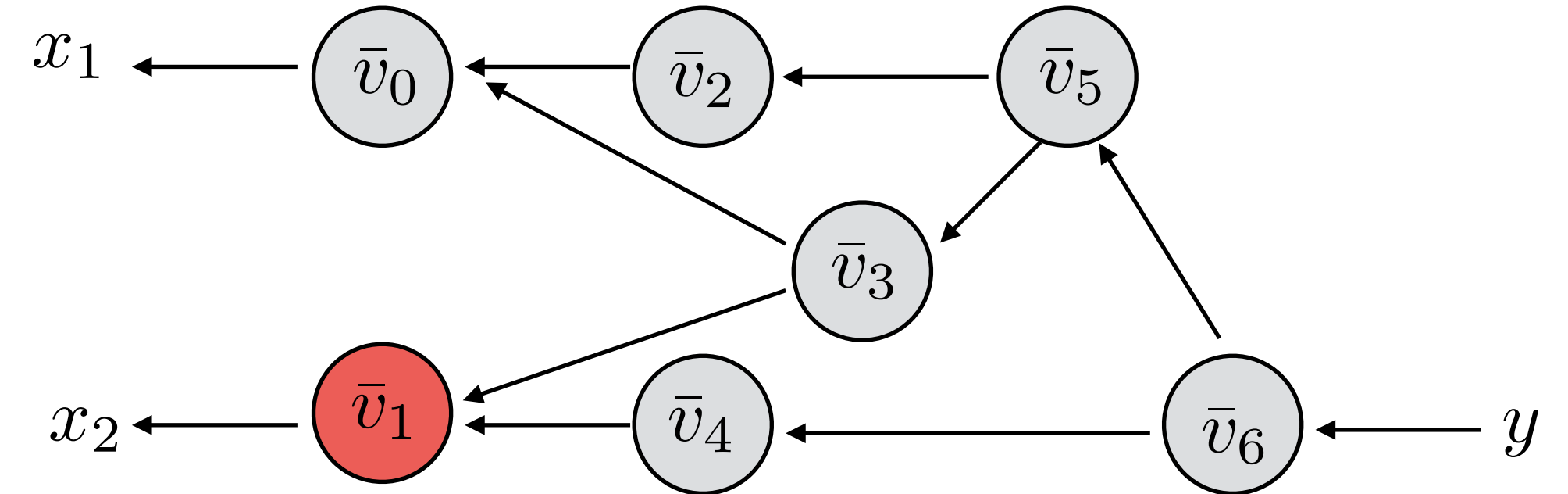
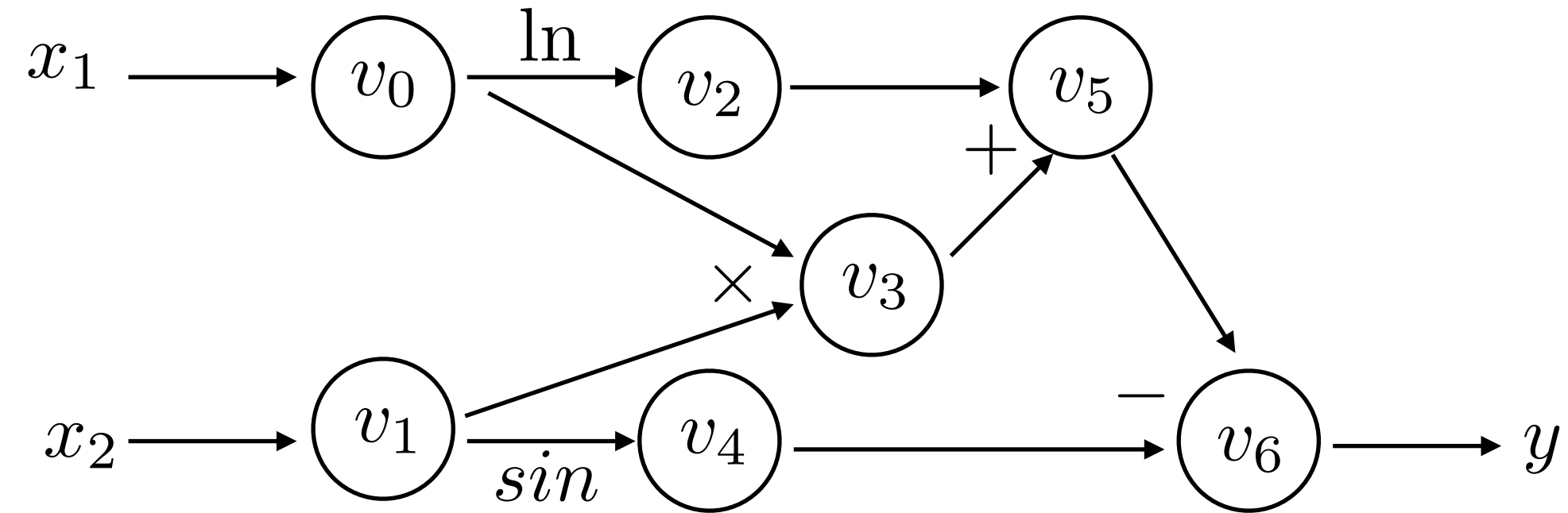
Backwards Derivative Trace:

Forward Evaluation Trace:

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

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

AutoDiff - Reverse Mode



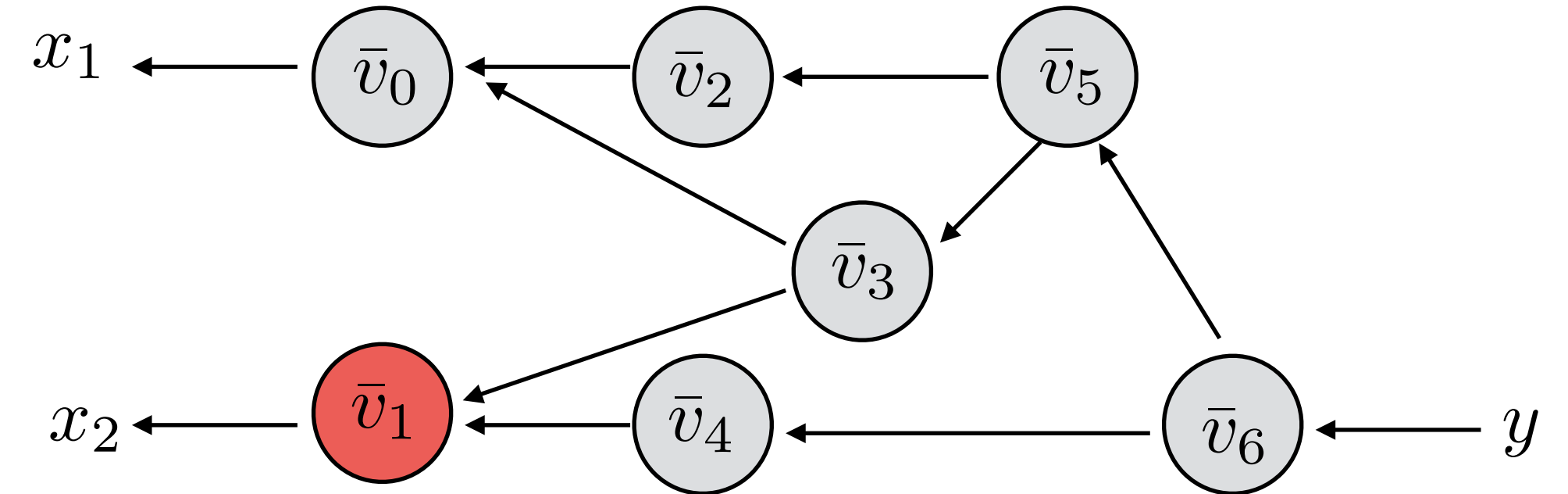
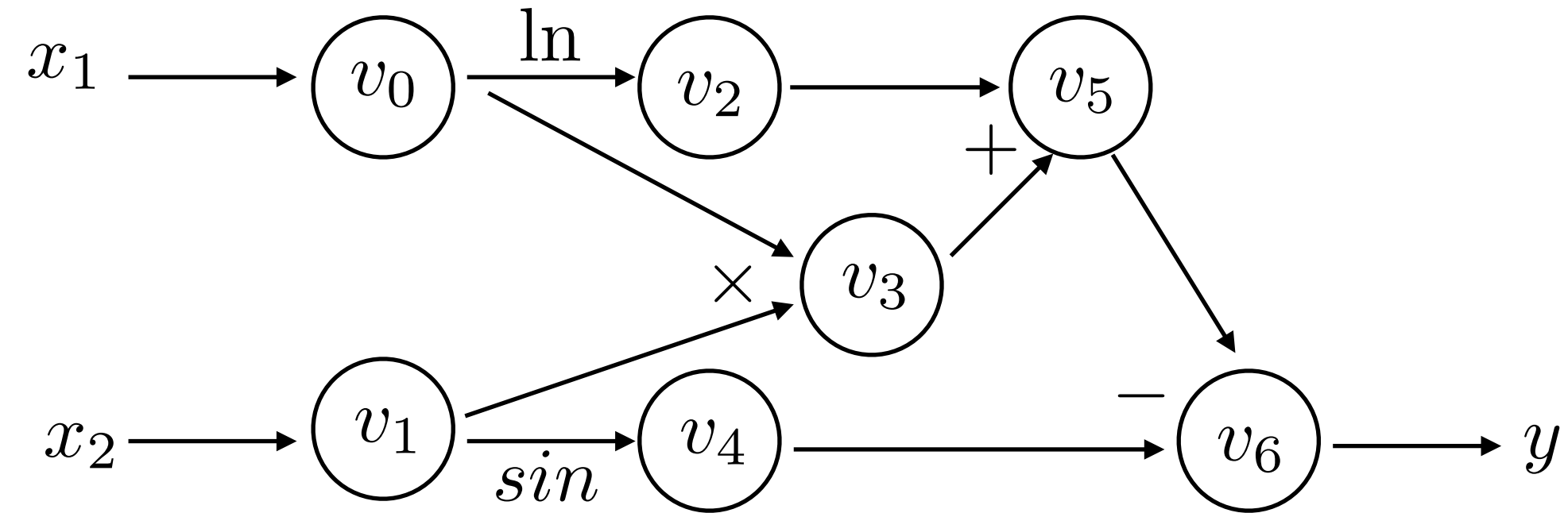
Backwards Derivative Trace:

Forward Evaluation Trace:

