Neural Network Introduction

LING 575K Deep Learning for NLP

Shane Steinert-Threlkeld

April 6 2022

Announcements

- HW1 due tomorrow night, upload readme and hw1.tar.gz to Canvas
  - NB: separate files!
  - Do not put readme inside of tar.gz
- indices_to_tokens: no error handling
- You can/should use `Vocabulary.from_text_files` to build your vocab object
  - Factory design pattern allows for different initialization signatures in Python
  - E.g. from_csv in pandas, from_pretrained in huggingface (later this course)
- Note on *args and **kwargs
  - https://book.pythontips.com/en/latest/args_and_kwargs.html

*args and **kwargs

```python
def add(a, b):
    return a + b


print(add(1, 2))  # 3
print(add(*(1, 2)))  # 3


def add_any(*args):
    return sum(args)


print(add_any(1, 2, 3))  # 6
print(add_any(1, 2, 3, 4))  # 10
```

*args and **kwargs

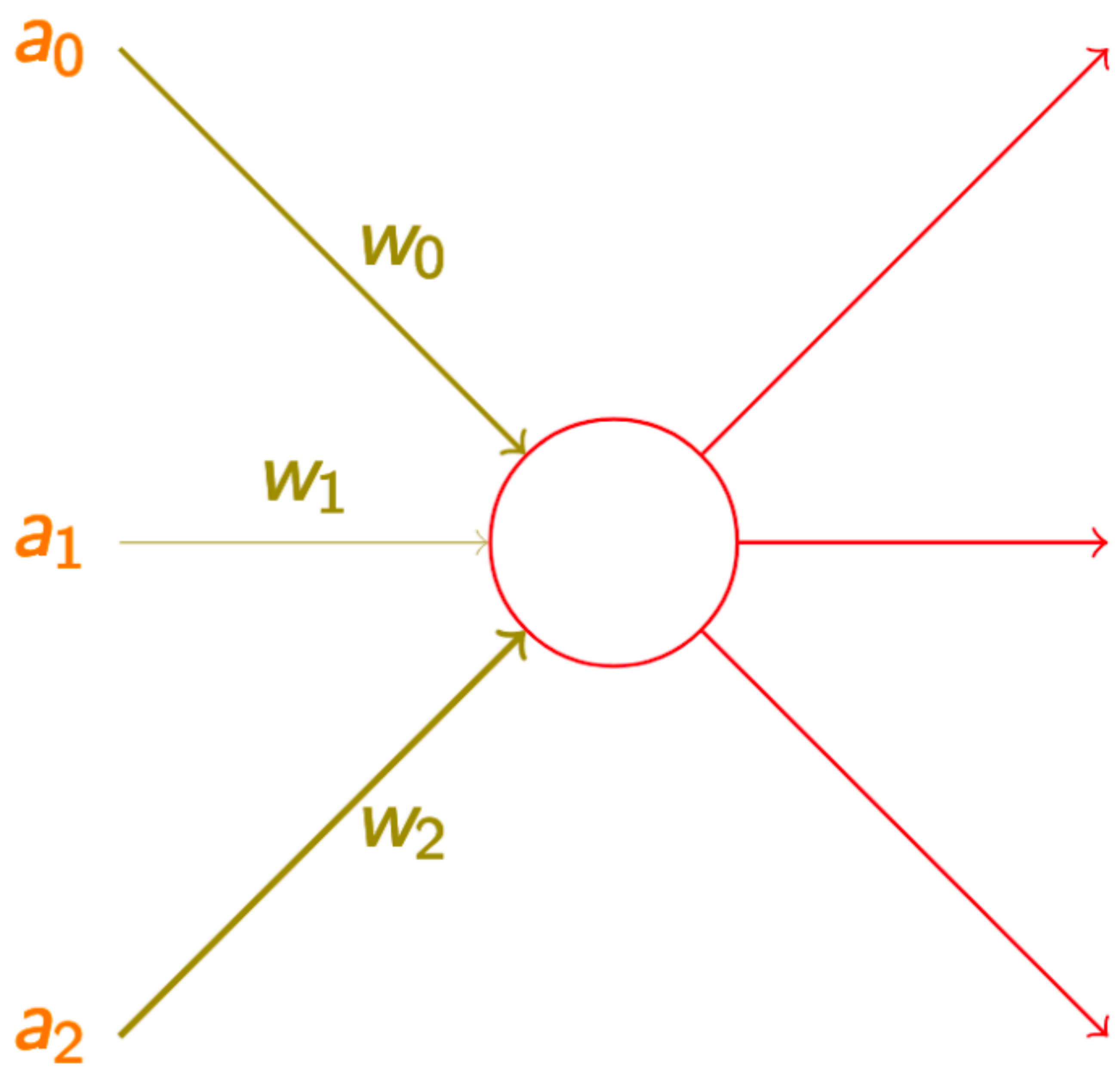
```python
def keywords(name="Shane", course="575k"):
    return f"{name} is teaching {course}"


print(keywords(name="Agatha"))
print(keywords(**{"name": "Agatha"}))


def keywords_any(**kwargs):
    for key, value in kwargs.items():
        print(f"{key}: {value}")

keywords_any(name="Shane", course="575k"))
keywords_any(name="Shane", course="575k", foo="bar"))
keywords_any(**{"name": "Shane", "course": "575k"}))
```

Plan for Today

- Last time:
  - Prediction-based word vectors
  - Skip-gram with negative sampling [model + loss]
- Today: intro to feed-forward neural networks
  - Basic computation + expressive power
  - Multilayer perceptrons
  - Mini-batches
  - Hyper-parameters and regularization

Computation: Basic Example

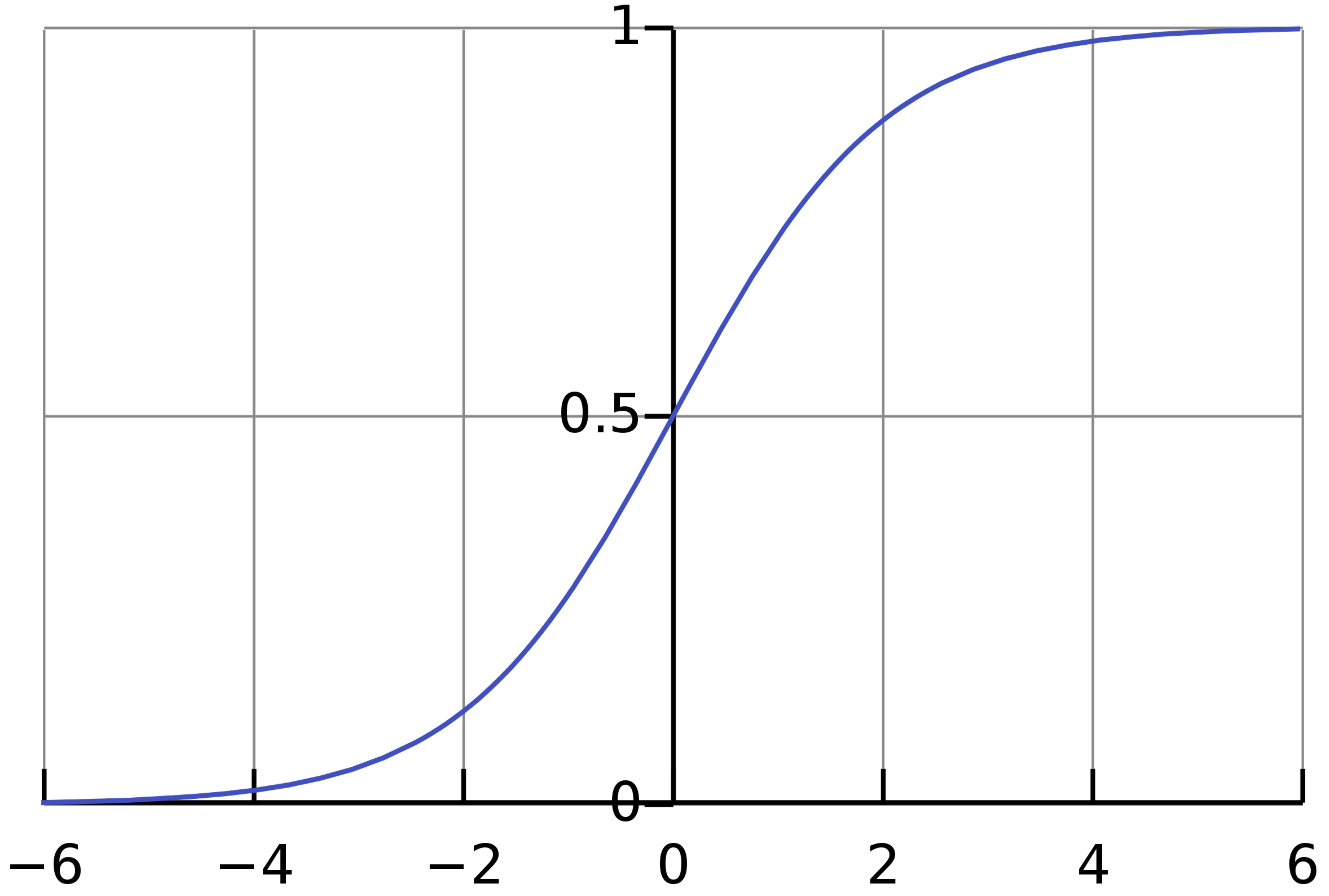
Artificial Neuron



$$a = f(a_0 \cdot w_0 + a_1 \cdot w_1 + a_2 \cdot w_2)$$

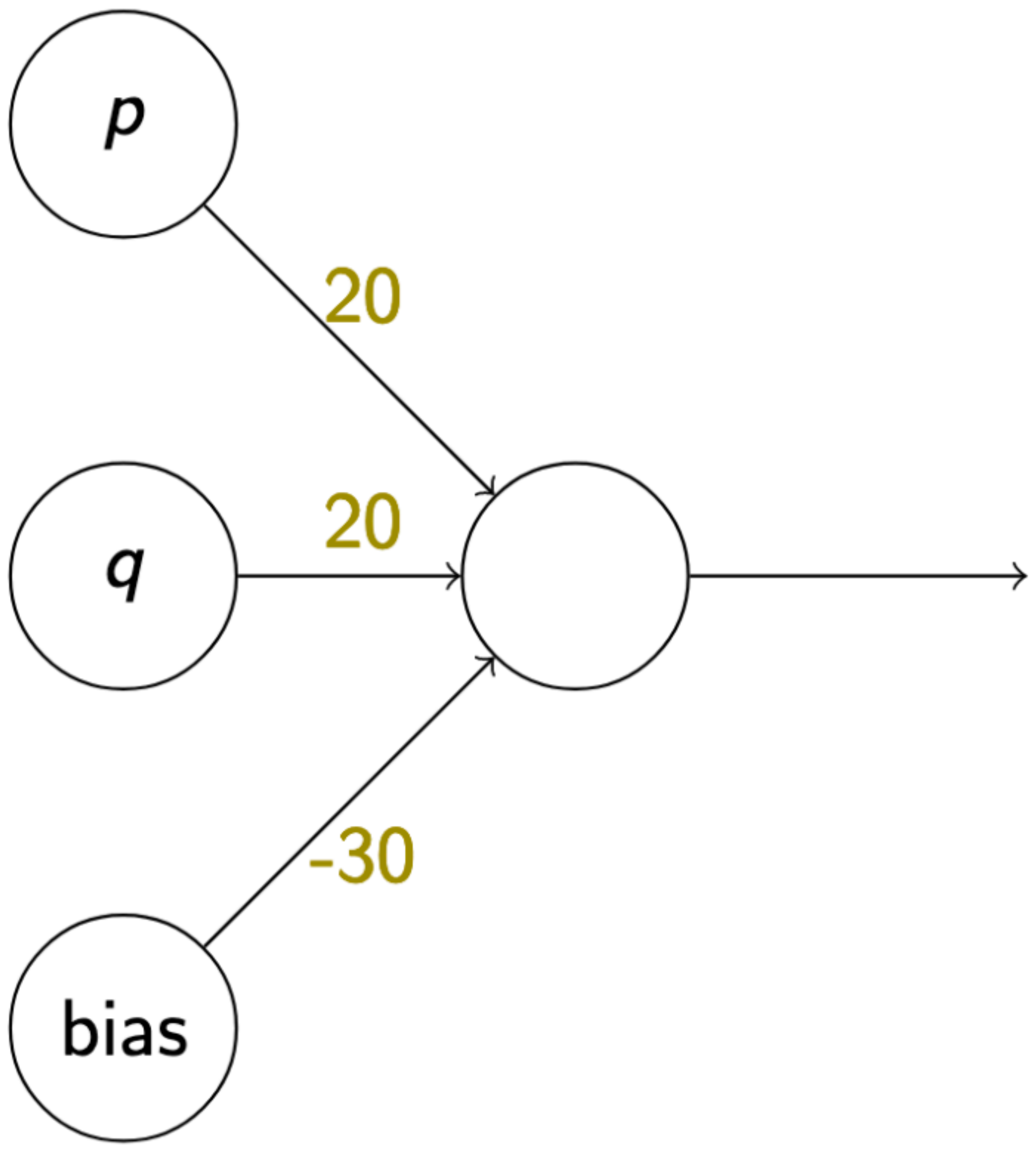
https://github.com/shanest/nn-tutorial

Activation Function: Sigmoid



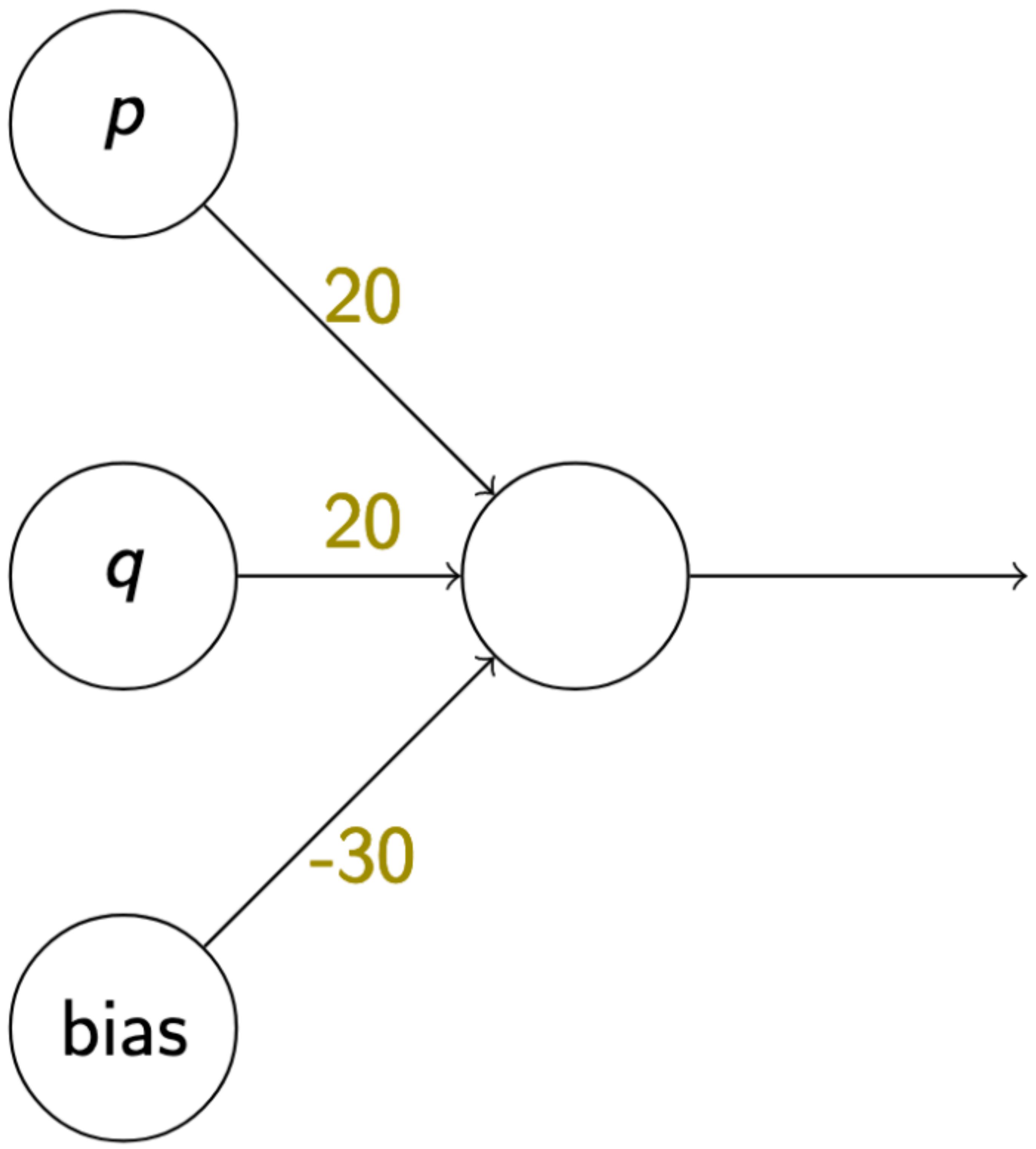
$$\sigma(x) = \frac{1}{1 + e^{-x}} = \frac{e^x}{e^x + 1}$$

Computing a Boolean function



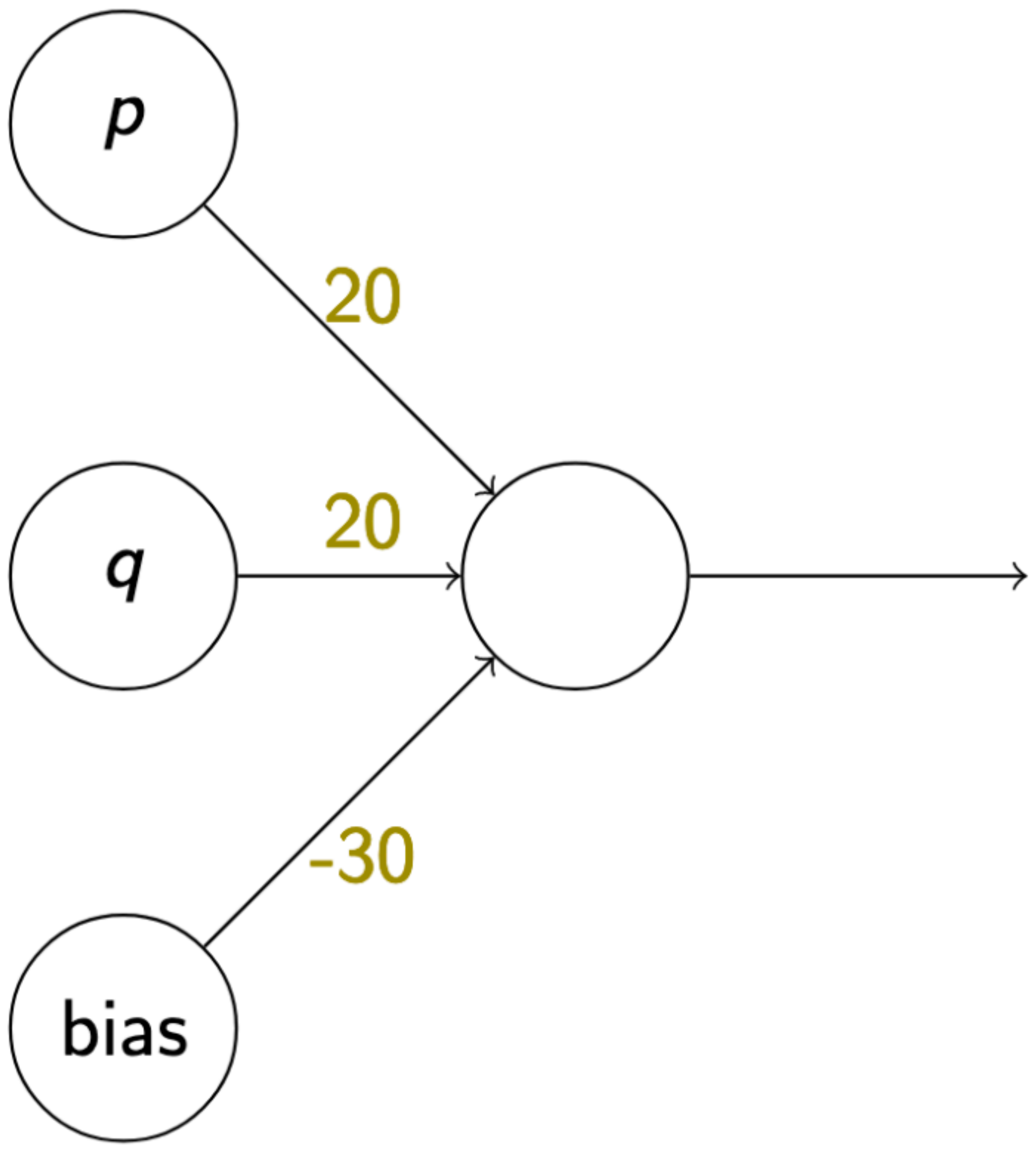
Computing a Boolean function

p	q	a



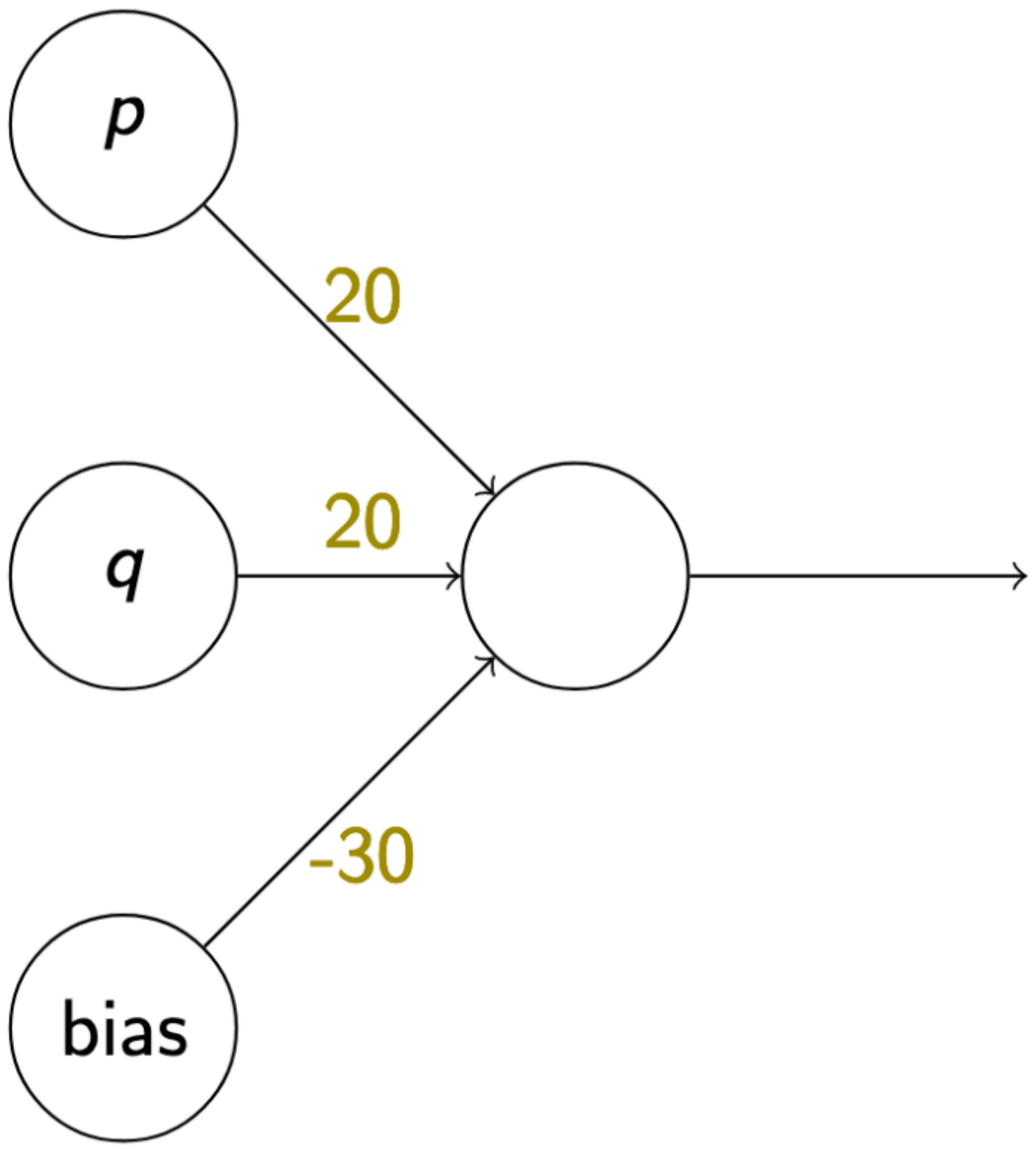
Computing a Boolean function

p	q	a
1	1	1



Computing a Boolean function

p	q	a
1	1	1
1	0	0



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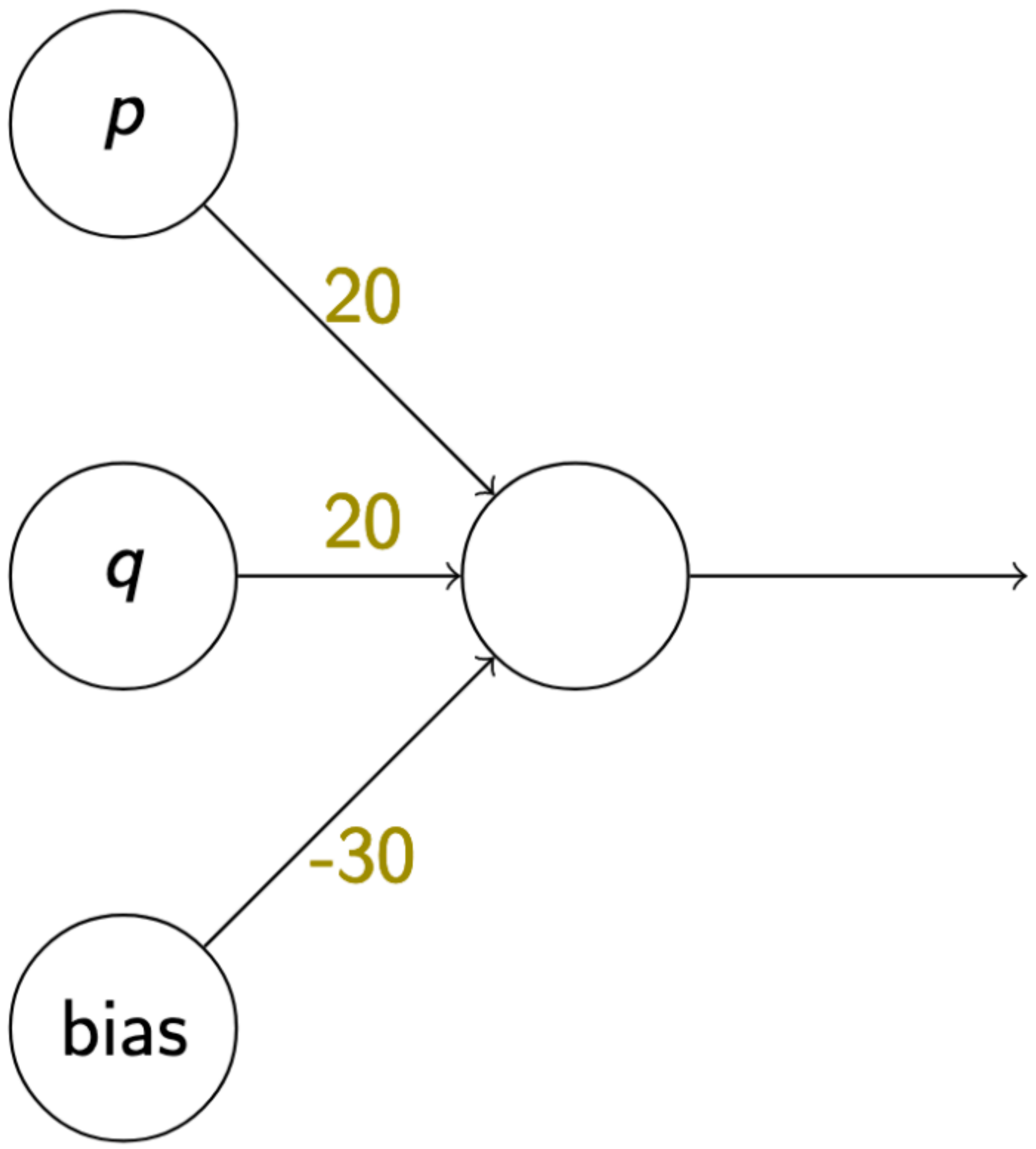