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

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

AutoDiff - Reverse Mode



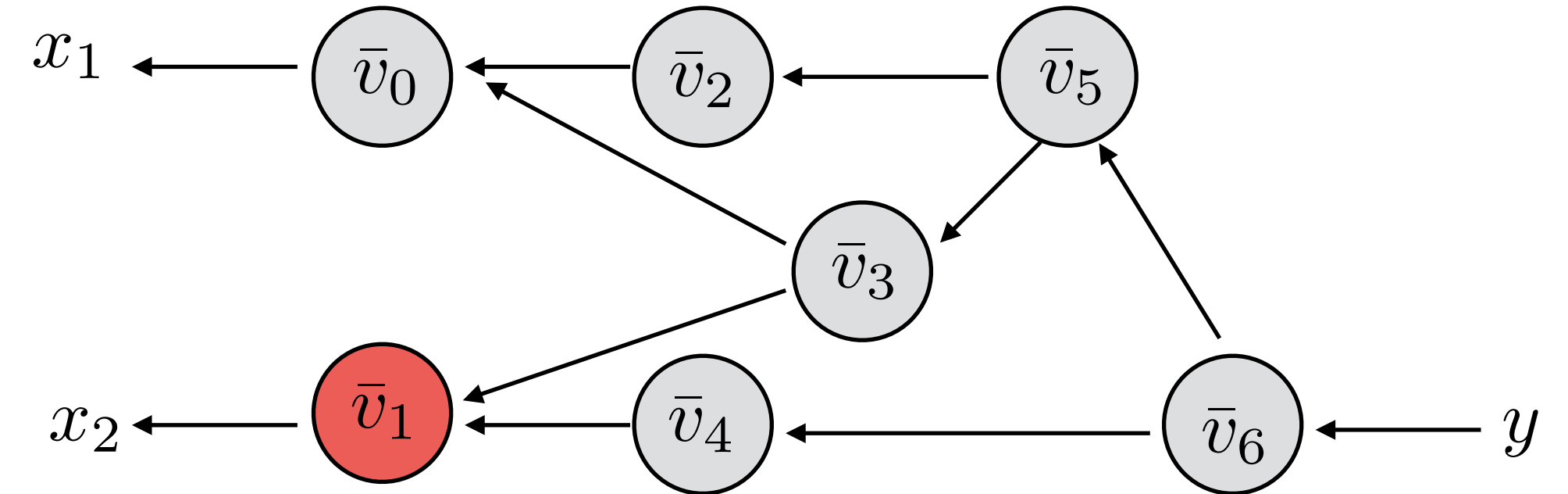
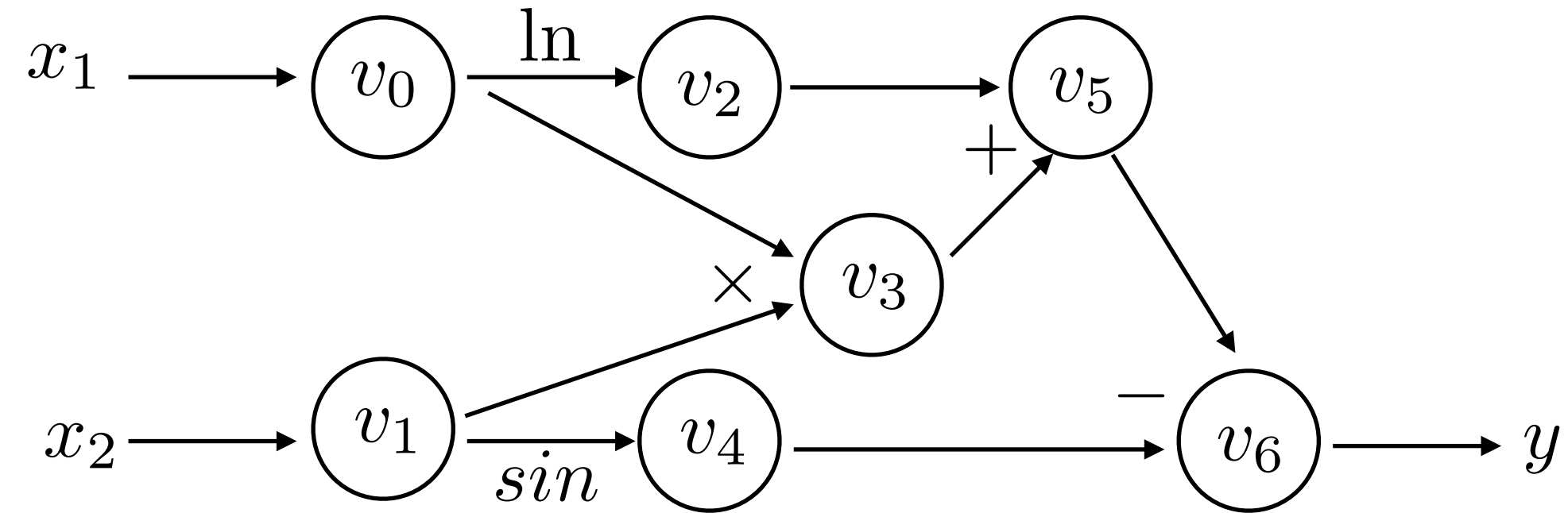
Backwards Derivative Trace:

Forward Evaluation Trace:

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

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

AutoDiff - Reverse Mode



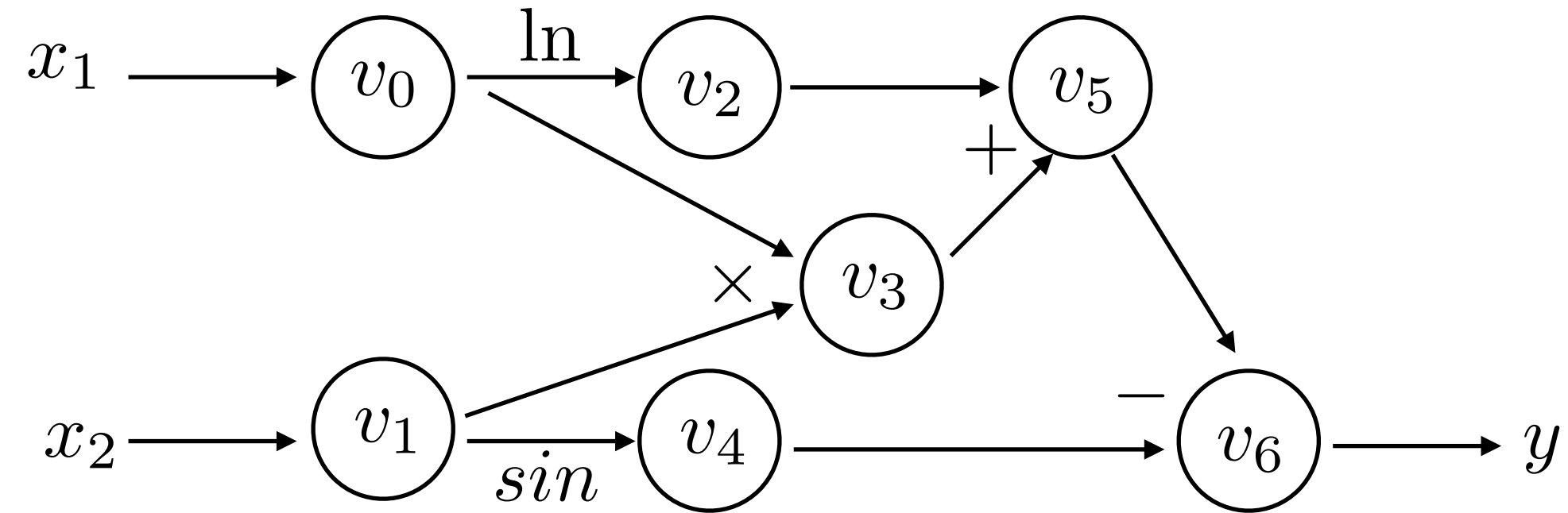
Backwards Derivative Trace:

Forward Evaluation Trace:

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

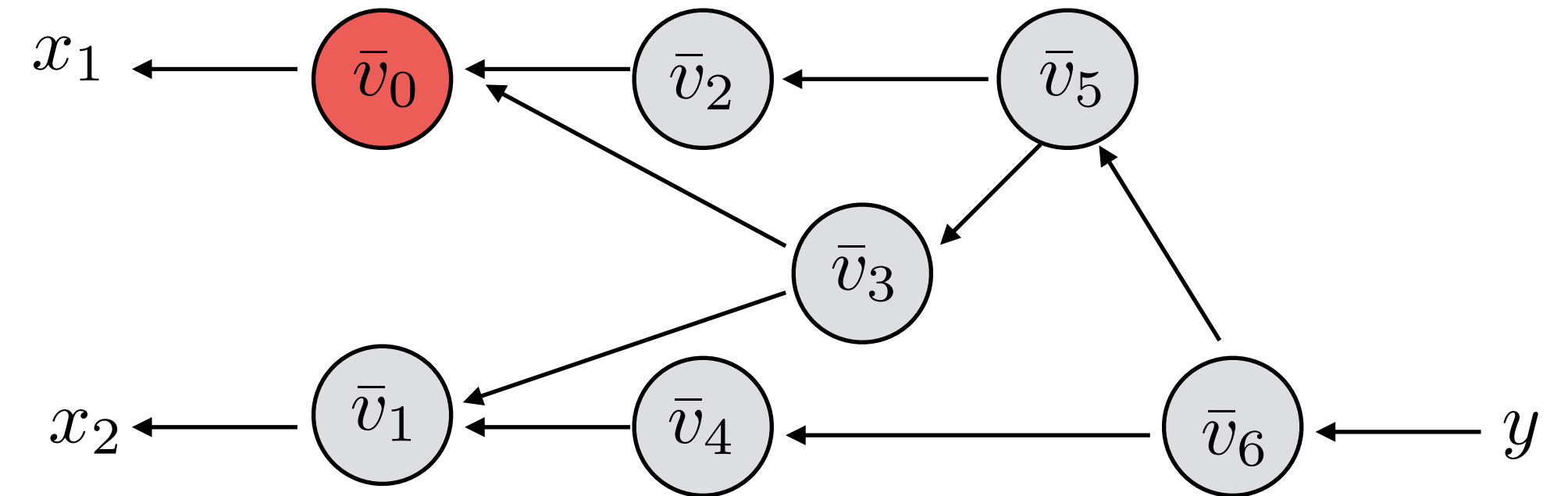
$\bar{v}_1 = \bar{v}_3 \frac{\partial v_3}{\partial v_1} + \bar{v}_4 \frac{\partial v_4}{\partial v_1} = \bar{v}_3 v_0 + \bar{v}_4 \cos(v_1)$	1.716
$\bar{v}_2 = \bar{v}_5 \frac{\partial v_5}{\partial v_2} = \bar{v}_5 \cdot (1)$	$1 \times 1 = 1$
$\bar{v}_3 = \bar{v}_5 \frac{\partial v_5}{\partial v_3}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

AutoDiff - Reverse Mode



Forward Evaluation Trace:

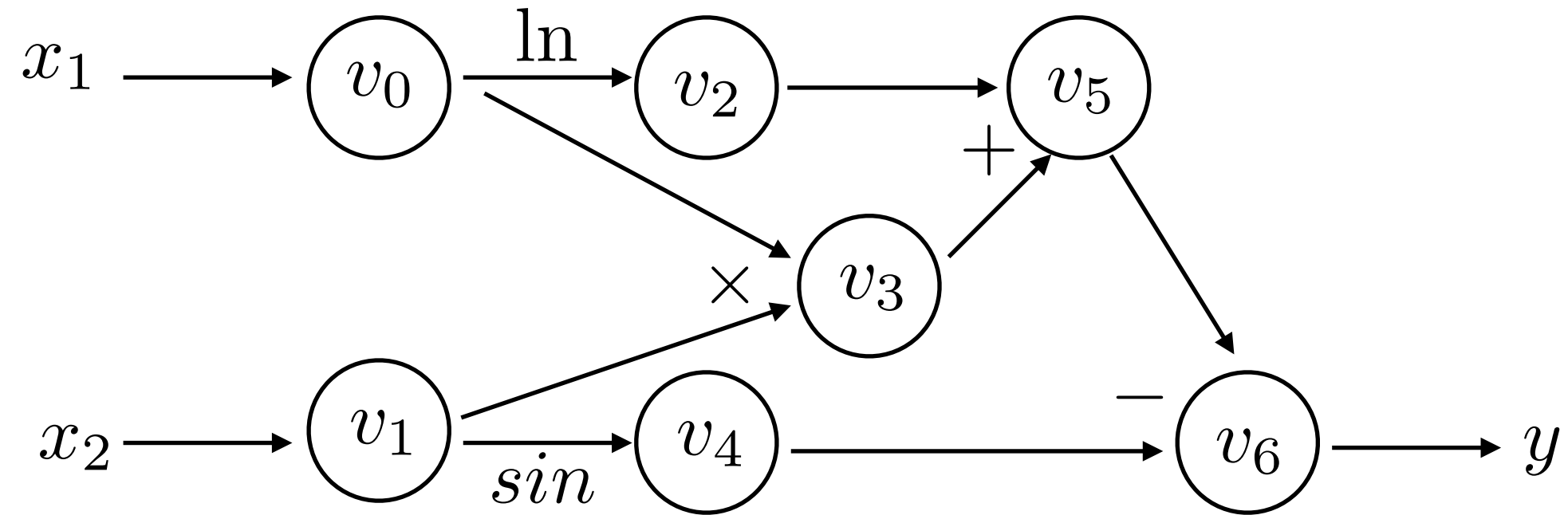
	$f(2, 5)$
$v_0 = x_1$	2
$v_1 = x_2$	5
$v_2 = \ln(v_0)$	$\ln(2) = 0.693$
$v_3 = v_0 \cdot v_1$	$2 \times 5 = 10$
$v_4 = \sin(v_1)$	$\sin(5) = 0.959$
$v_5 = v_2 + v_3$	$0.693 + 10 = 10.693$
$v_6 = v_5 - v_4$	$10.693 + 0.959 = 11.652$
$y = v_6$	11.652



Backwards Derivative Trace:

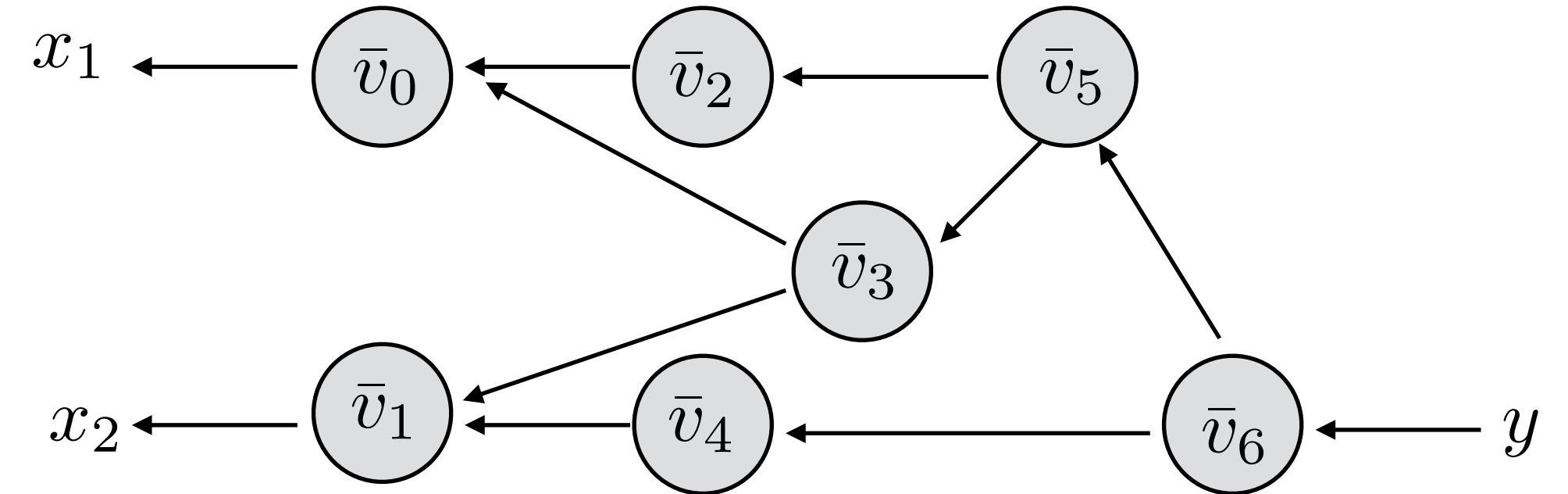
$\bar{v}_0 = \bar{v}_3 \frac{\partial v_3}{\partial v_0} + \bar{v}_2 \frac{\partial v_2}{\partial v_0} = \bar{v}_3 v_1 + \bar{v}_2 \frac{1}{v_0}$	5.5
$\bar{v}_1 = \bar{v}_3 \frac{\partial v_3}{\partial v_1} + \bar{v}_4 \frac{\partial v_4}{\partial v_1} = \bar{v}_3 v_0 + \bar{v}_4 \cos(v_1)$	1.716
$\bar{v}_2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

AutoDiff - Reverse Mode



Forward Evaluation Trace:

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



Backwards Derivative Trace:

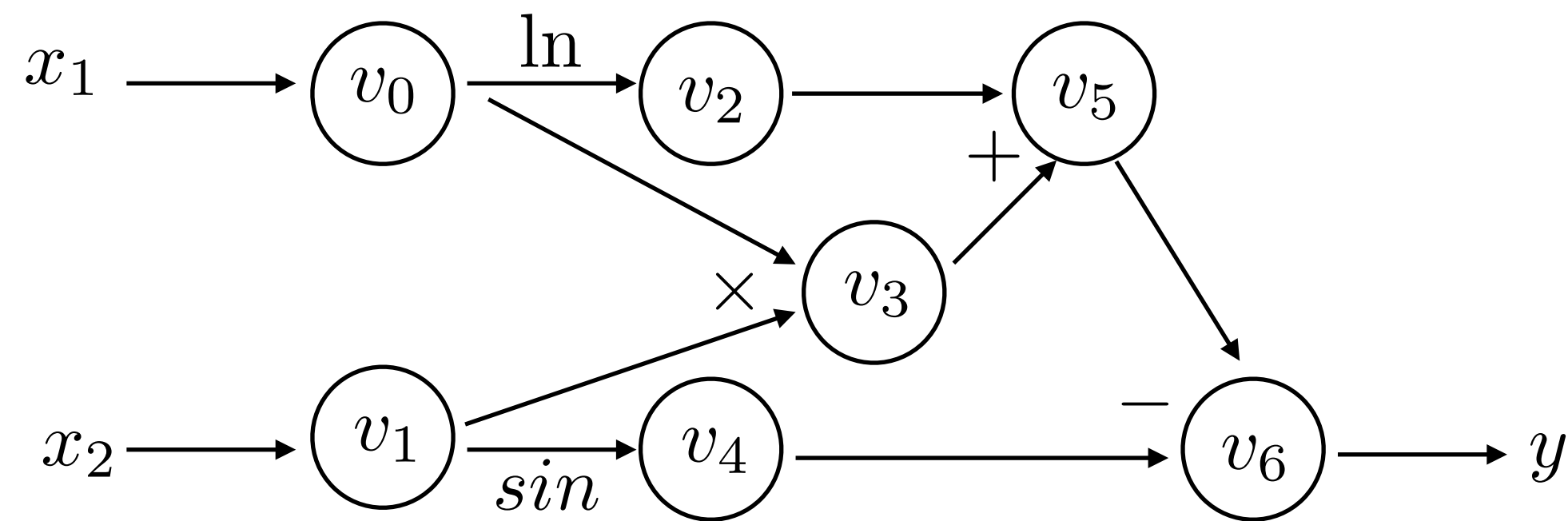
$\bar{v}_0 = \bar{v}_3 \frac{\partial v_3}{\partial v_0} + \bar{v}_2 \frac{\partial v_2}{\partial v_0} = \bar{v}_3 v_1 + \bar{v}_2 \frac{1}{v_0}$	5.5
$\bar{v}_1 = \bar{v}_3 \frac{\partial v_3}{\partial v_1} + \bar{v}_4 \frac{\partial v_4}{\partial v_1} = \bar{v}_3 v_0 + \bar{v}_4 \cos(v_1)$	1.716
$\bar{v}_2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

Automatic Differentiation (AutoDiff)

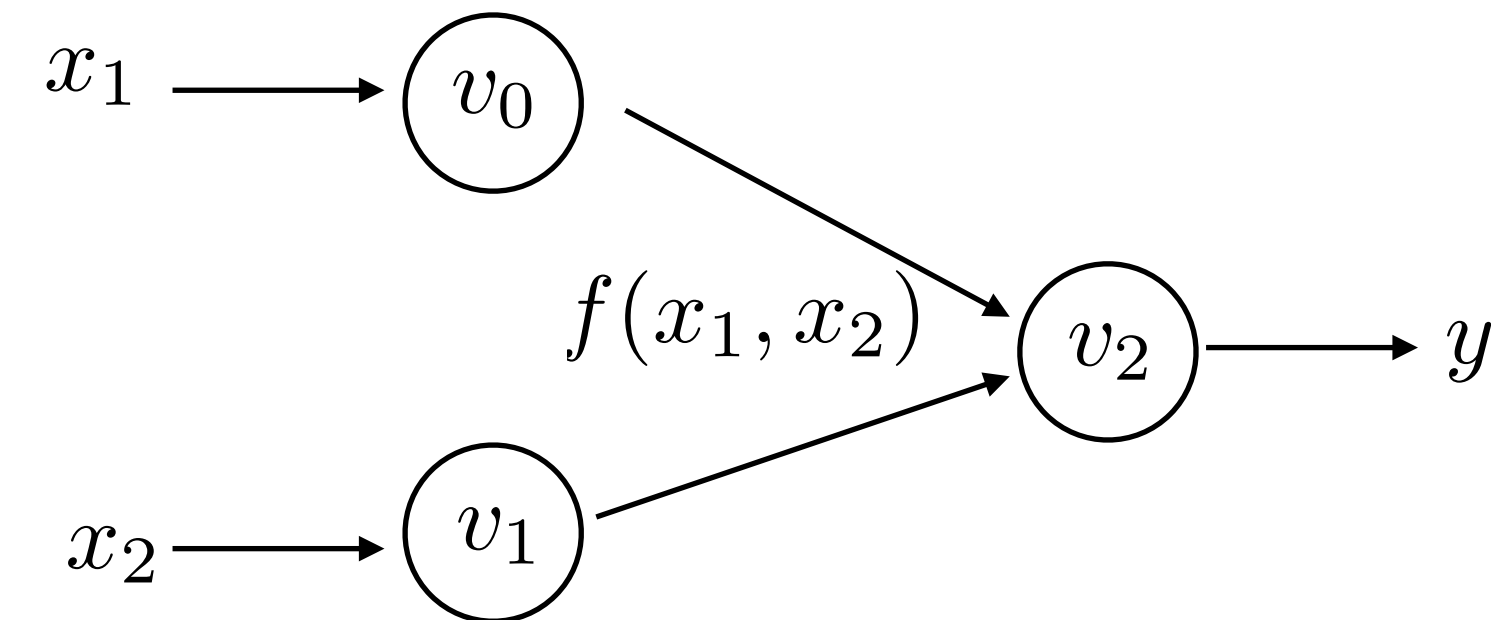
$$y = f(x_1, x_2) = \ln(x_1) + x_1x_2 - \sin(x_2)$$