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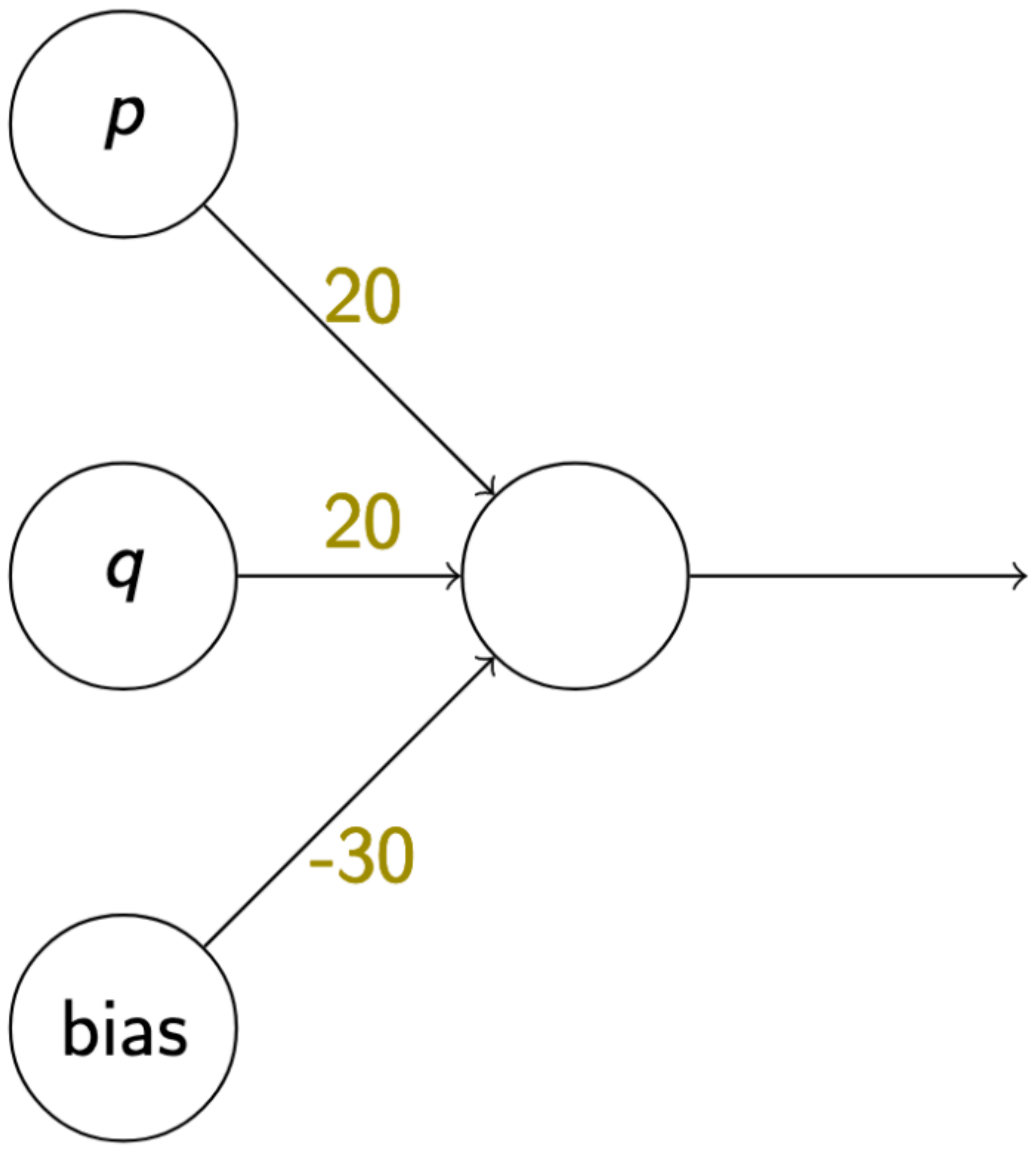
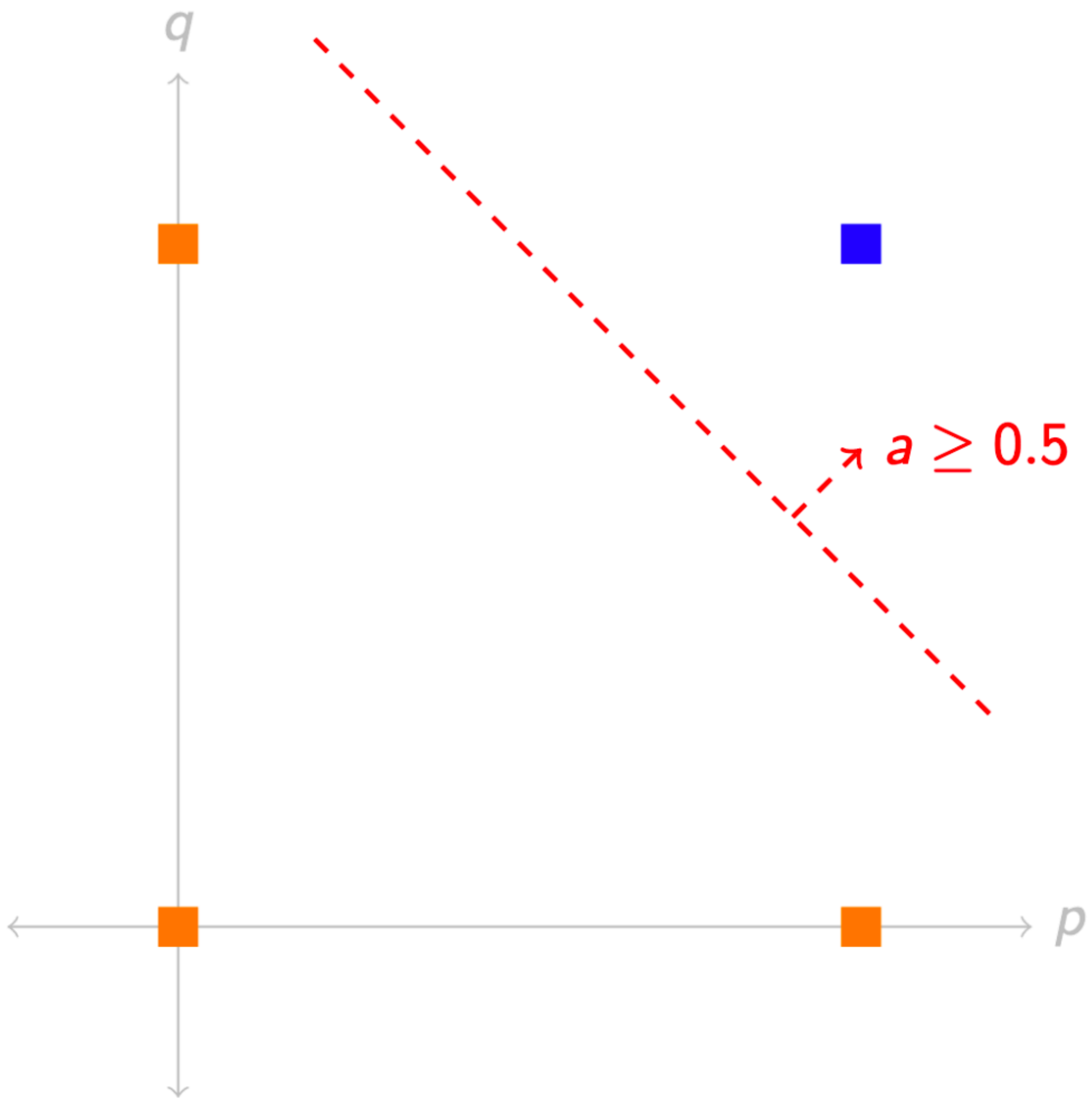
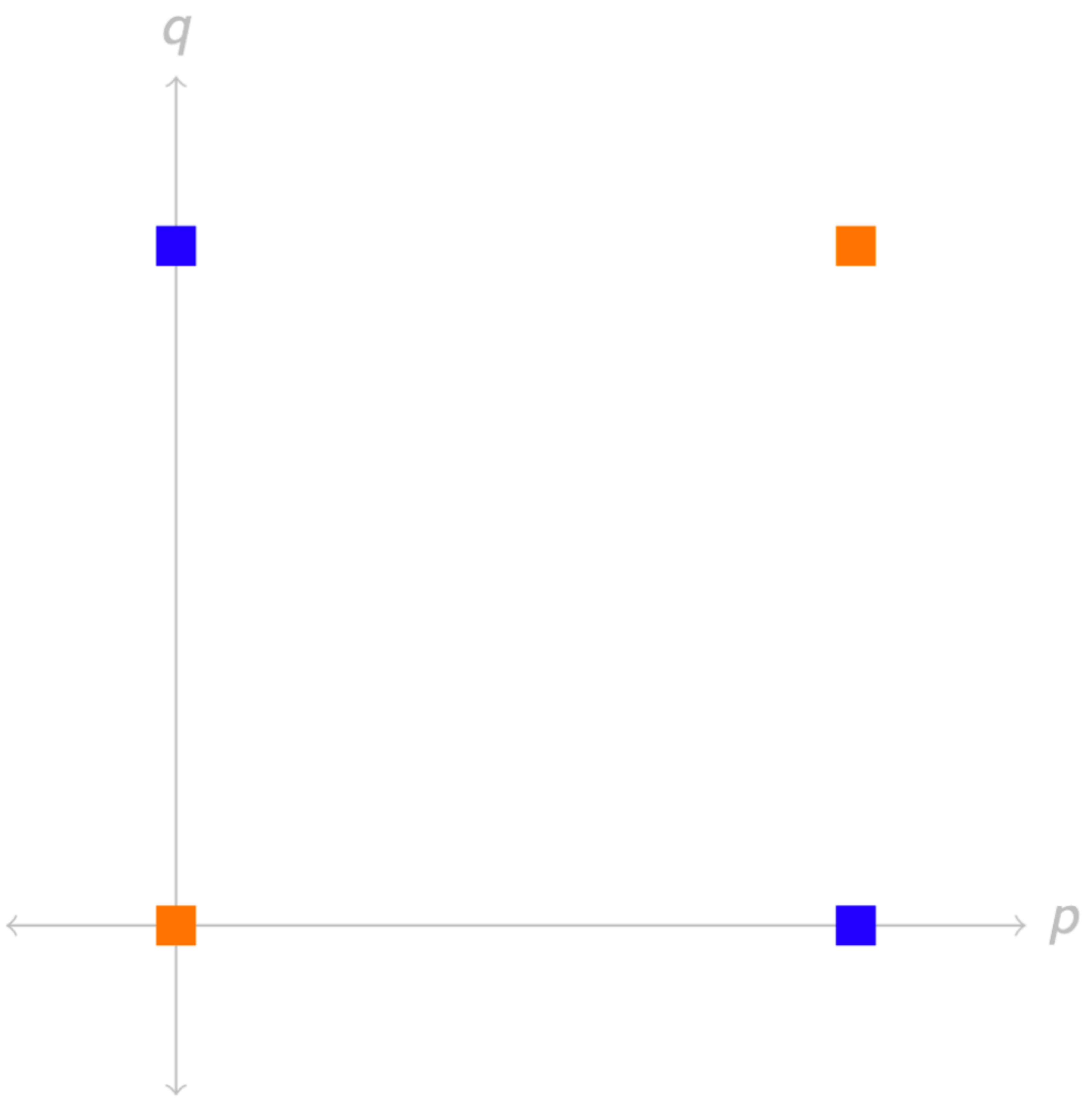


Computing 'and'



The XOR problem



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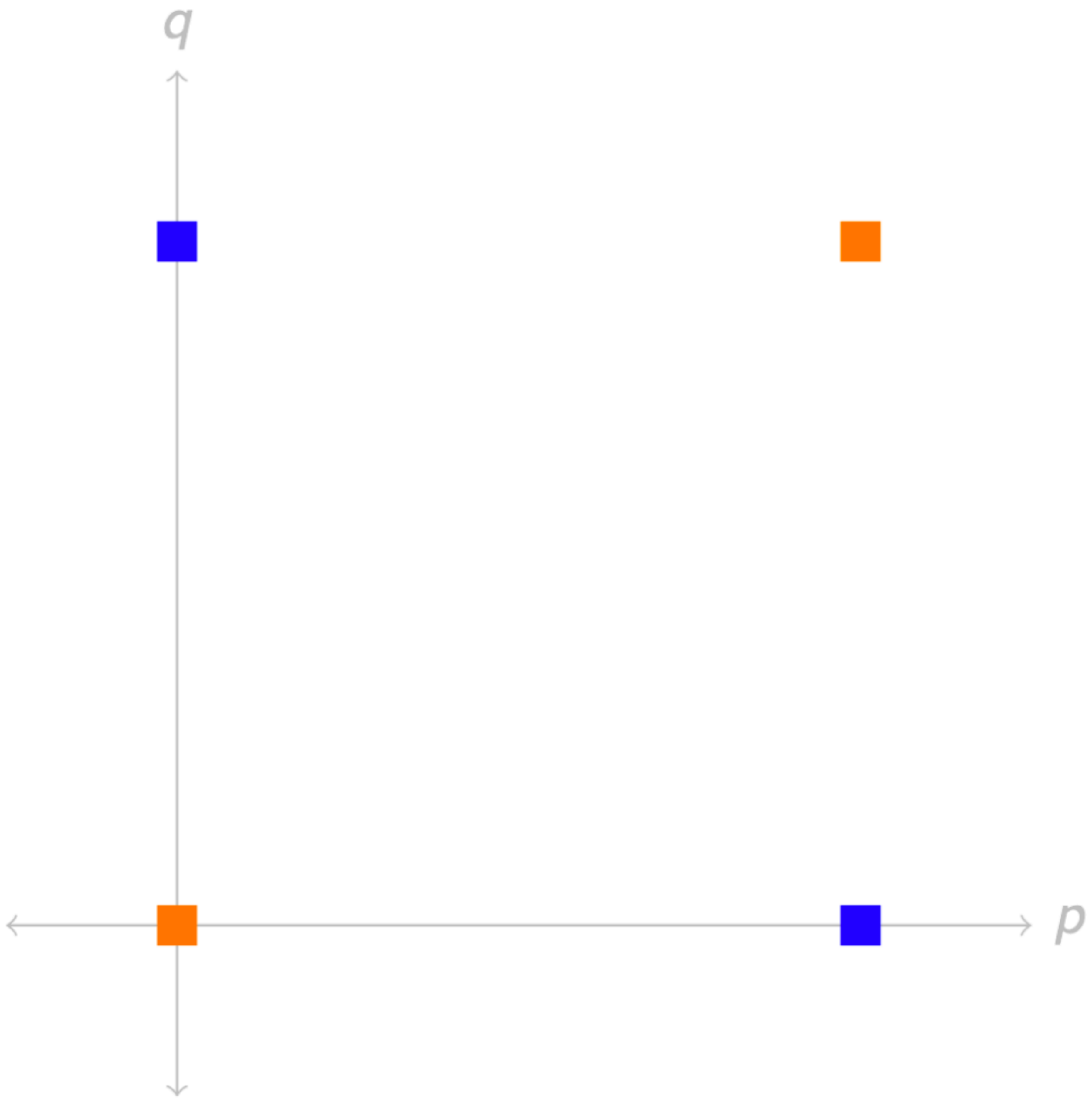
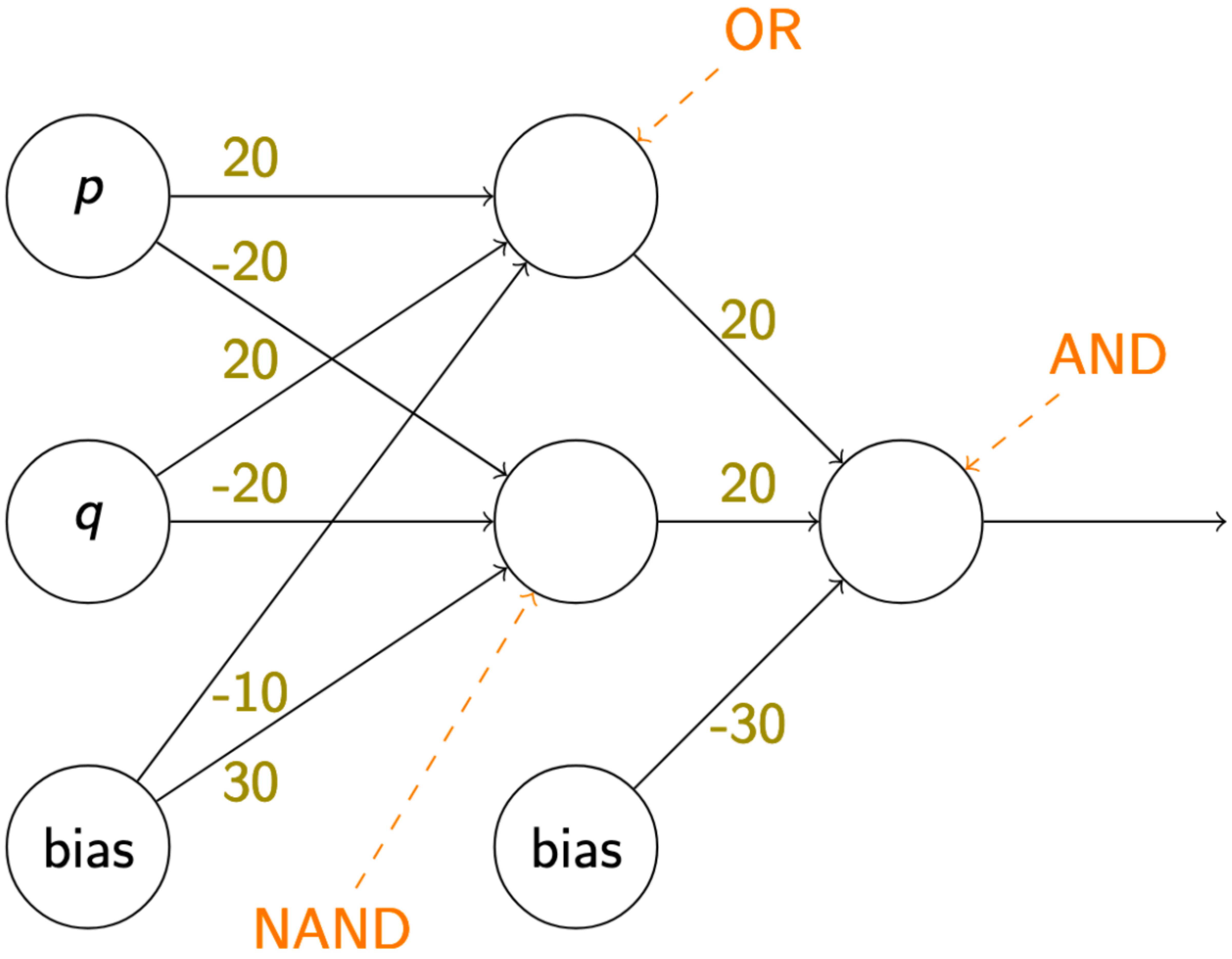