AutoDiff can be done at various **granularities**

Elementary function granularity:



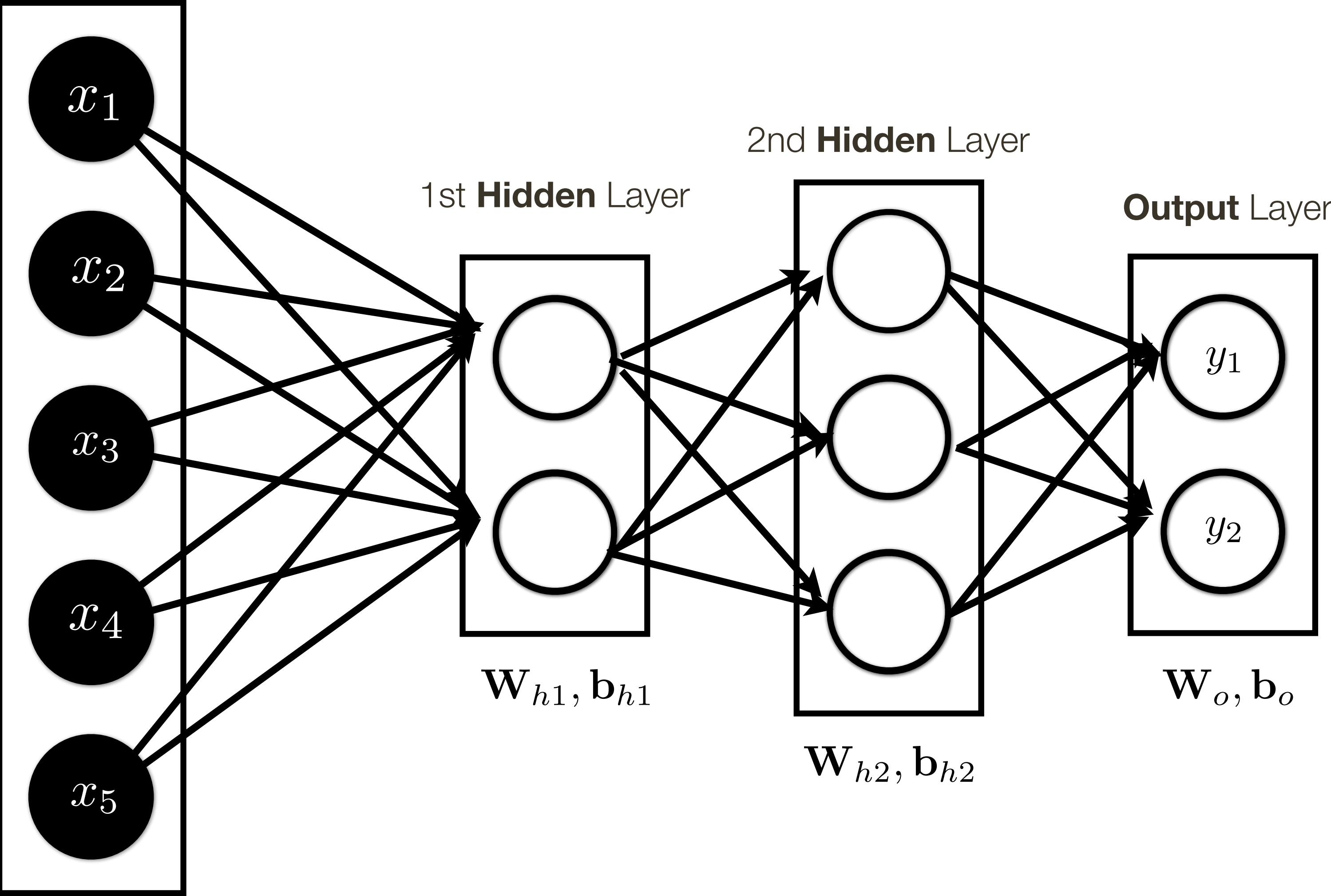
Complex function granularity:



Backpropagation Practical Issues

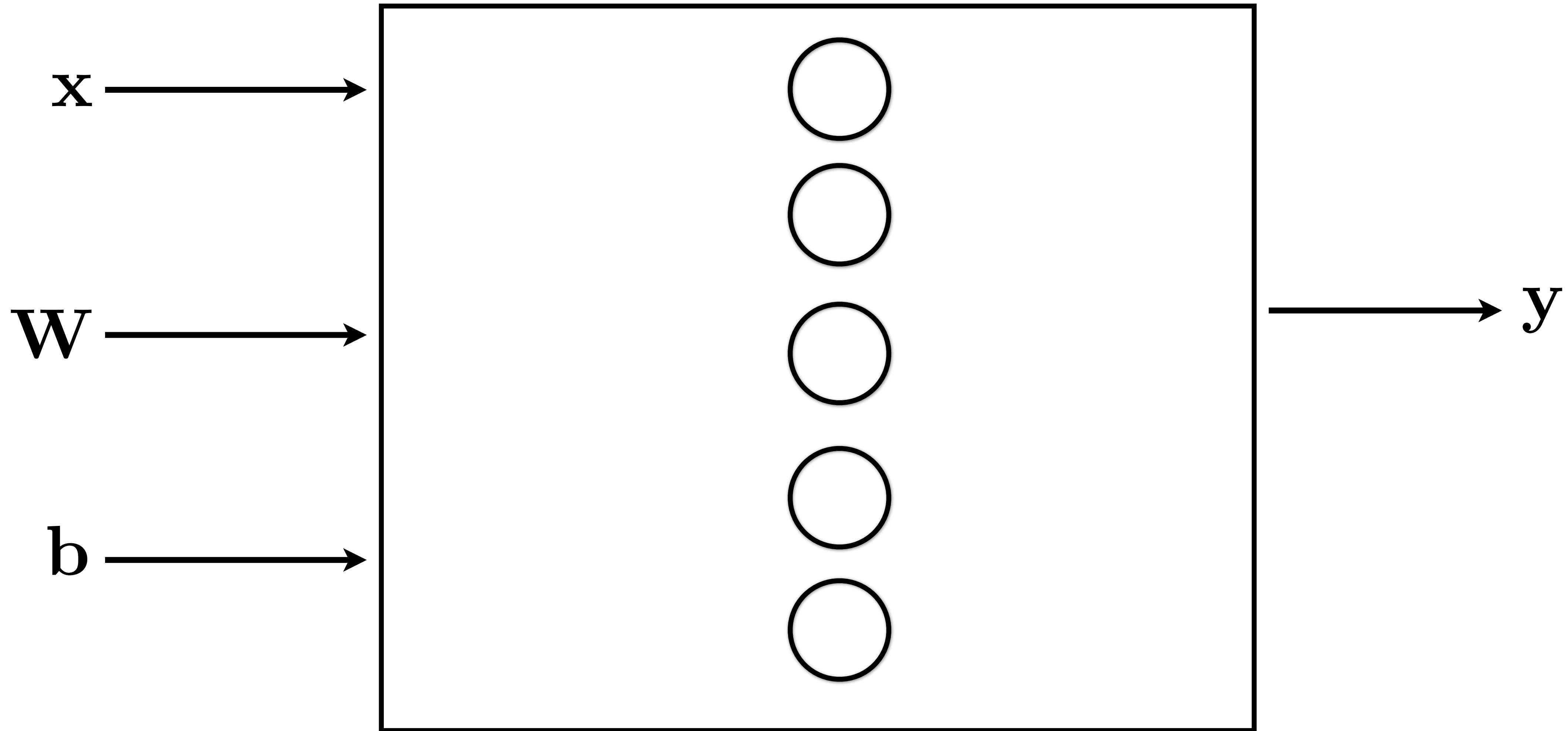
Input Layer

Easier to deal with in **vector form**



Backpropagation Practical Issues

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

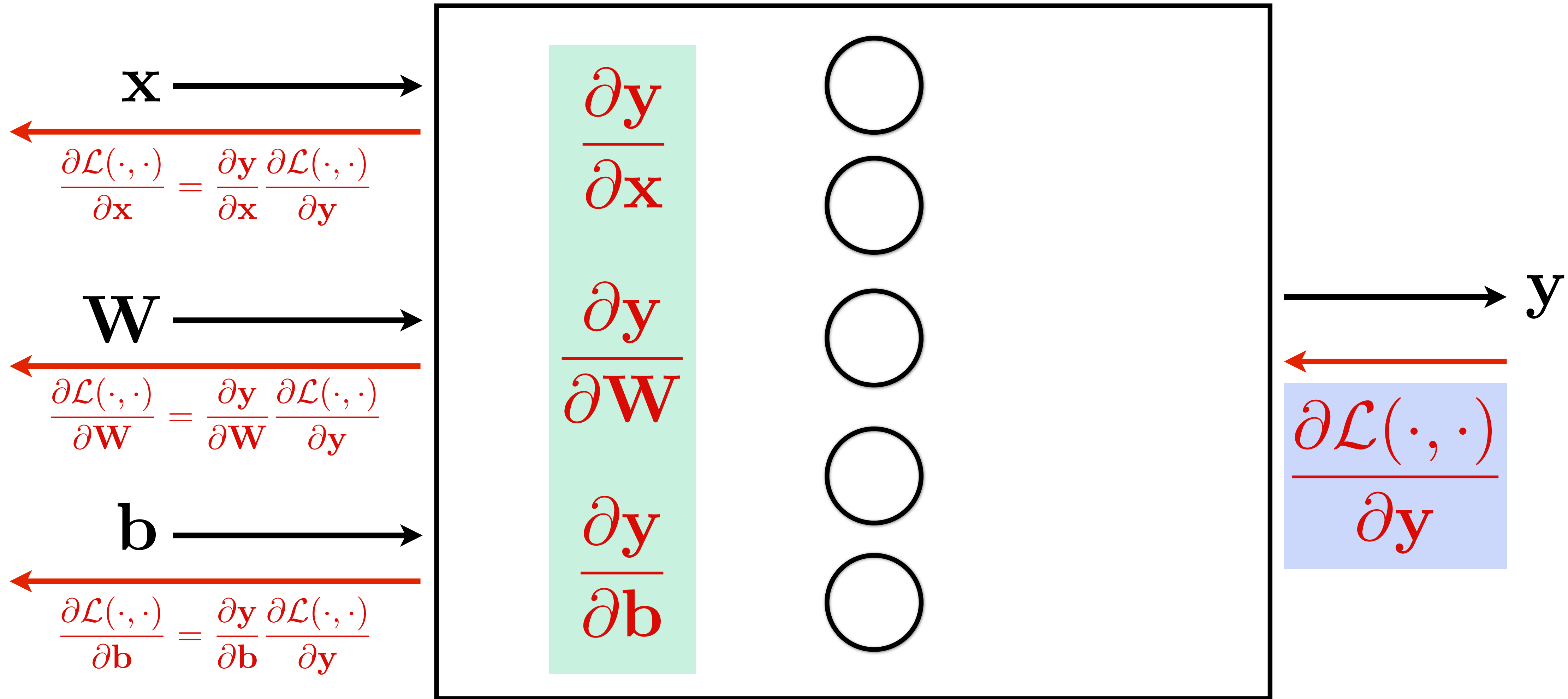


Backpropagation Practical Issues

“**local**” Jacobians
(matrix of partial derivatives, e.g. size $|x| \times |y|$)