XOR is not linearly separable

Computing XOR



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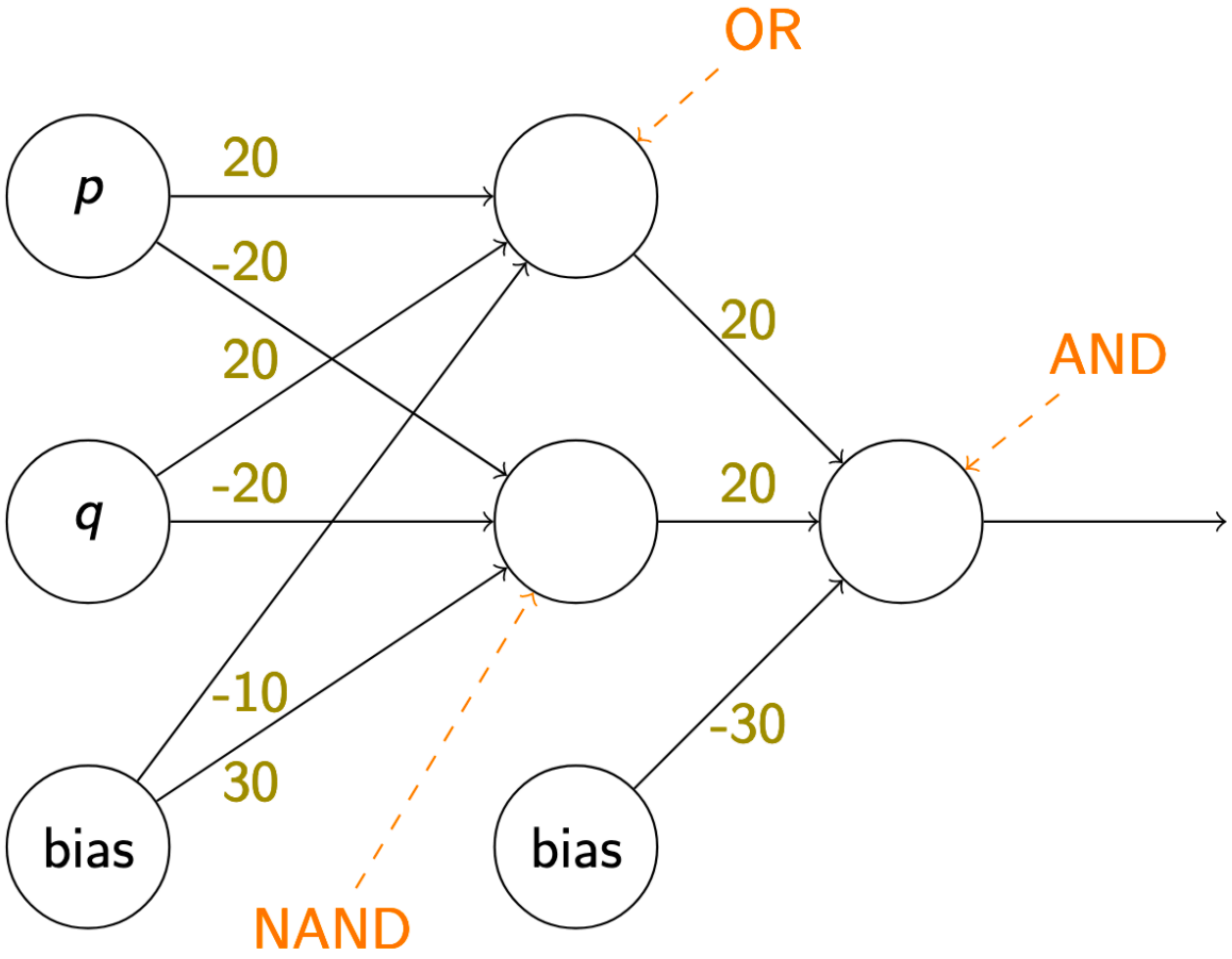
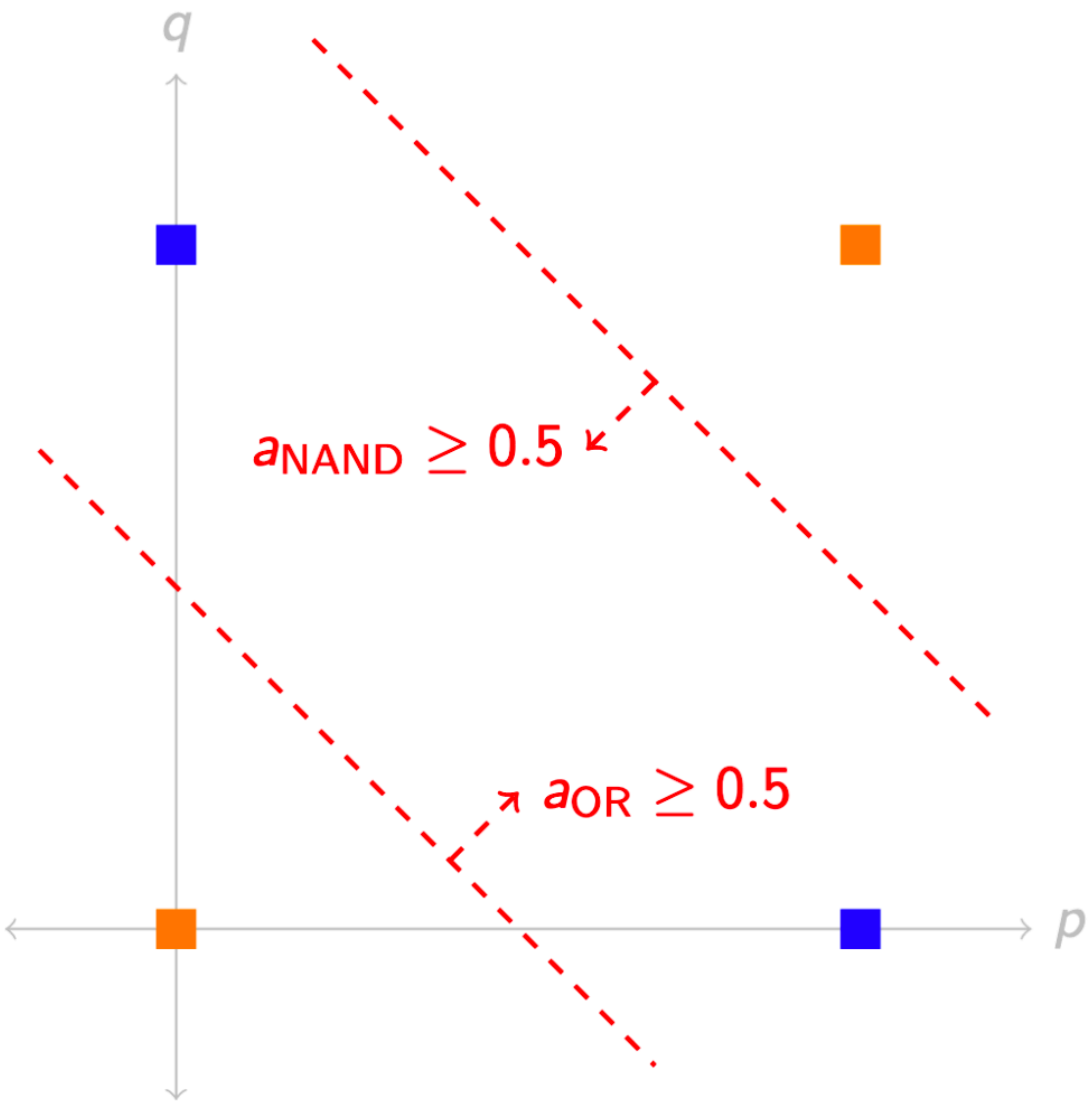


Exercise: show that
NAND behaves as described.

Computing XOR



Key Ideas

- Hidden layers compute high-level / abstract features of the input
  - Via training, will *learn which features* are helpful for a given task
  - Caveat: doesn't always learn much more than shallow features
- Doing so *increases the expressive power* of a neural network
  - Strictly more functions can be computed with hidden layers than without

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- Let $f : [0,1]^m \to \mathbb{R}$ be continuous and $\epsilon > 0$. Then there is a one-hidden-layer neural network g with sigmoid activation such that $|f(\mathbf{x}) - g(\mathbf{x})| < \epsilon$ for all $\mathbf{x} \in [0,1]^m$.

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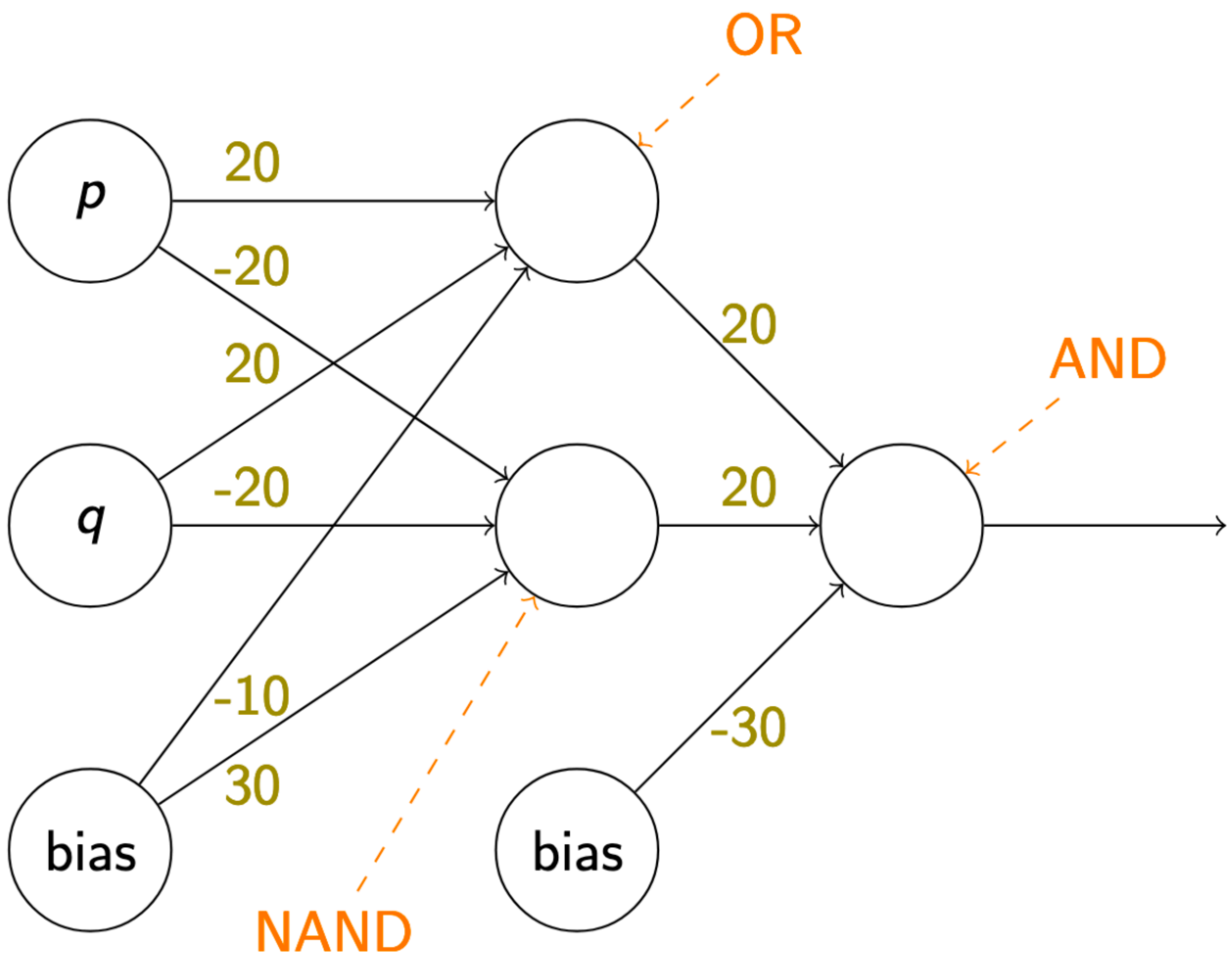
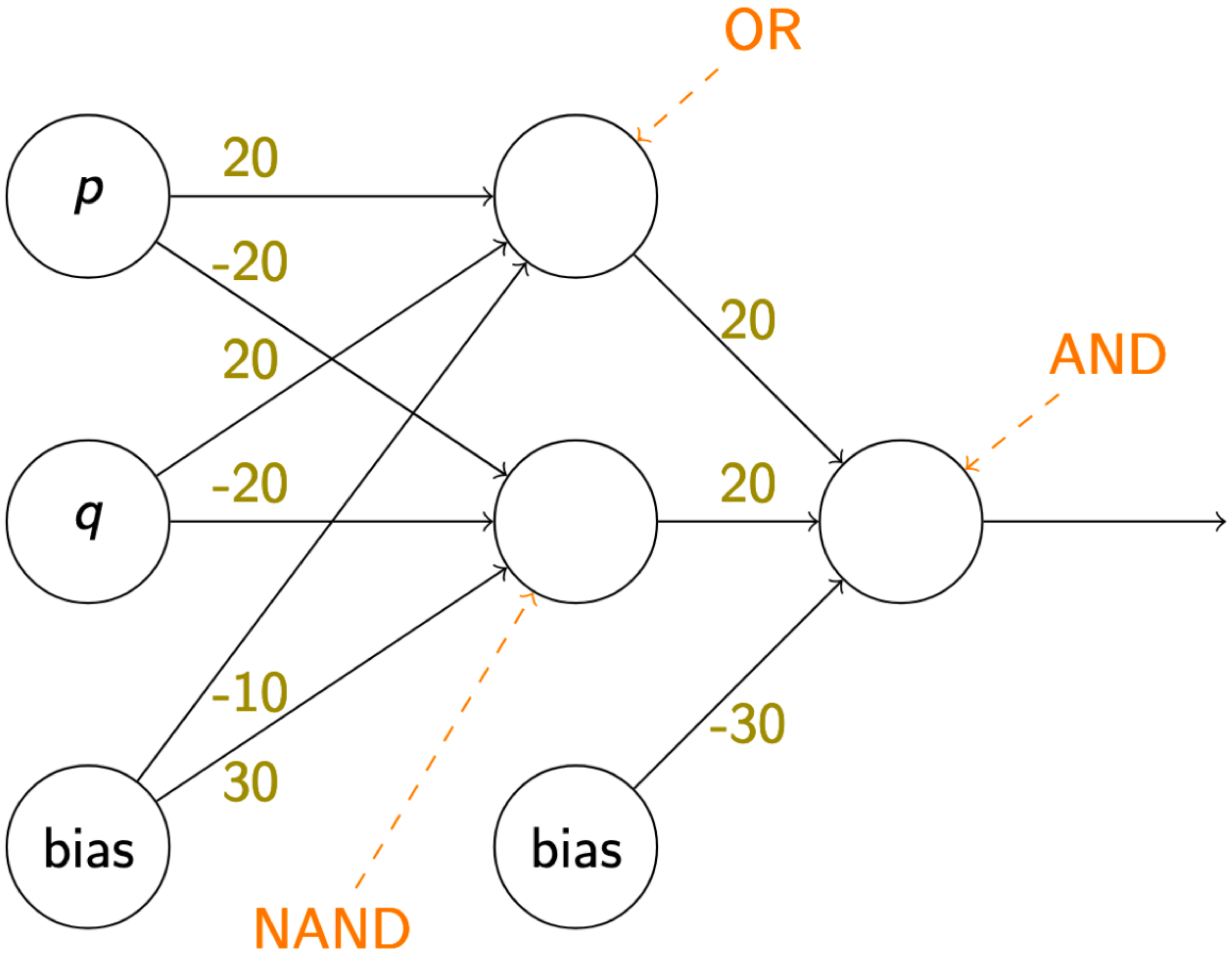
- Nice walkthrough: http://neuralnetworksanddeeplearning.com/chap4.html

Feed-forward networks
aka Multi-layer perceptrons (MLP)

XOR Network

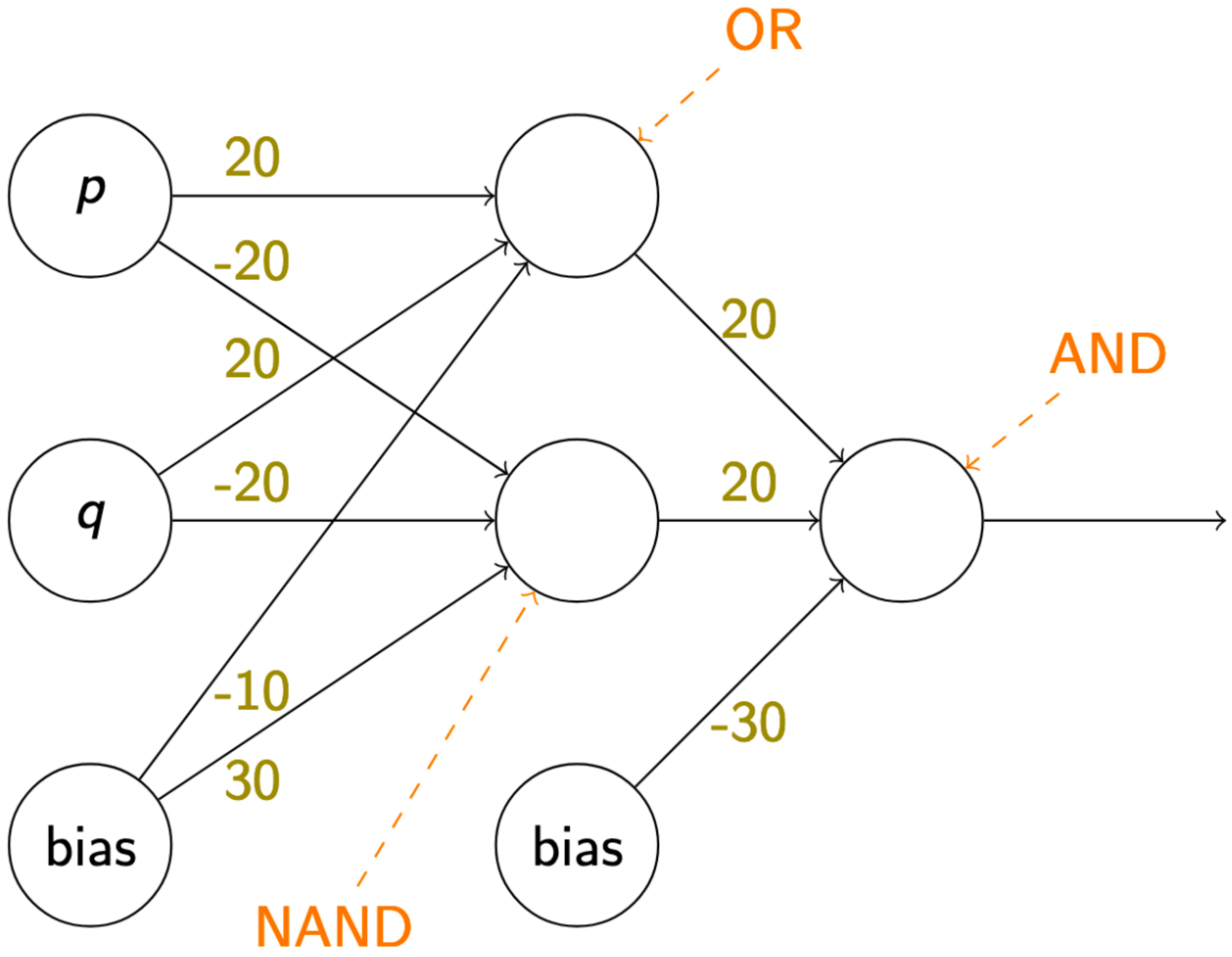


XOR Network



$$a_{\text{and}} = \sigma\left(w^{\text{and}}_{\text{or}} \cdot a_{\text{or}} + w^{\text{and}}_{\text{nand}} \cdot a_{\text{nand}} + b^{\text{and}}\right)$$

XOR Network



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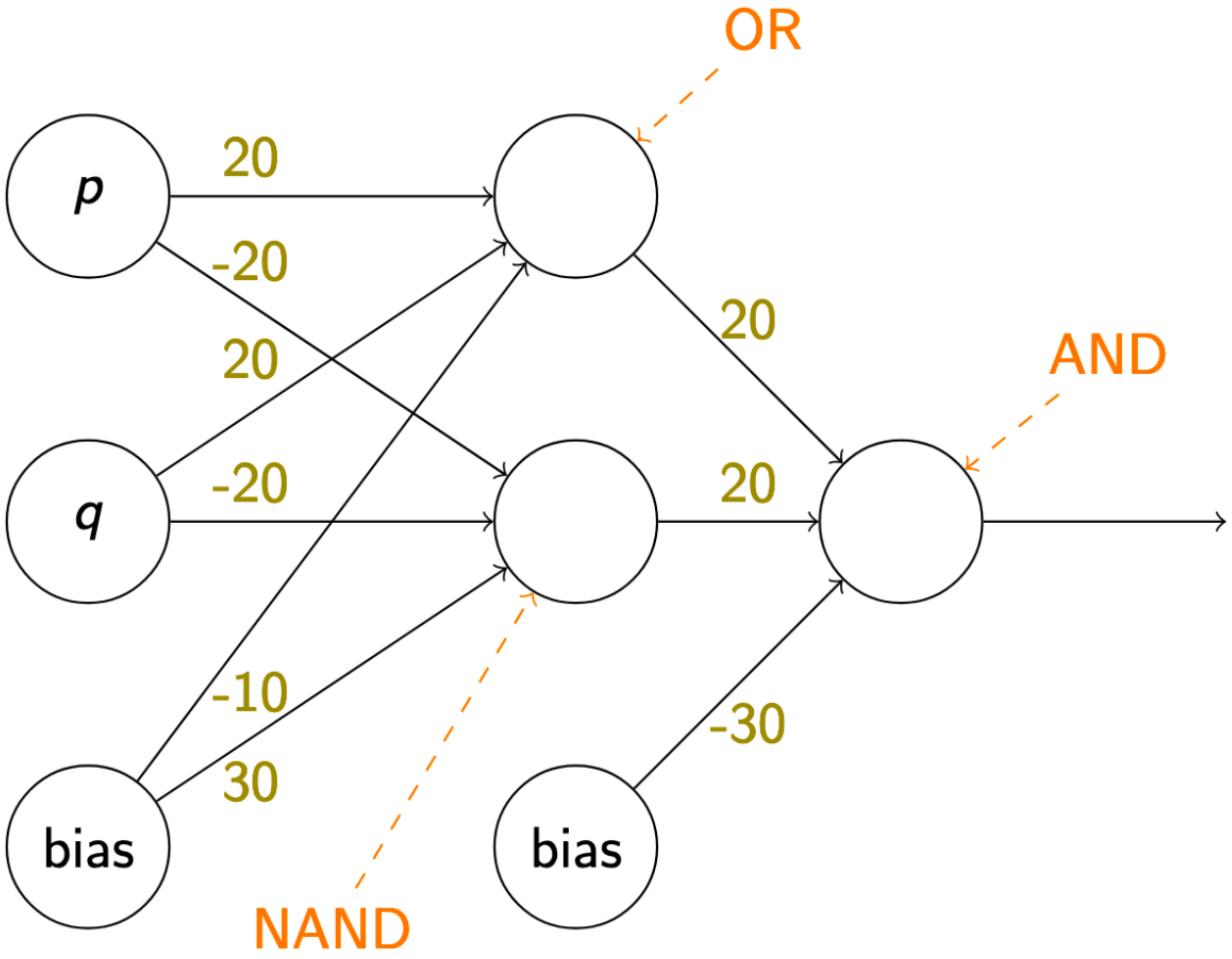

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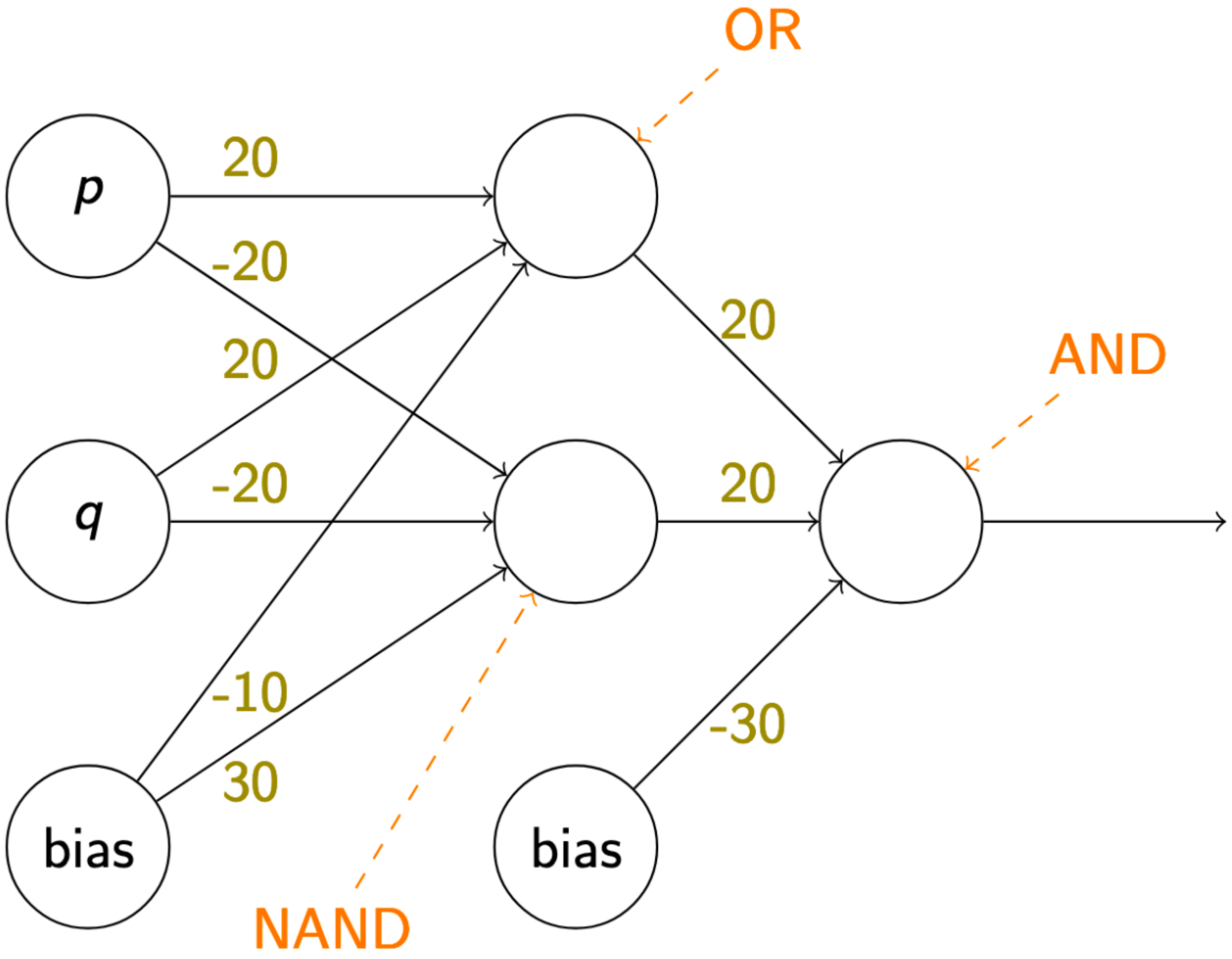

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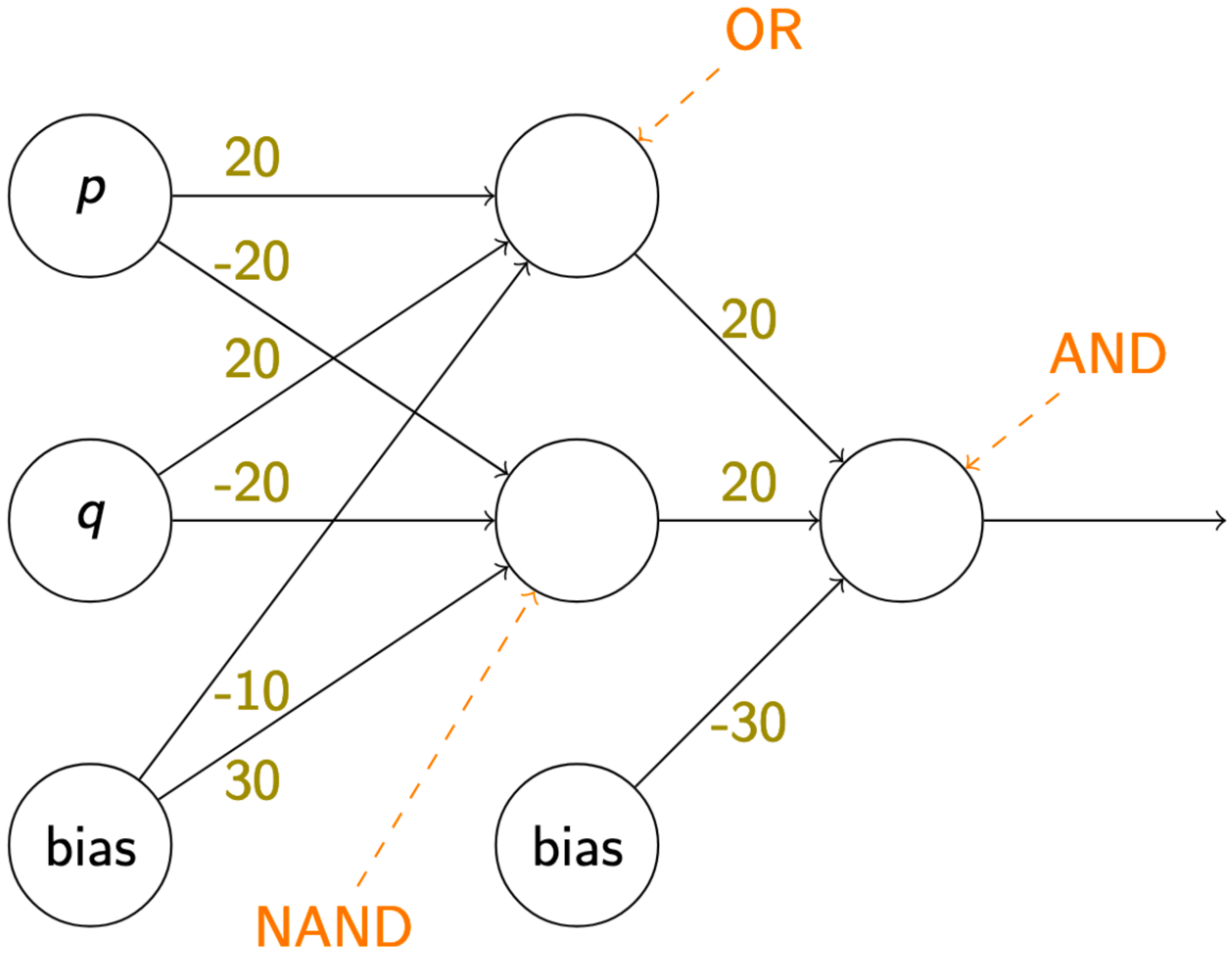
$$a_{\text{or}} = \sigma\left(w^{\text{or}}_{p} \cdot a_p + w^{\text{or}}_{q} \cdot a_q + b^{\text{or}}\right)$$

XOR Network



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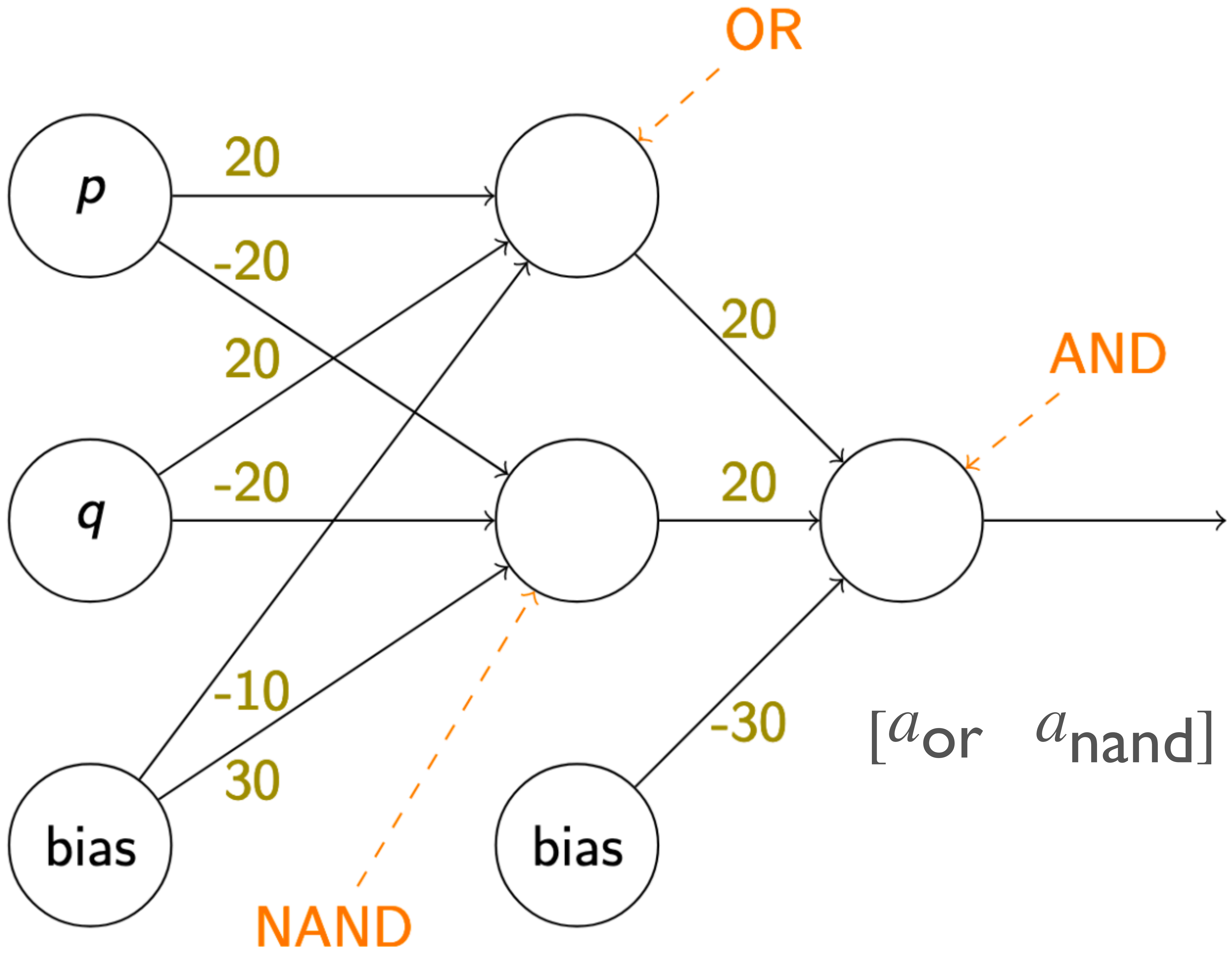
XOR Network