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

“**backprop**” Gradient

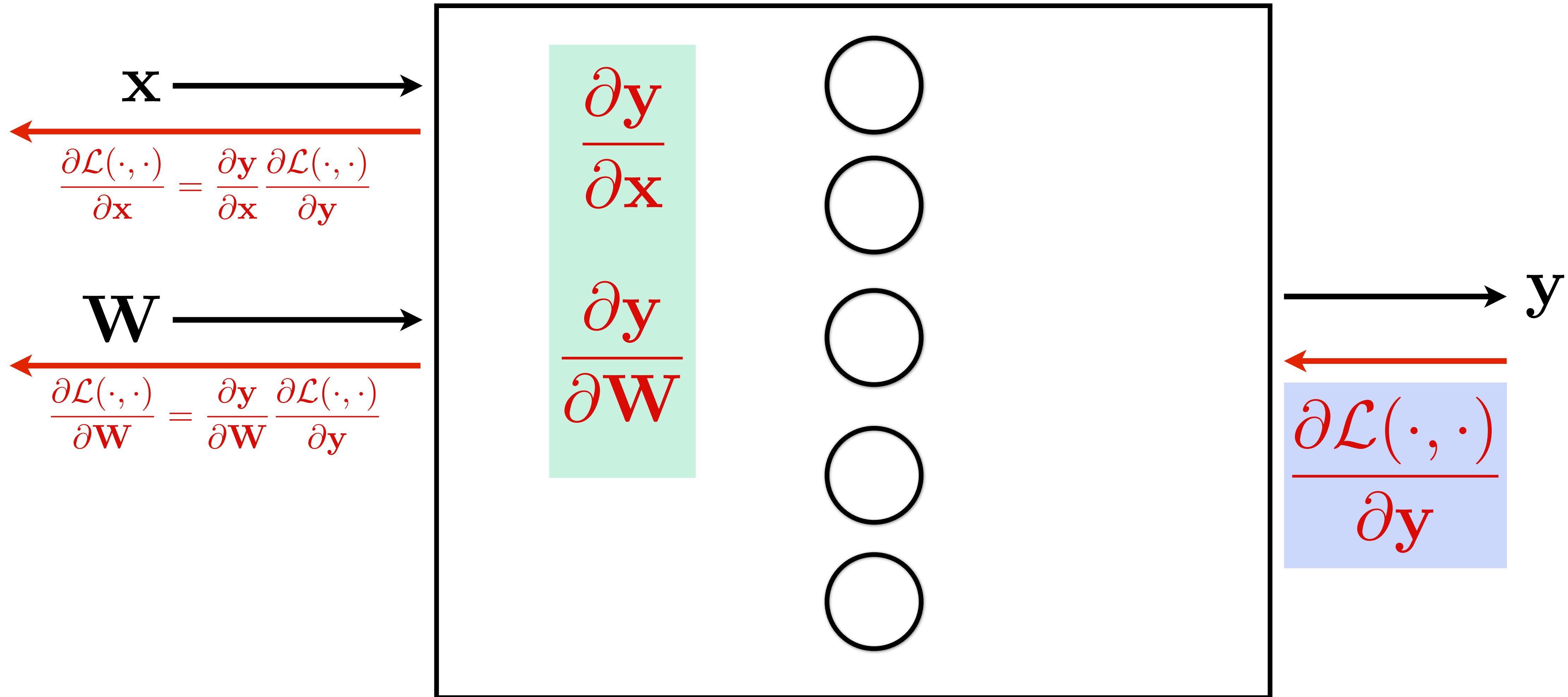


Backpropagation Practical Issues

“**local**” Jacobians
(matrix of partial derivatives, e.g. size $|x| \times |y|$)

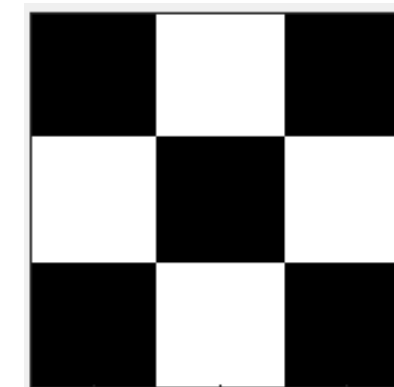
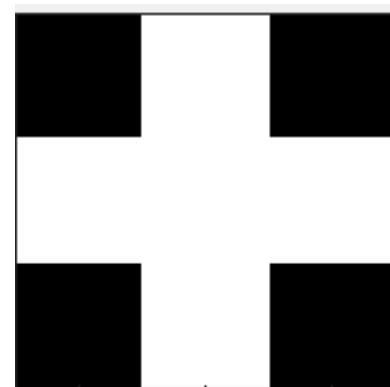
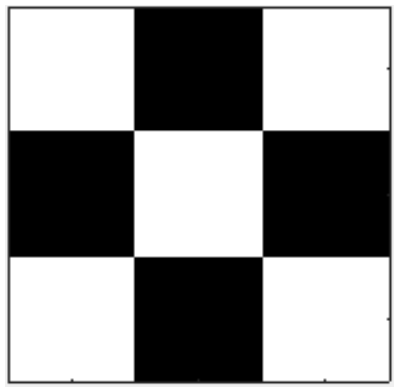
“**backprop**” Gradient

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



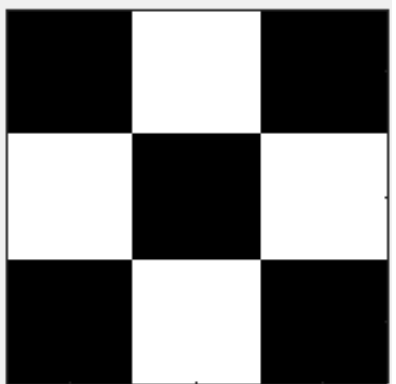
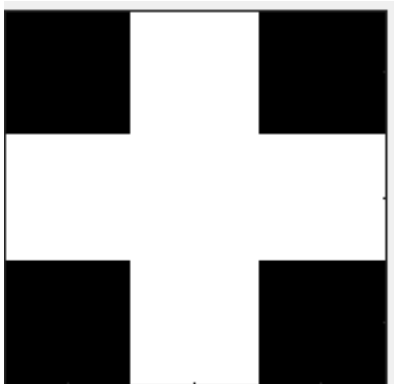
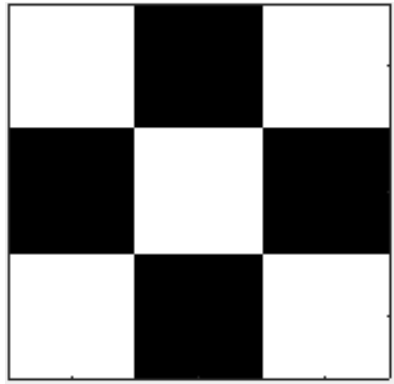
Example: Let's Build (world smallest) Neural Network

Lets create a neural network that will be able to differentiate (classify) these patterns of simple 3x3 pixel images

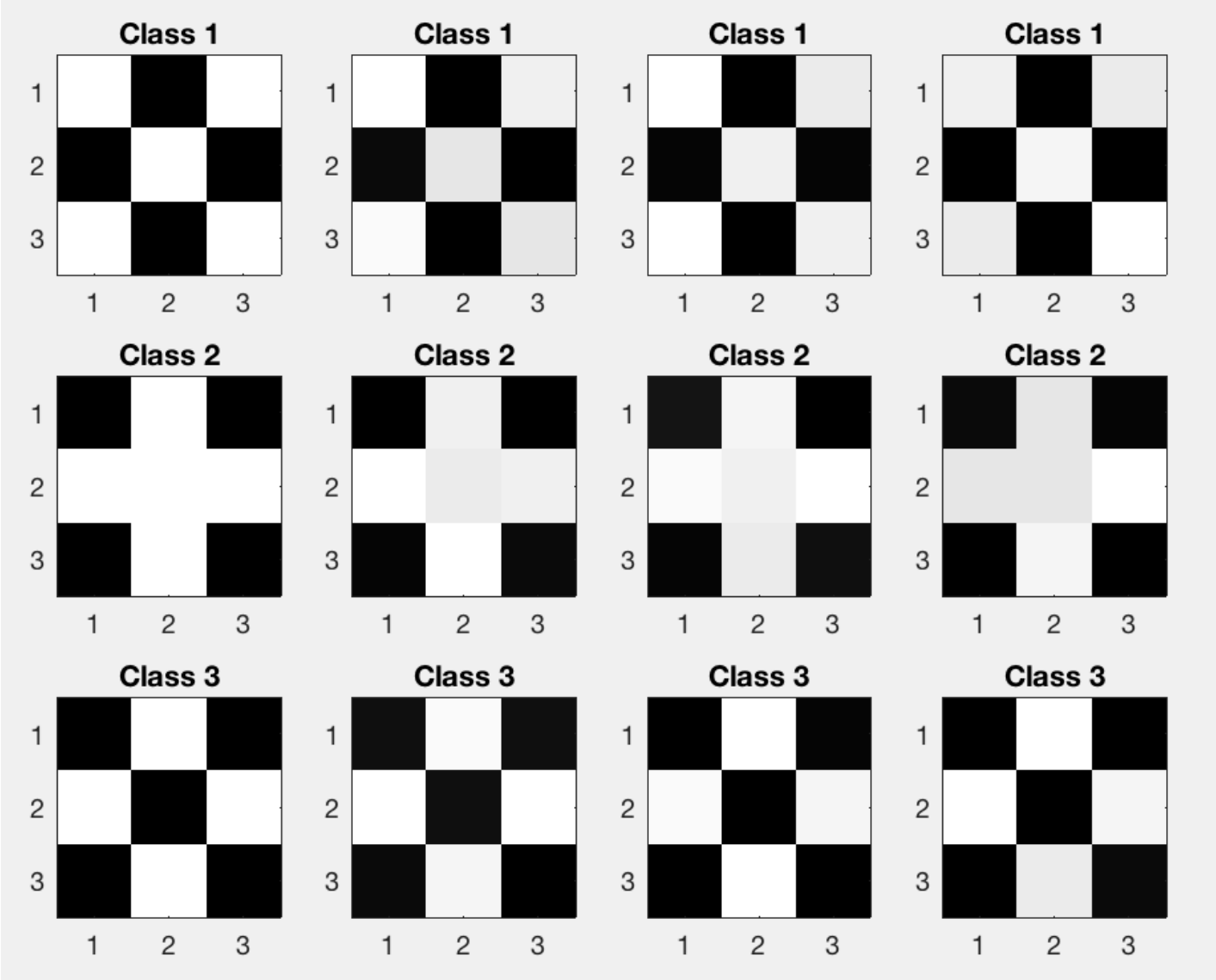


Example: Let's Build (world smallest) Neural Network

Lets create a neural network that will be able to differentiate (classify) these patterns of simple 3x3 pixel images