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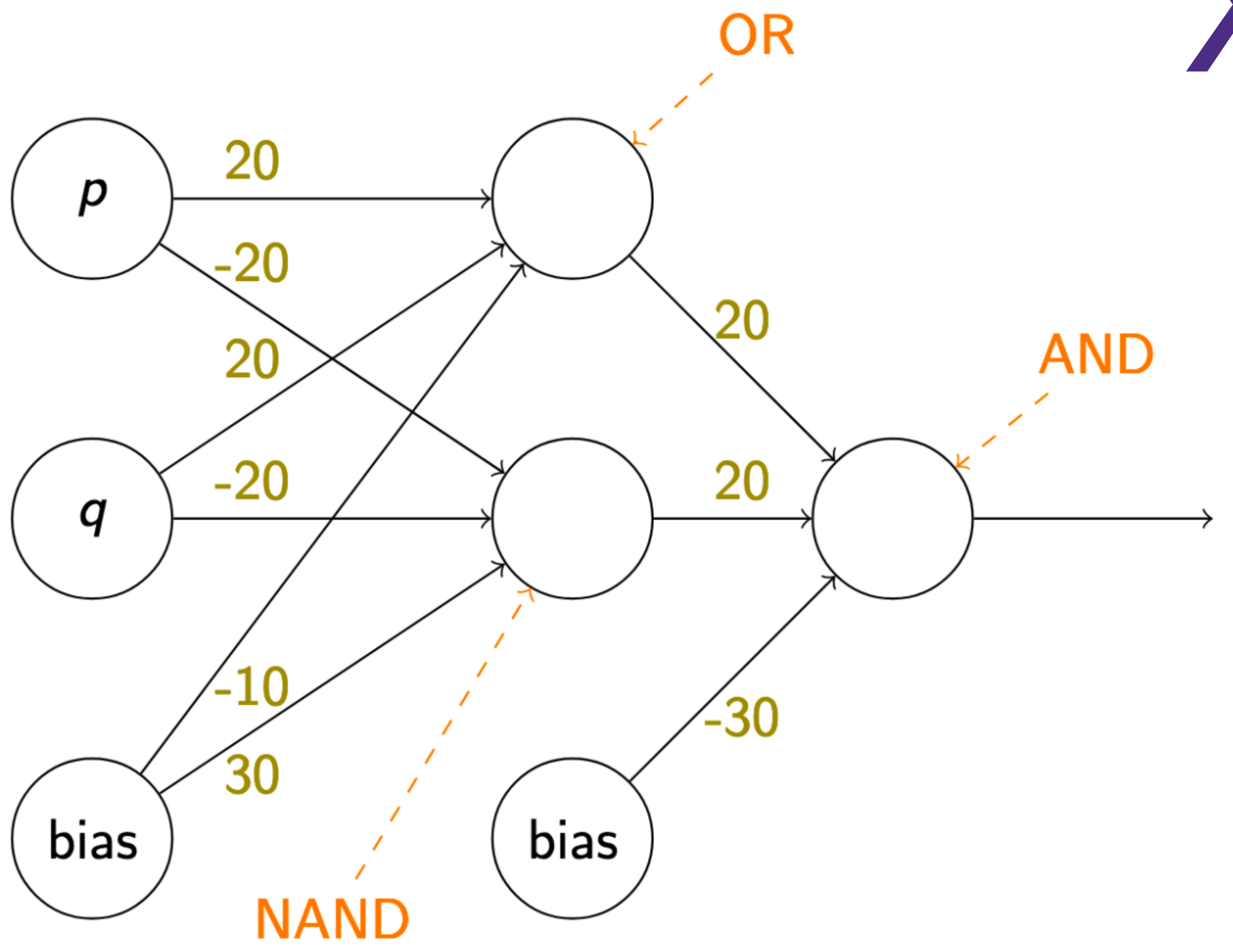
$$\begin{bmatrix} a_{\text{or}} & a_{\text{nand}} \end{bmatrix} = \sigma\left(\begin{bmatrix} a_p & a_q \end{bmatrix} \begin{bmatrix} w^{\text{or}}_p & w^{\text{nand}}_p \\ w^{\text{or}}_q & w^{\text{nand}}_q \end{bmatrix} + \begin{bmatrix} b^{\text{or}} & b^{\text{nand}} \end{bmatrix}\right)$$

XOR Network



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$$a_{\text{and}} = \sigma\left(\sigma\left(\begin{bmatrix} a_p & a_q \end{bmatrix} \begin{bmatrix} w^{\text{or}}_p & w^{\text{nand}}_p \\ w^{\text{or}}_q & w^{\text{nand}}_q \end{bmatrix} + \begin{bmatrix} b^{\text{or}} & b^{\text{nand}} \end{bmatrix}\right) \begin{bmatrix} w^{\text{and}}_{\text{or}} \\ w^{\text{and}}_{\text{nand}} \end{bmatrix} + b^{\text{and}}\right)$$

Generalizing

$$a_{\text{and}} = \sigma\left(\sigma\left(\begin{bmatrix} a_p & a_q \end{bmatrix} \begin{bmatrix} w_p^{\text{or}} & w_p^{\text{nand}} \\ w_q^{\text{or}} & w_q^{\text{nand}} \end{bmatrix} + \begin{bmatrix} b^{\text{or}} & b^{\text{nand}} \end{bmatrix}\right) \begin{bmatrix} w_{\text{or}}^{\text{and}} \\ w_{\text{nand}}^{\text{and}} \end{bmatrix} + b^{\text{and}}\right)$$

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$$\hat{y} = f_2\left(f_1\left(xW^1 + b^1\right)W^2 + b^2\right)$$

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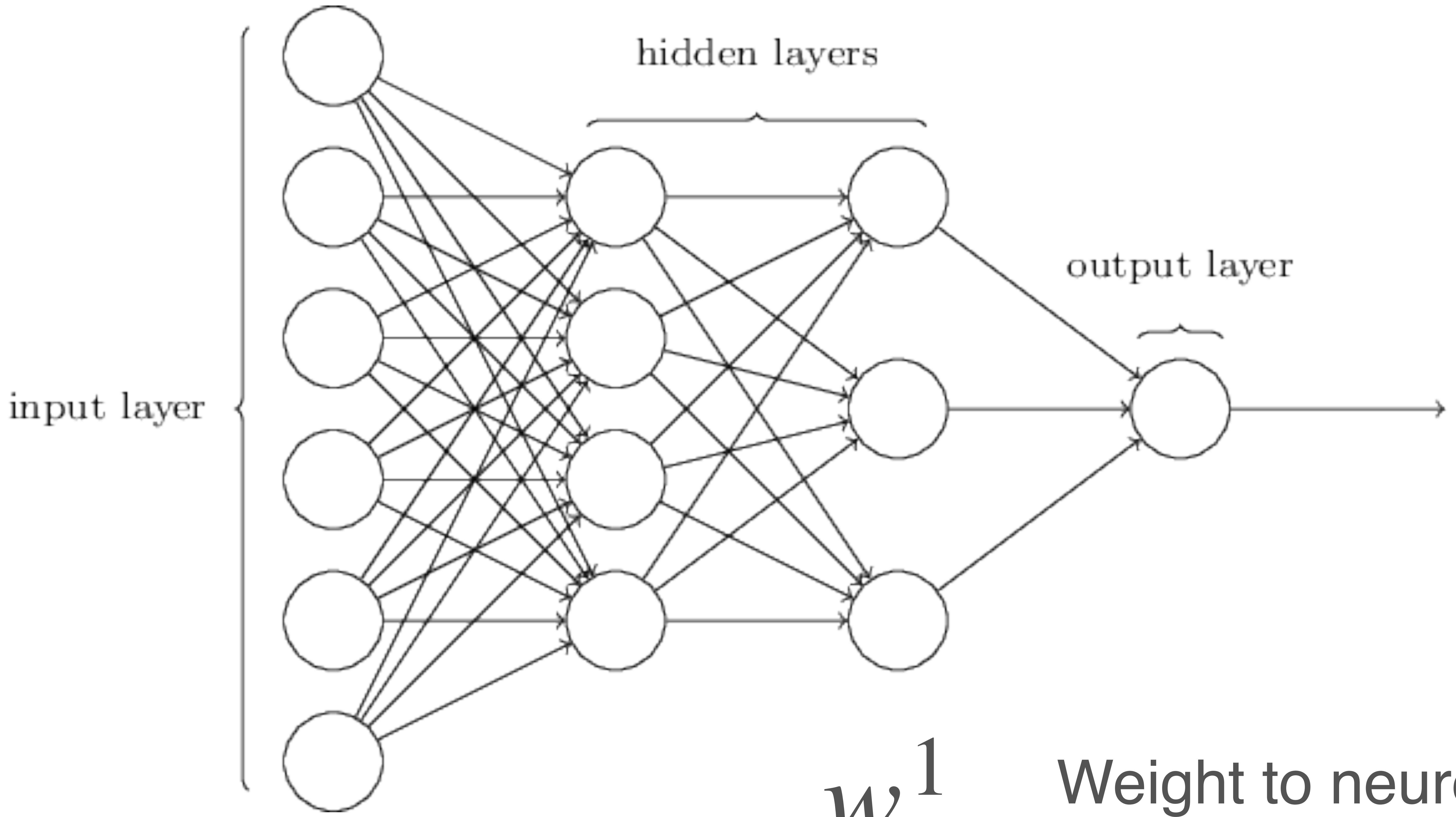
$$\hat{y} = f_n\left(f_{n-1}\left(\cdots f_2\left(f_1\left(xW^1 + b^1\right) W^2 + b^2\right)\cdots\right) W^n + b^n\right)$$

Some terminology

- Our XOR network is a *feed-forward neural network* with *one hidden layer*
  - Aka a multi-layer perceptron (MLP)
- Input nodes: 2; output nodes: 1
- Activation function: sigmoid

General MLP



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$$w_{ij}^{1}$$

Weight to neuron j in layer 1 from neuron i in layer 0

General MLP

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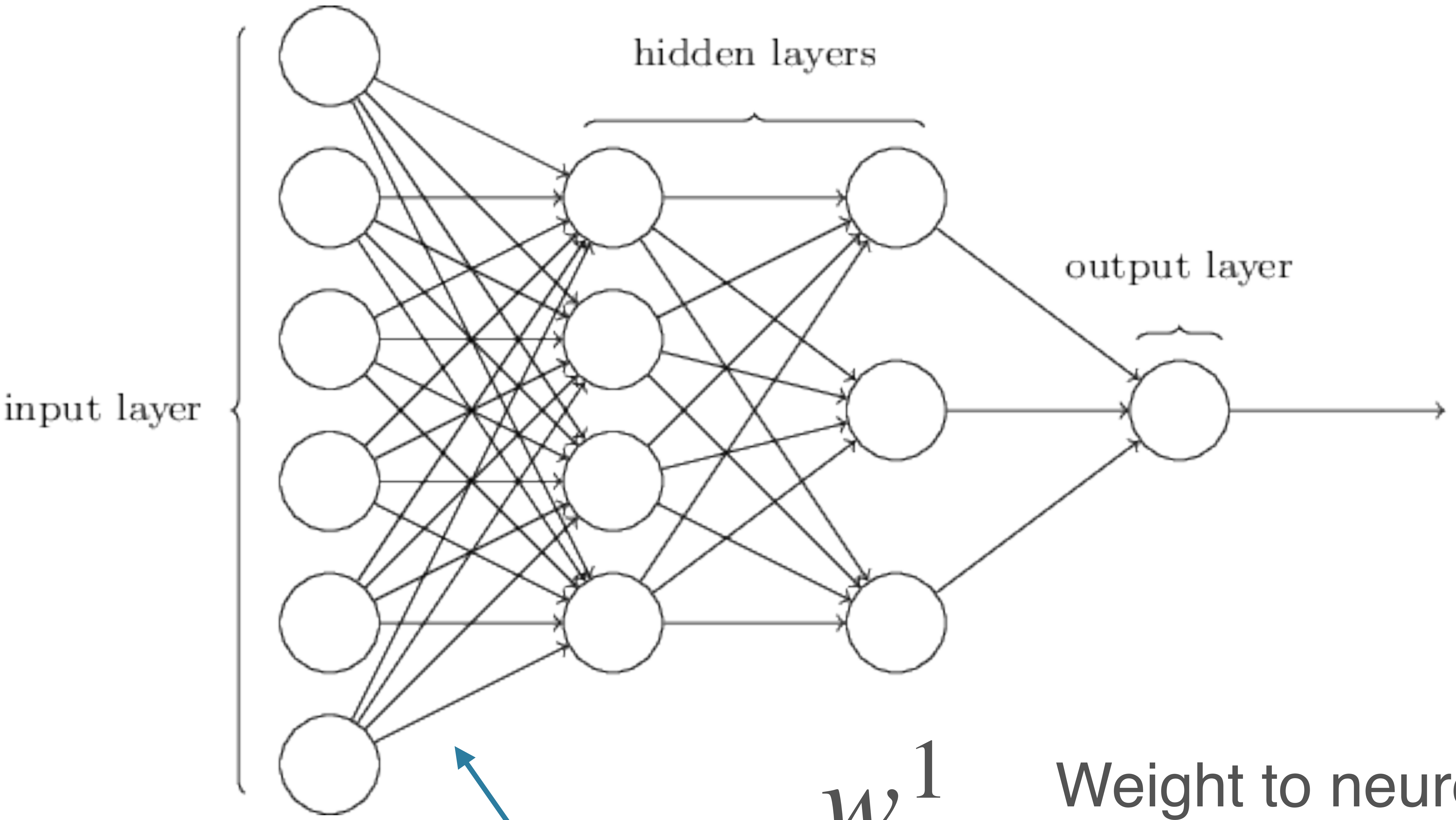

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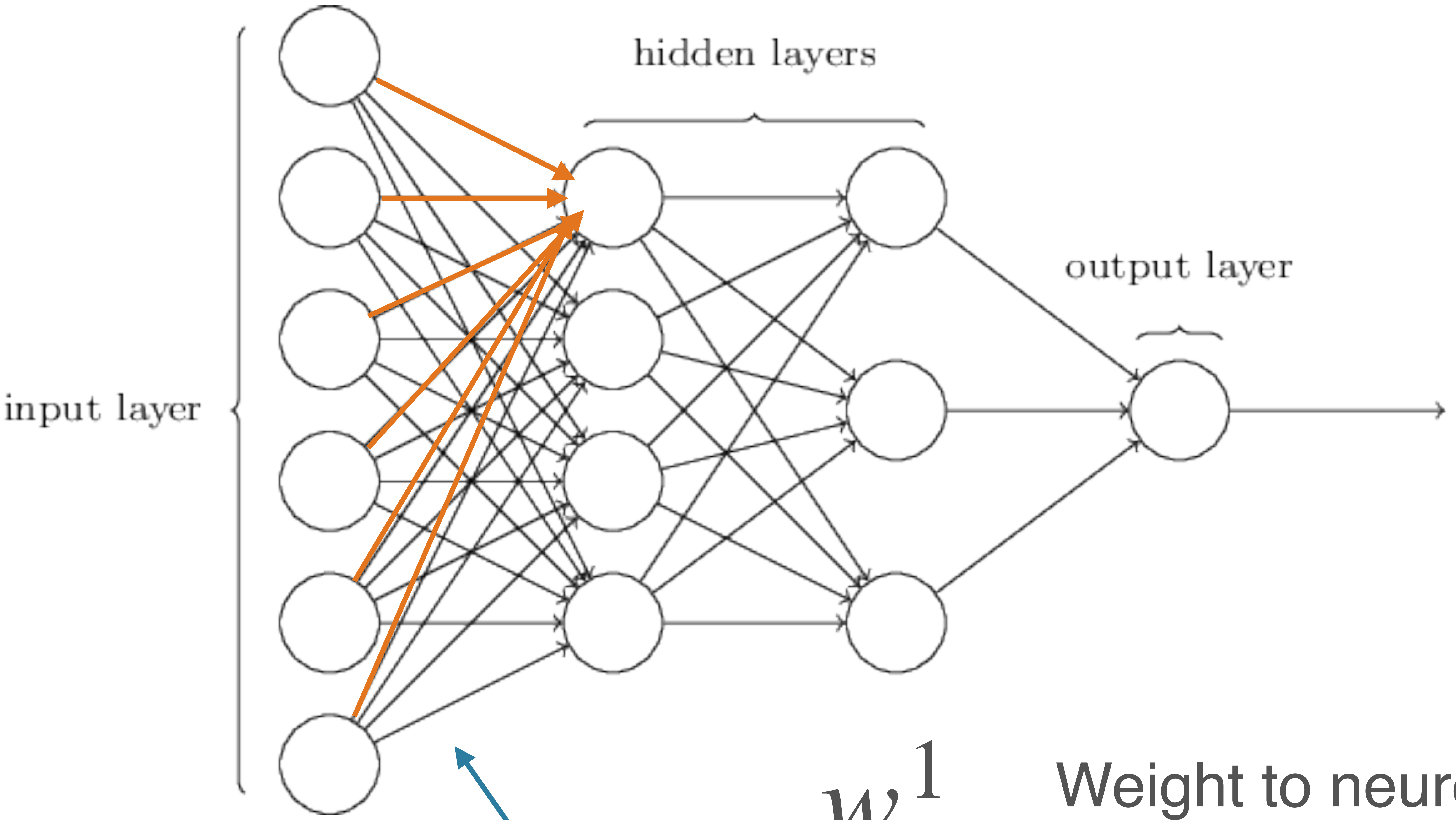

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$$x = \begin{bmatrix} x_0 & x_1 & \cdots & x_{n_0} \end{bmatrix}$$

Shape: $(1, n_0)$

General MLP

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Shape: (n_0, n_1)

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Parameters of an MLP

- Weights and biases
  - For each layer l: $n_l(n_{l-1} + 1)$
  - $n_l n_{l-1}$ weights; n_l biases
- With *n* hidden layers (considering the output as a hidden layer):

$$\sum_{i=1}^{n} n_i(n_{i-1} + 1)$$

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- Input size, output size
  - Usually fixed by your problem / dataset
  - Input: image size, vocab size; number of “raw” features in general
  - Output: 1 for binary classification or simple regression, number of labels for classification, …

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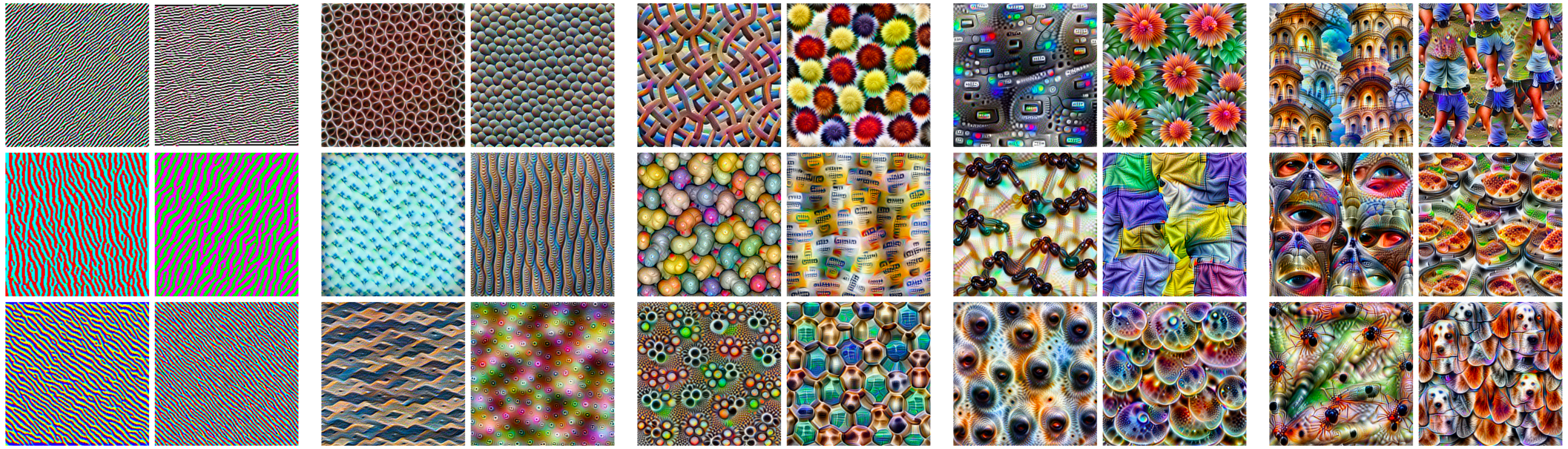
- Others: initialization, regularization (and associated values), learning rate / training, …

The Deep in Deep Learning

- The Universal Approximation Theorem says that one hidden layer suffices for arbitrarily-closely approximating a given function
- Empirical drawbacks: Super-exponentially many neurons; hard to discover
- “Deep and narrow” >> “Shallow and wide”
  - In principle allows hierarchical features to be learned
  - More well-behaved w/r/t optimization



Edges (layer conv2d0) **Textures** (layer mixed3a) **Patterns** (layer mixed4a) **Parts** (layers mixed4b & mixed4c) **Objects** (layers mixed4d & mixed4e)

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Activation Functions

- Note: *non-linear* activation functions are essential
- MLP: linear transformation, followed by a point-wise non-linearity, repeated several times over
- Without the non-linearity, would just have several linear transformations
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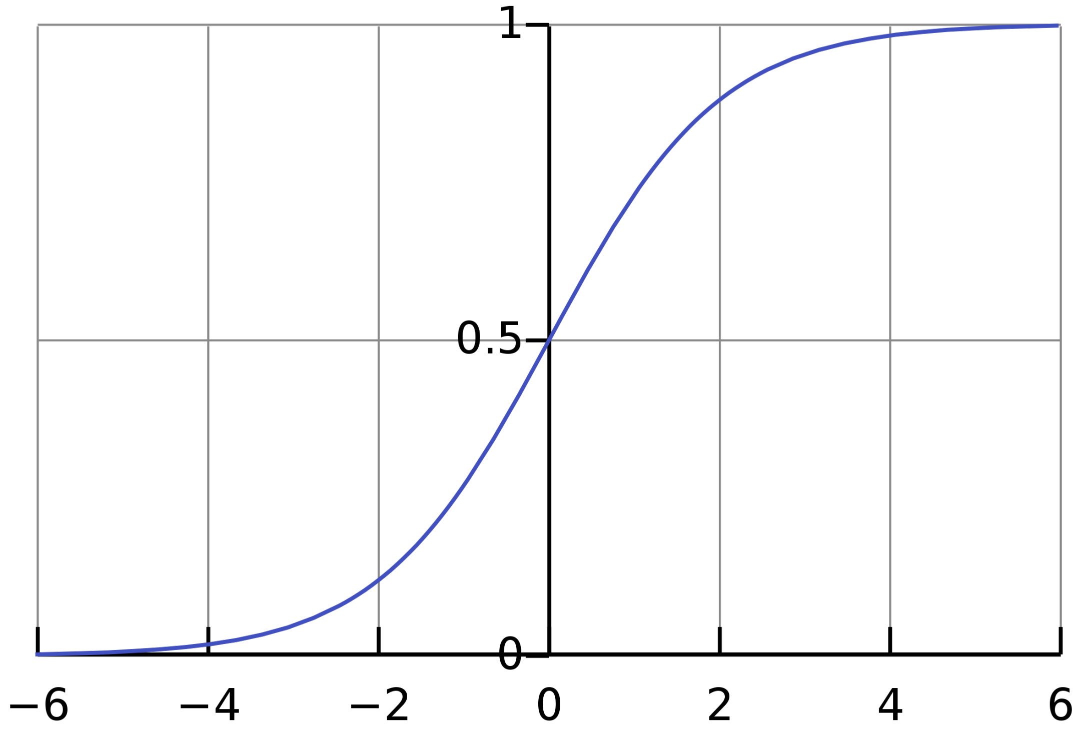
- Without the non-linearity, would just have several linear transformations
  - Composition of linear transformations is *also* linear!

$$\hat{y} = f_n\left(f_{n-1}\left(\cdots f_2\left(f_1\left(xW^1 + b^1\right)W^2 + b^2\right)\cdots\right)W^n + b^n\right)$$

Activation Functions: Hidden Layer

sigmoid



$$\sigma(x) = \frac{1}{1+e^{-x}} = \frac{e^x}{e^x+1}$$

Activation Functions: Hidden Layer

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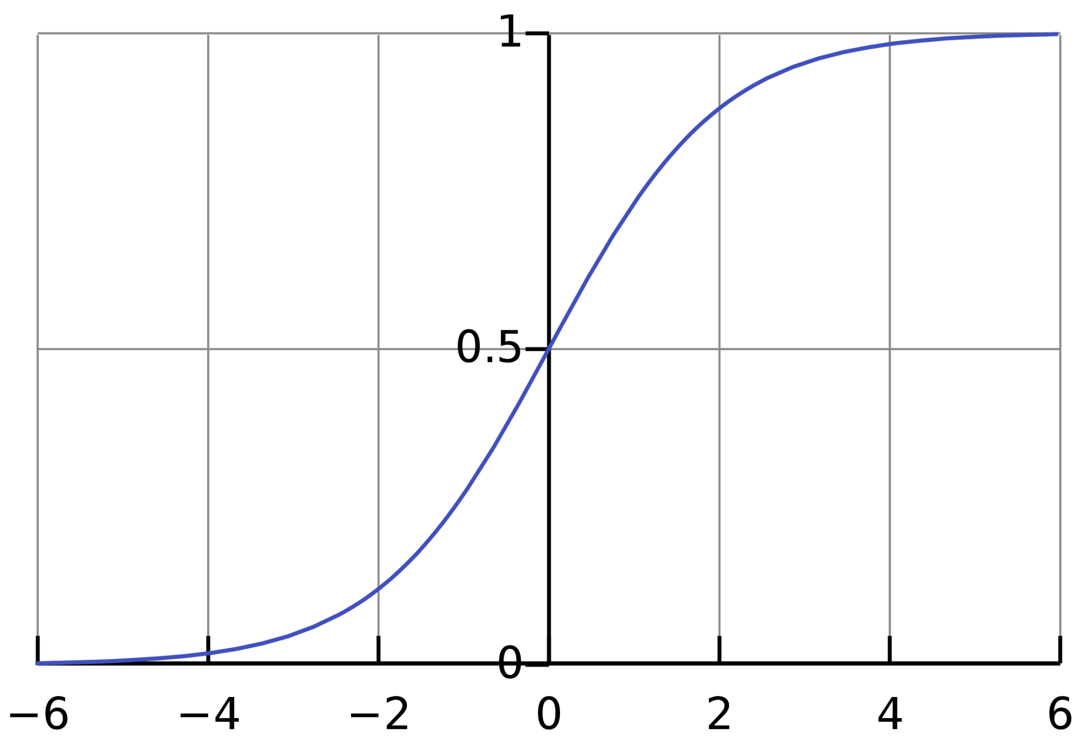

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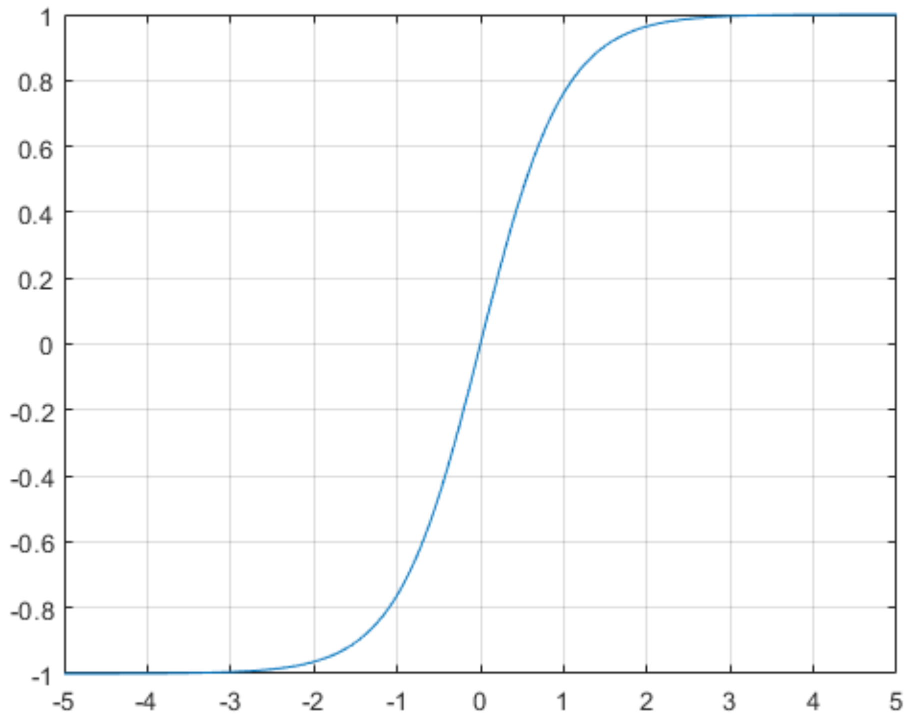

$$\tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}} = 2\sigma(2x) - 1$$

Activation Functions: Hidden Layer

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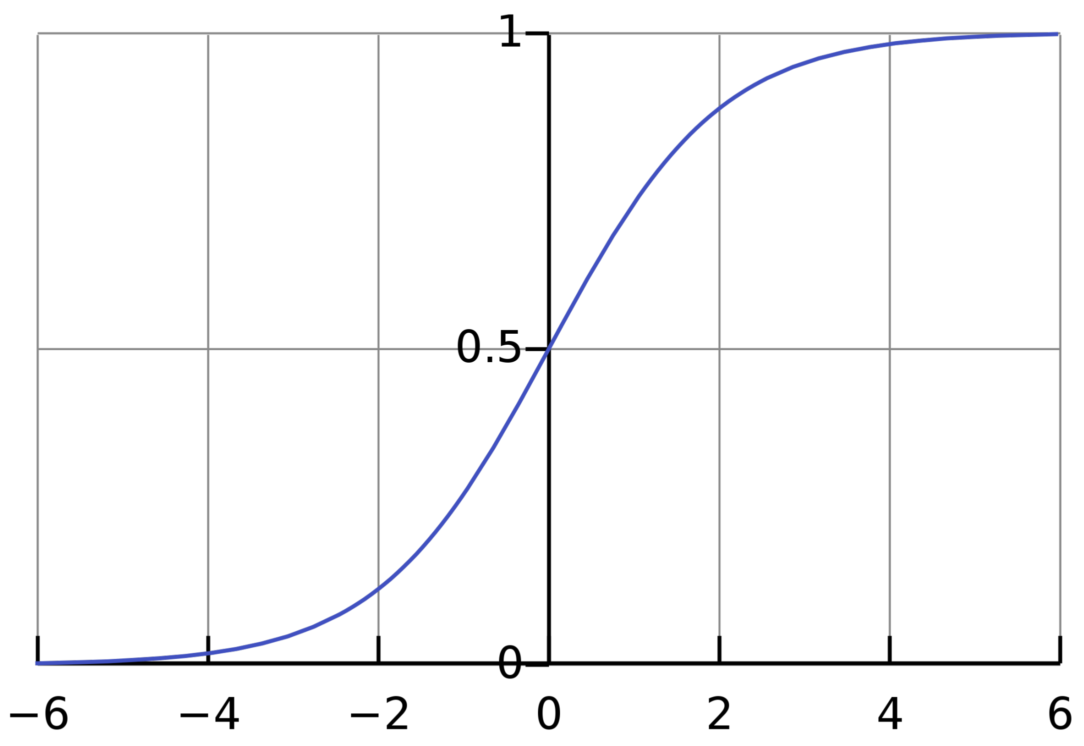

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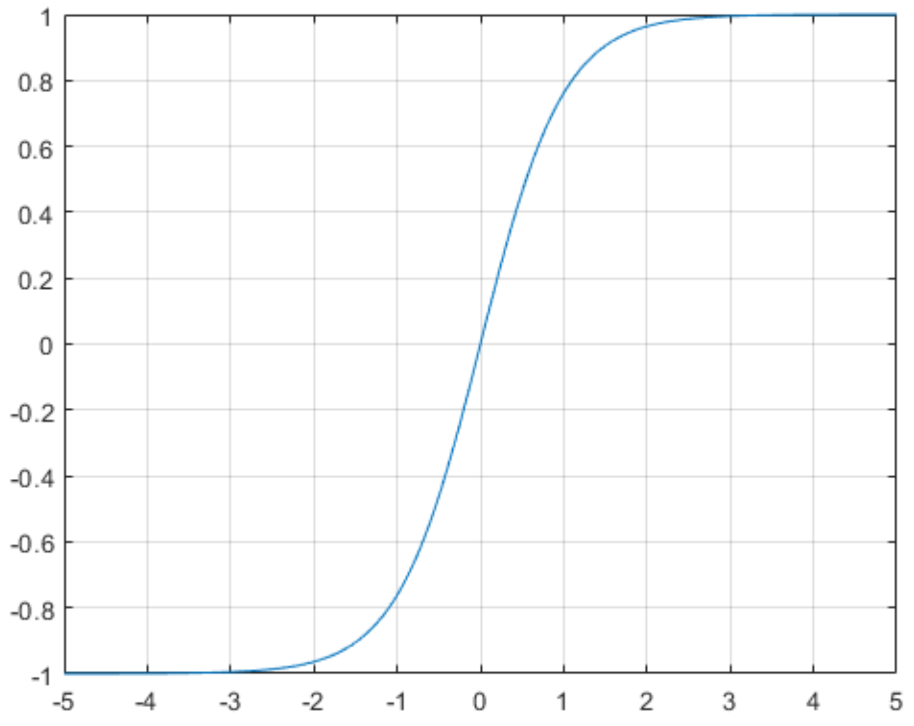