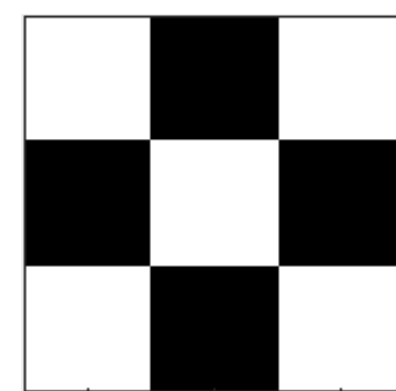
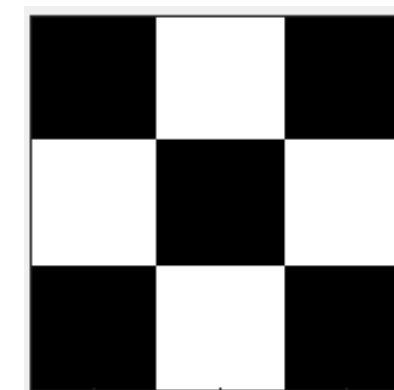
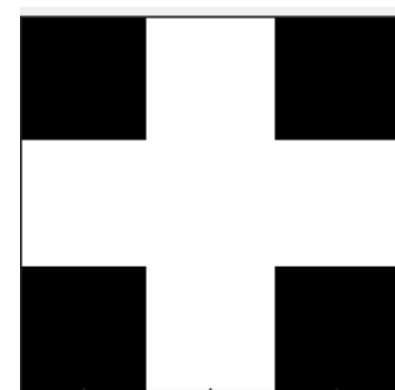
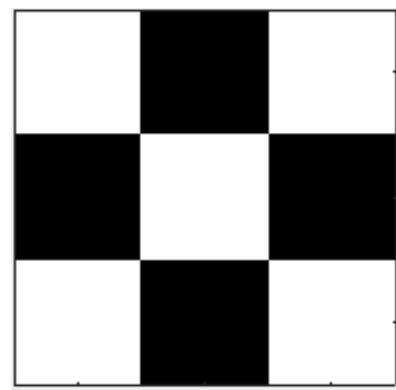


We will need some labeled data



Example: Let's Build (world smallest) Neural Network

Lets create a neural network that will be able to differentiate (classify) these patterns of simple 3x3 pixel images

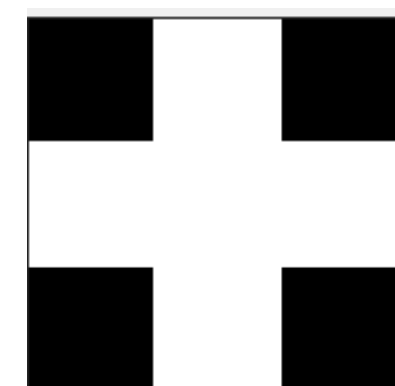
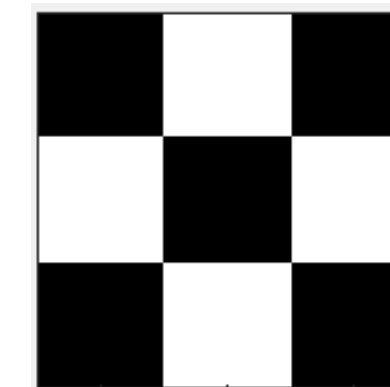
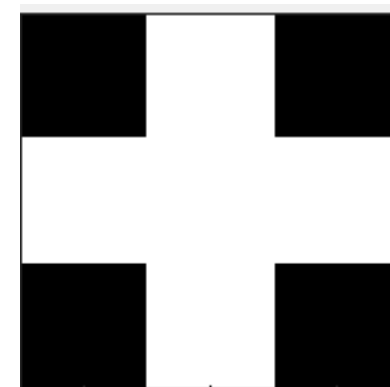
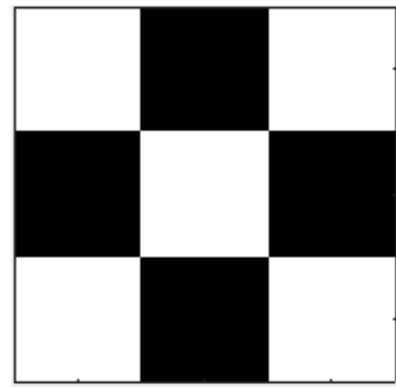


Neural Network

Class 1

Example: Let's Build (world smallest) Neural Network

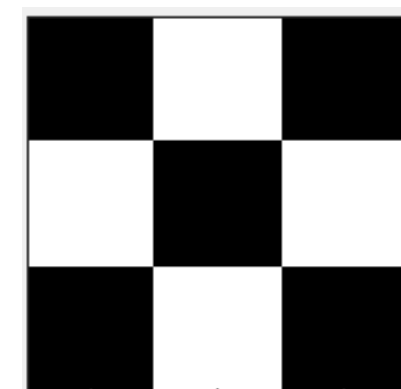
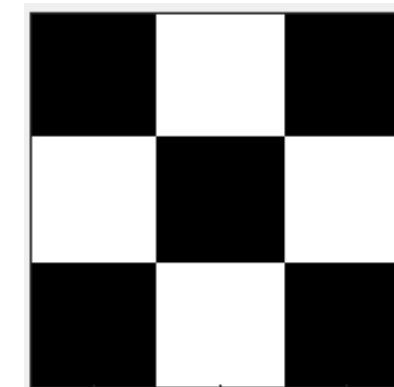
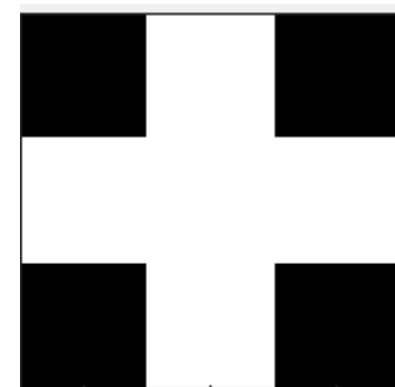
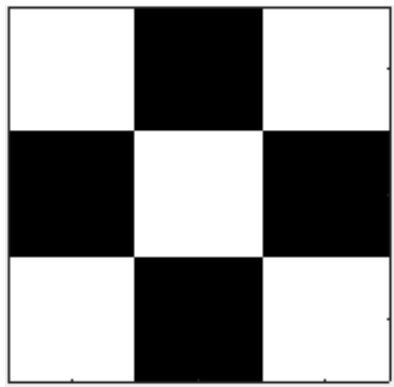
Lets create a neural network that will be able to differentiate (classify) these patterns of simple 3x3 pixel images



Class **2**

Example: Let's Build (world smallest) Neural Network

Lets create a neural network that will be able to differentiate (classify) these patterns of simple 3x3 pixel images

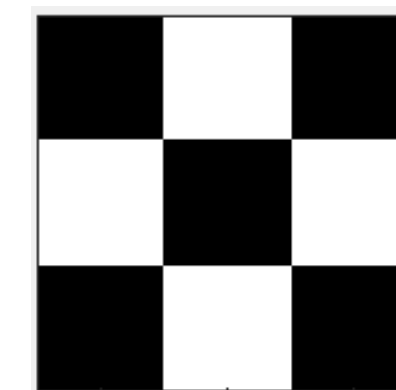
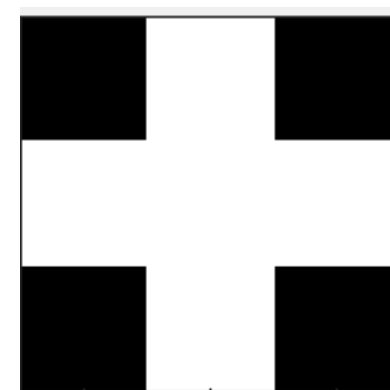
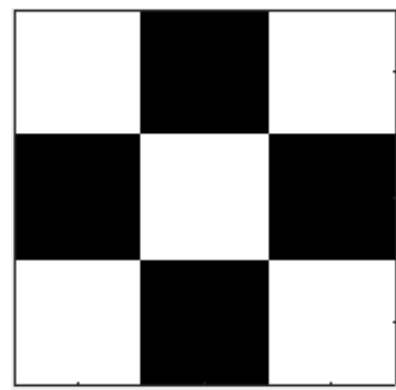


Neural Network

Class **3**

Example: Let's Build (world smallest) Neural Network

Lets create a neural network that will be able to differentiate (classify) these patterns of simple 3x3 pixel images



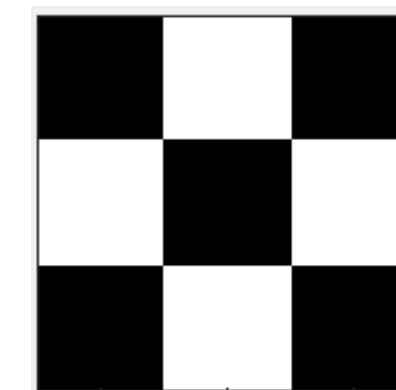
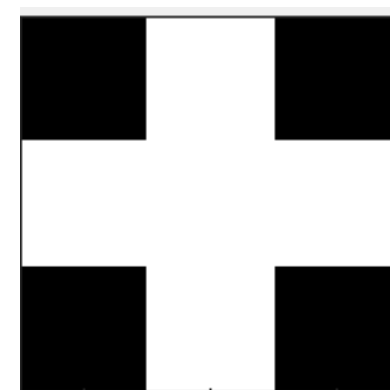
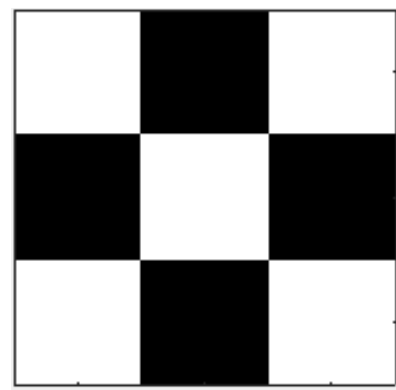
What do we need to do?



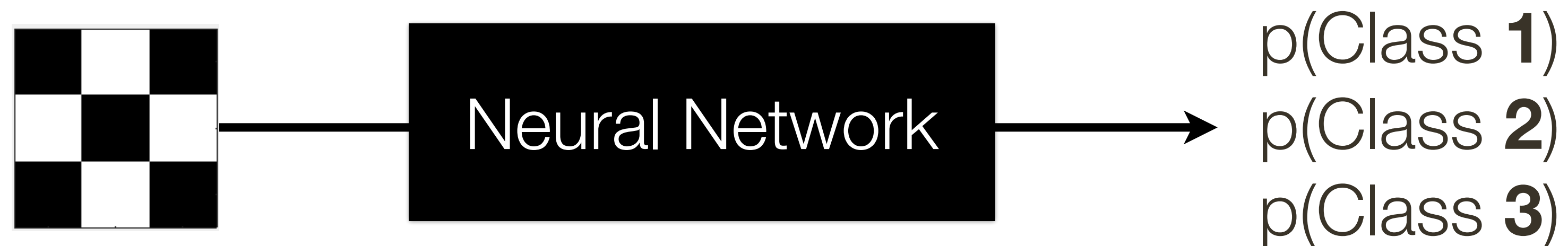
First, lets re-formulate the problem

Example: Let's Build (world smallest) Neural Network

Lets create a neural network that will be able to differentiate (classify) these patterns of simple 3x3 pixel images



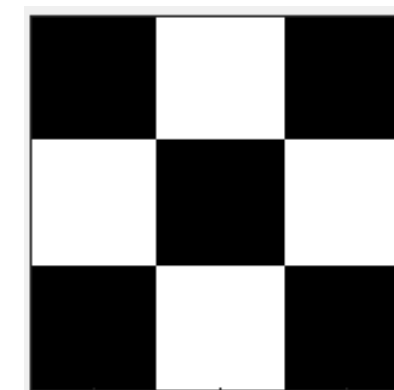
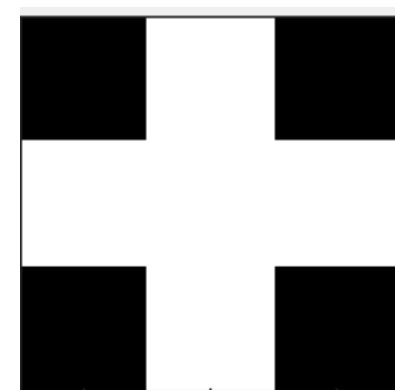
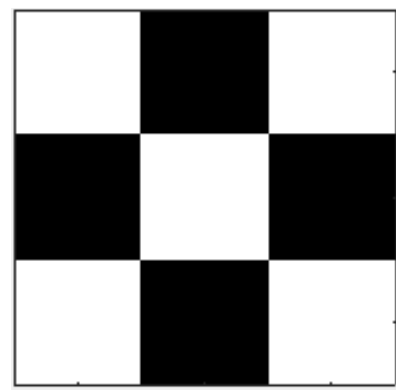
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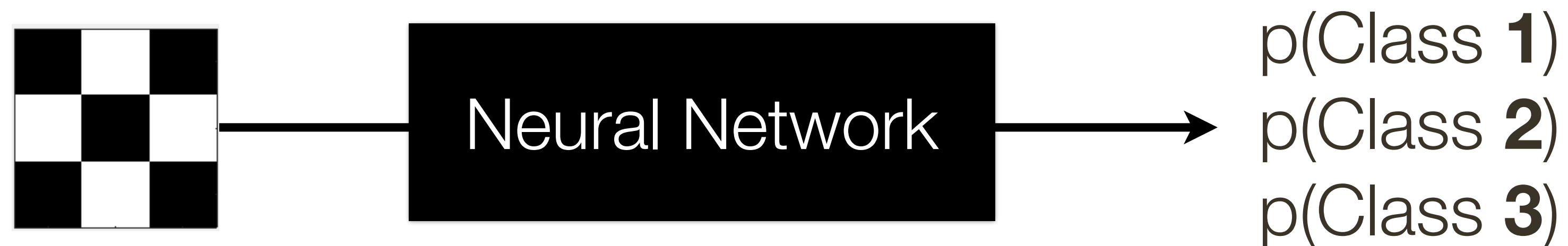
First, lets re-formulate the problem

Example: Let's Build (world smallest) Neural Network

Lets create a neural network that will be able to differentiate (classify) these patterns of simple 3x3 pixel images



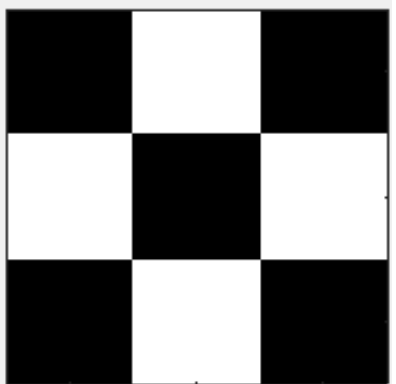
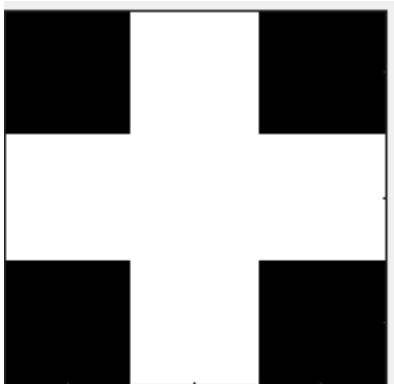
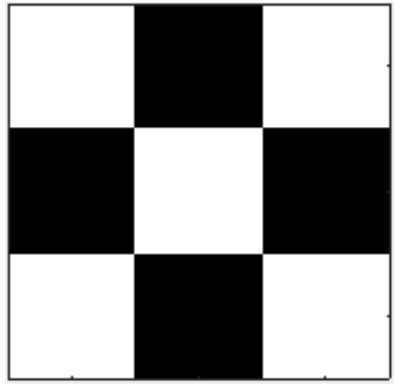
Now, lets build a **network!**



How many inputs should the network have? How neuron outputs?

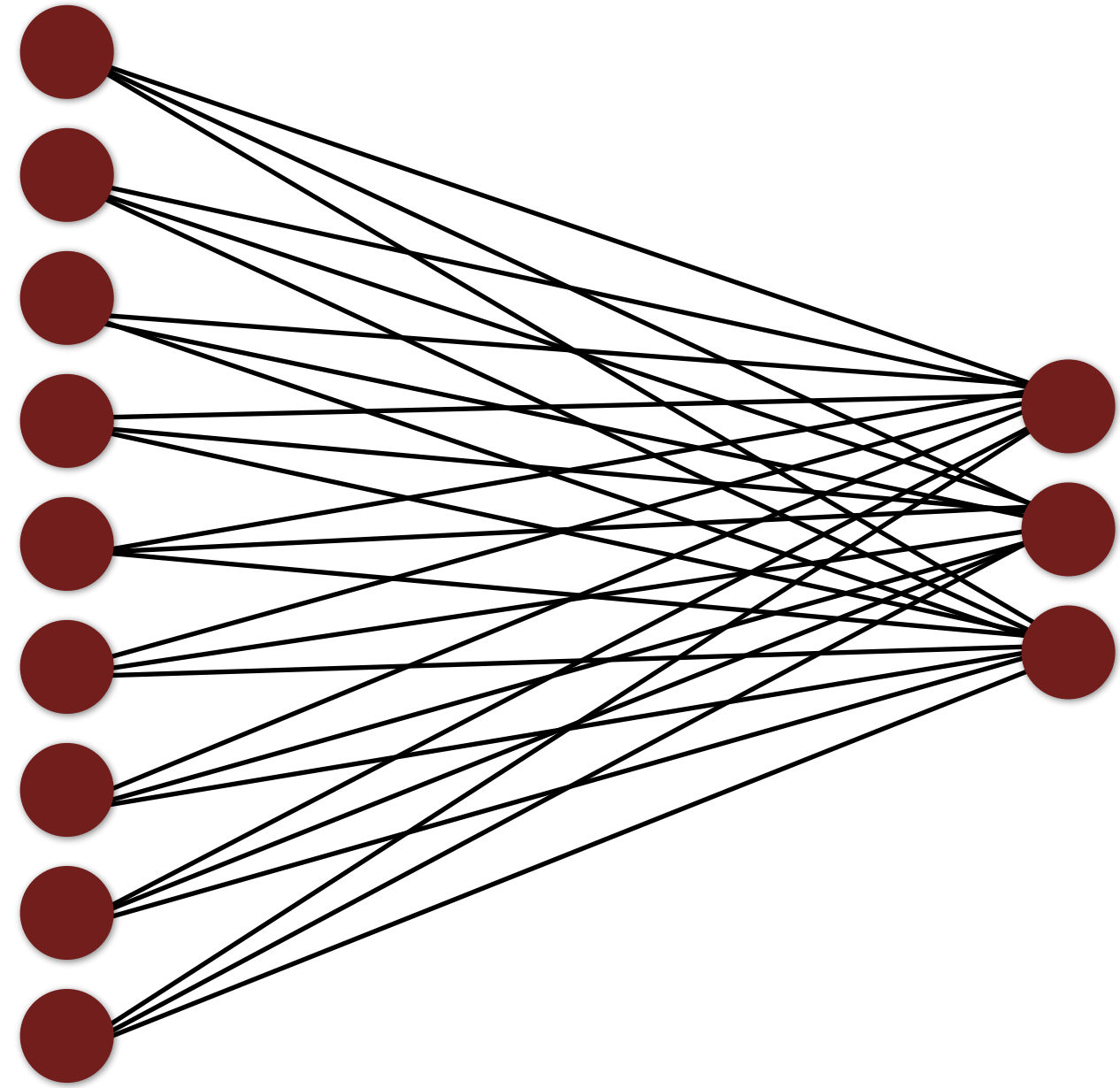
Example: Let's Build (world smallest) Neural Network

Lets create a neural network that will be able to differentiate (classify) these patterns of simple 3x3 pixel images



Input Layer

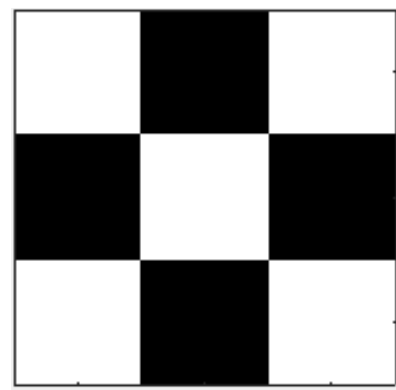
Output Layer



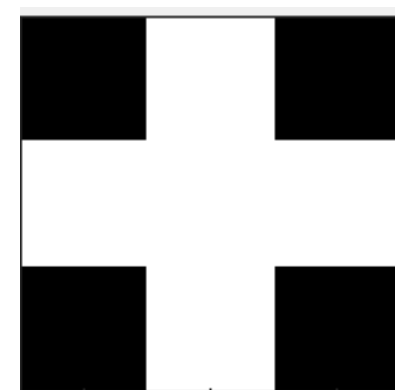
What else is missing for us to train it?

Example: Let's Build (world smallest) Neural Network

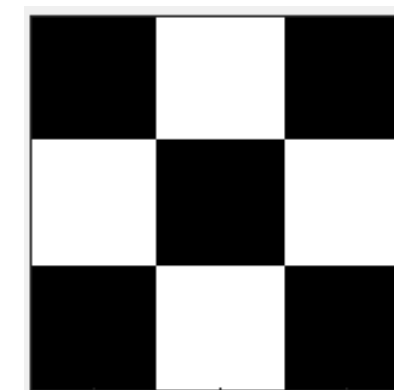
Lets create a neural network that will be able to differentiate (classify) these patterns of simple 3x3 pixel images



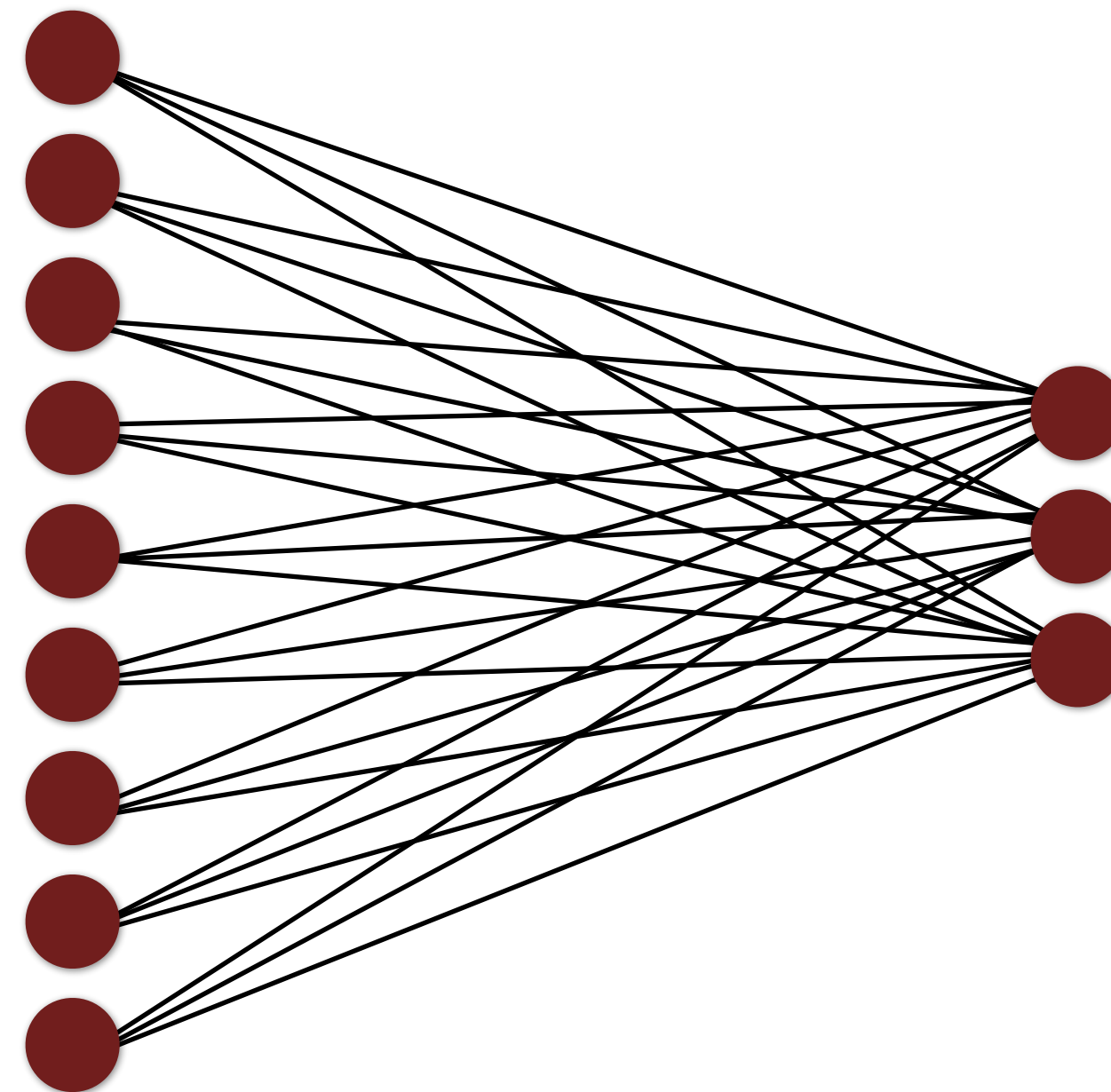
Input Layer



Output Layer



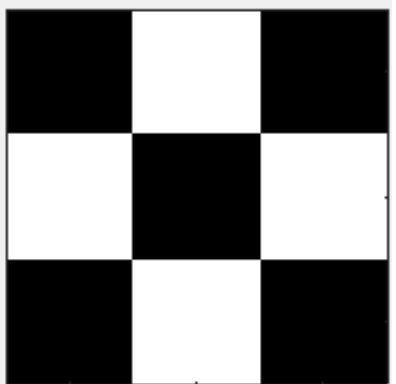
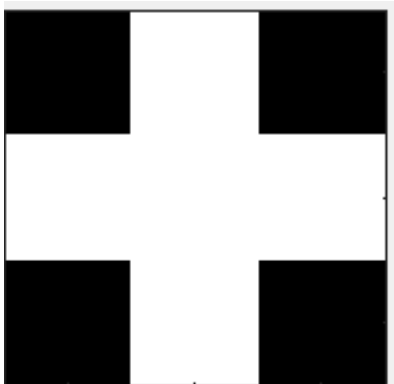
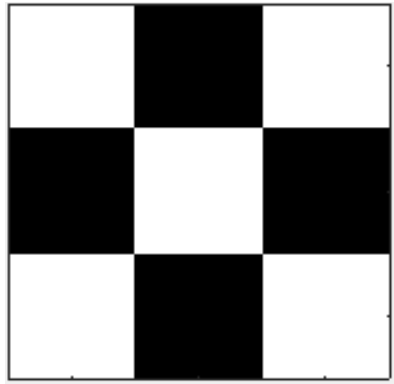
Loss



$$L_i = -\log \left(\frac{e^{f_{y_i}}}{\sum_j e^{f_{y_j}}} \right)$$

Example: Let's Build (world smallest) Neural Network

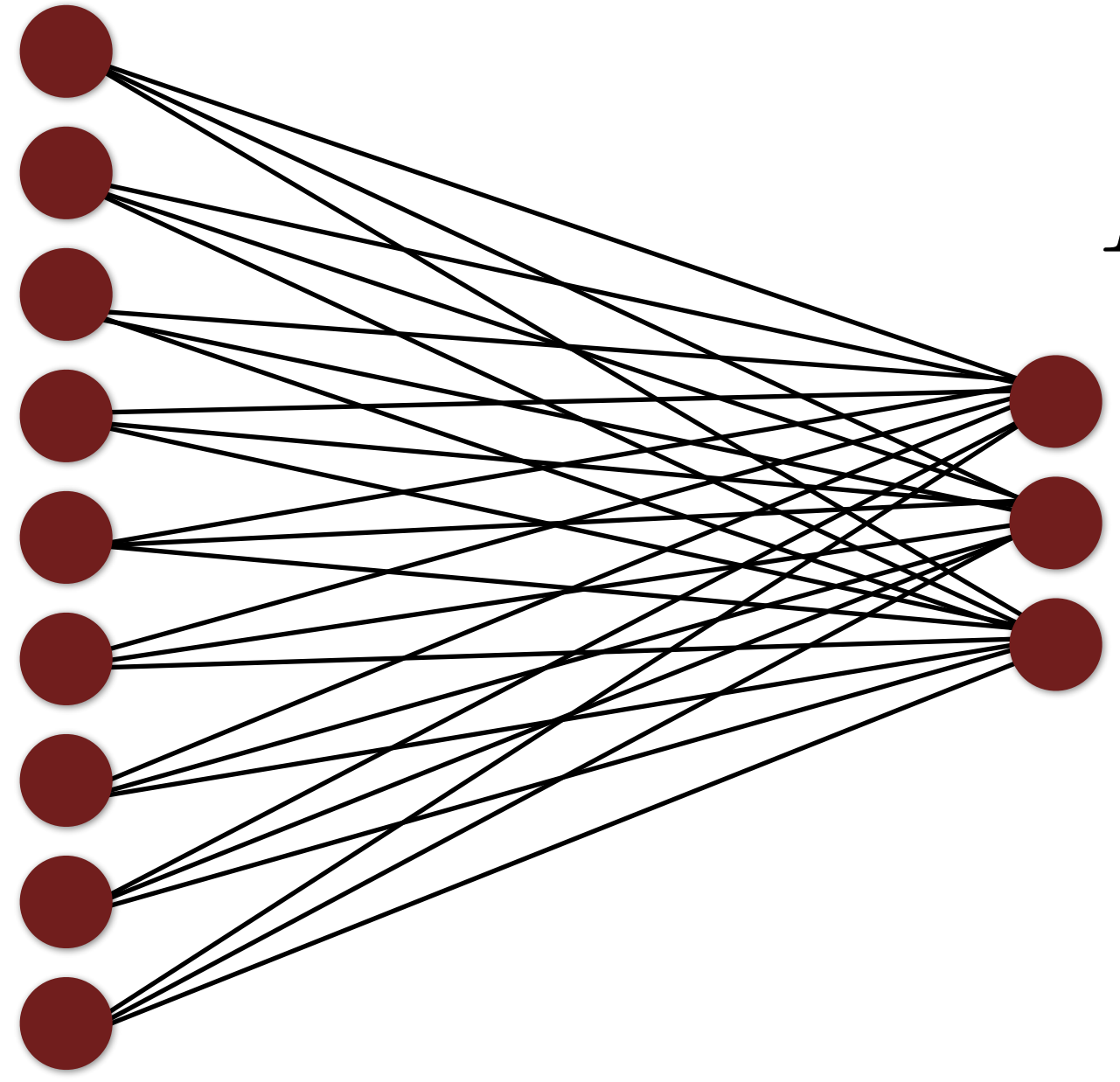
Lets create a neural network that will be able to differentiate (classify) these patterns of simple 3x3 pixel images



Input Layer

Output Layer

Loss



$$L_1 = -\log \left(\frac{e^{\sum_{i=1}^9 \sigma(w_{1,i}x_i + b_1)}}{\sum_{j=1}^3 e^{\sum_{i=1}^9 \sigma(w_{1,i}x_i + b_1)}} \right)$$