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Problem: derivative “saturates” (nearly 0) everywhere except near origin

Activation Functions: Hidden Layer

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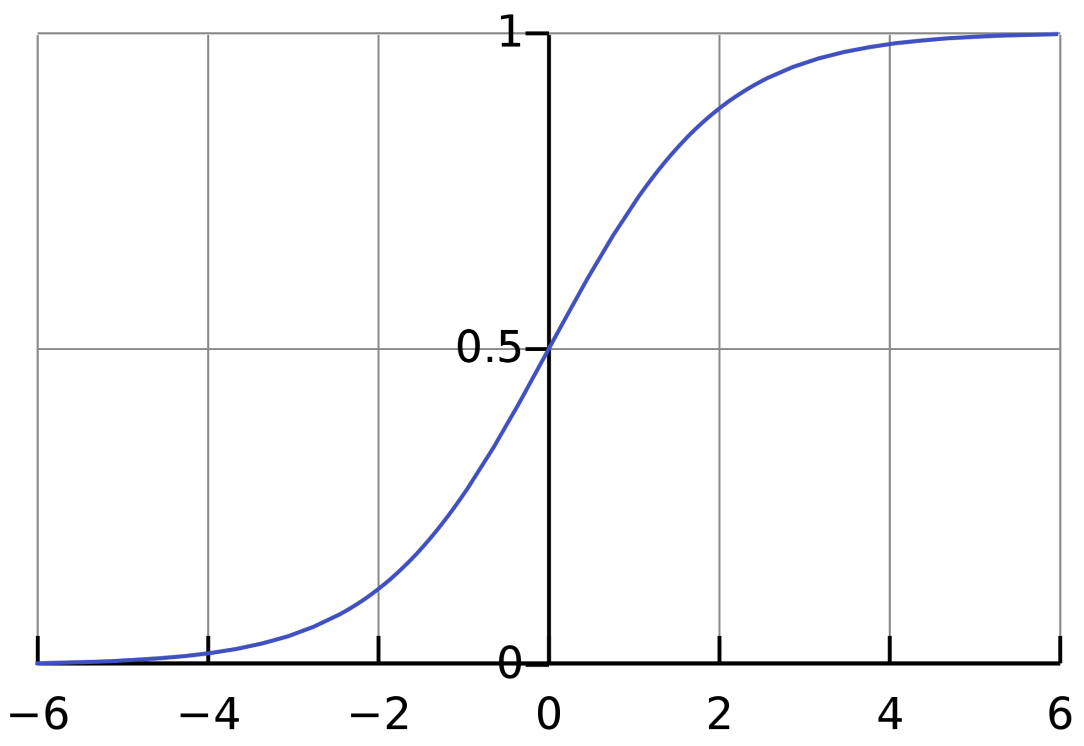

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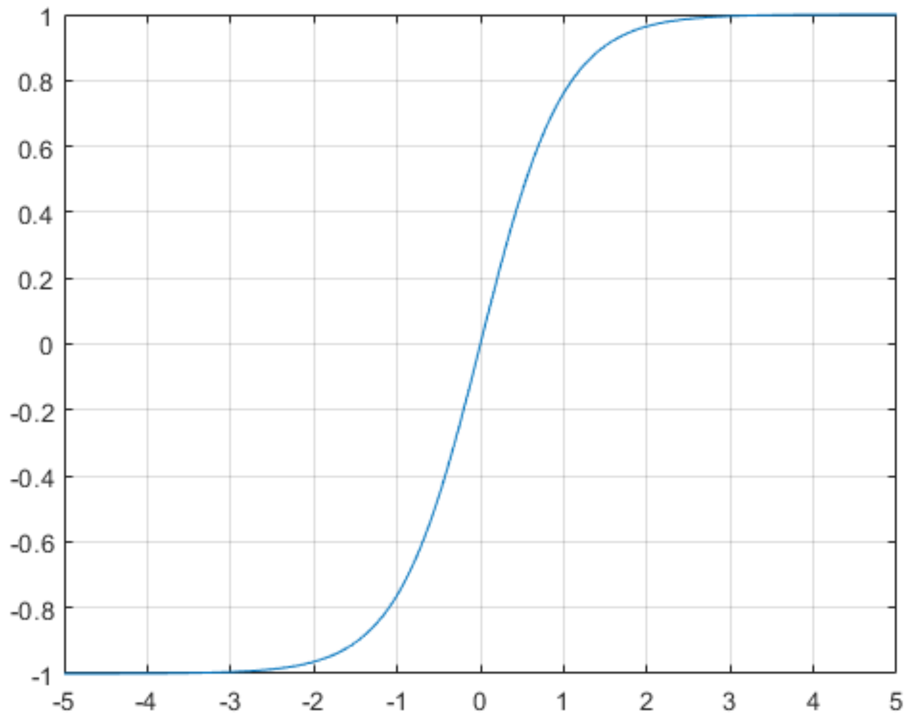

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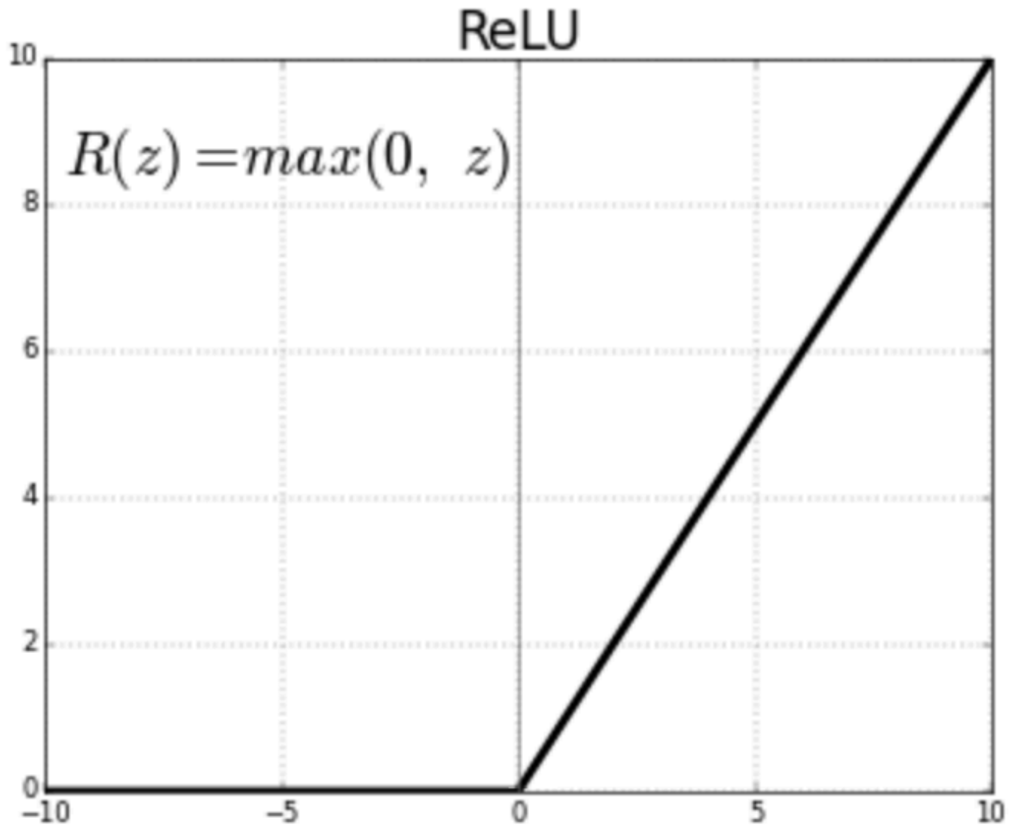

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Activation Functions: Hidden Layer

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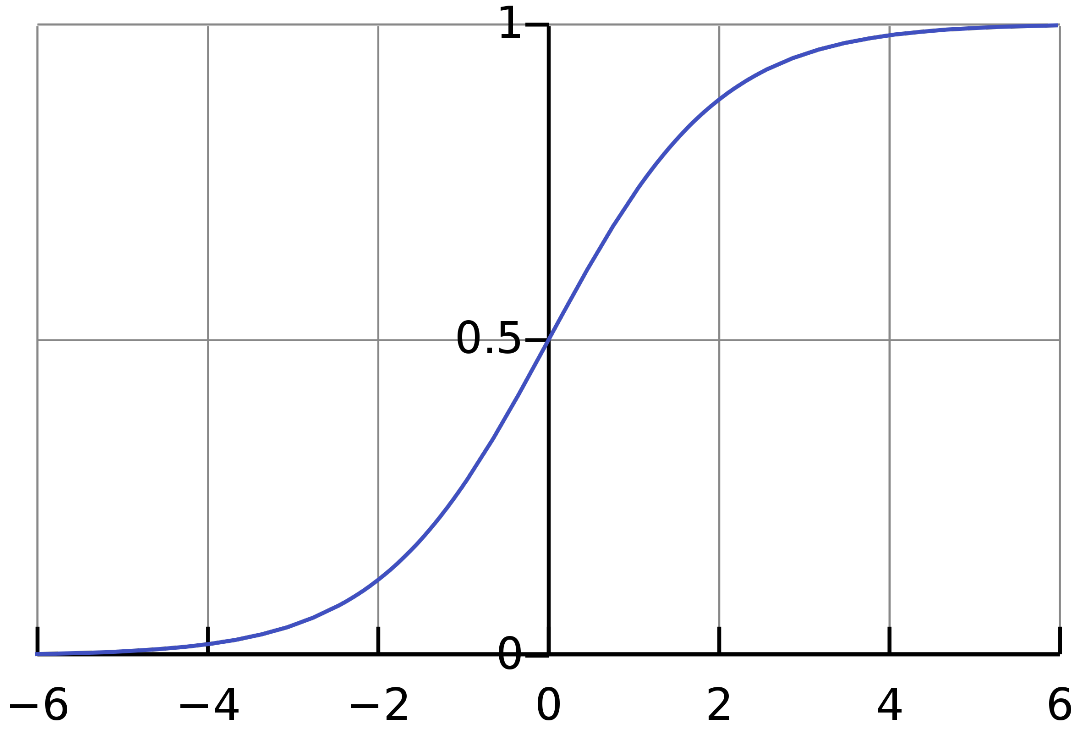

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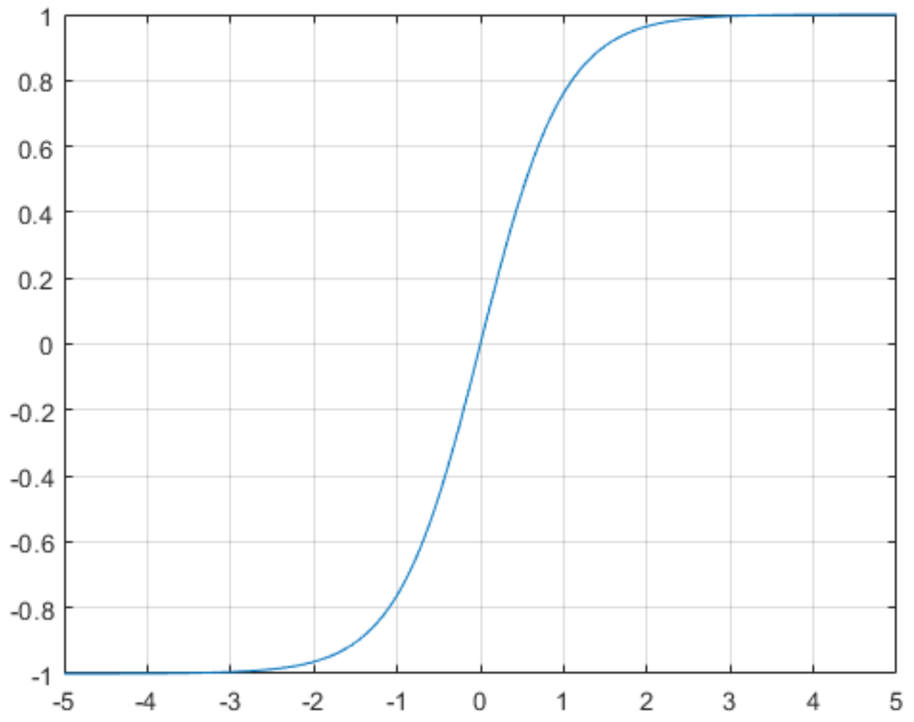

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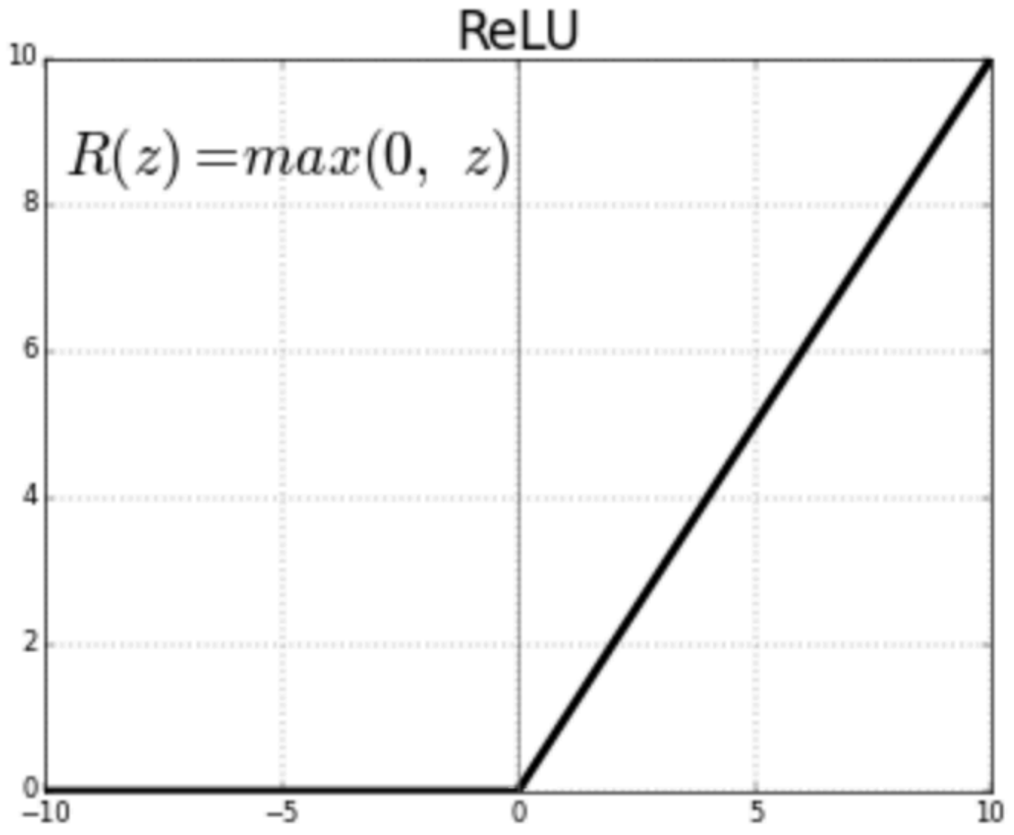

Problem: derivative "saturates" (nearly 0) everywhere except near origin

- Use ReLU by default
- Generalizations:
  - Leaky
  - ELU
  - Softplus
  - …

Activation Functions: Output Layer

- Depends on the task!
- Regression (continuous output(s)): none!
  - Just use final linear transformation
- Binary classification: sigmoid
  - Also for *multi-label* classification
- Multi-class classification: softmax
  - Terminology: the inputs to a softmax are called *logits*
  - [there are sometimes other uses of the term, so beware]

$$\text{softmax}(x)_i = \frac{e^{x_i}}{\sum_j e^{x_j}}$$

Mini-batch computation

Computing with a Single Input

$$\hat{y} = f_n\left(f_{n-1}\left(\cdots f_2\left(f_1\left(xW^1 + b^1\right)W^2 + b^2\right)\cdots\right)W^n + b^n\right)$$

$$x = \begin{bmatrix} x_0 & x_1 & \cdots & x_{n_0} \end{bmatrix}$$

Shape: $(1, n_0)$

$$b^1 = \begin{bmatrix} b_0^1 & b_1^1 & \cdots & b_{n_1}^1 \end{bmatrix}$$

Shape: $(1, n_1)$

$$W^1 = \begin{bmatrix} w_{00}^1 & w_{10}^1 & \cdots & w_{0n_1}^1 \\ w_{10}^1 & w_{11}^1 & \cdots & w_{1n_1}^1 \\ \vdots & \vdots & \ddots & \vdots \\ w_{n_00}^1 & w_{n_01}^1 & \cdots & w_{n_0n_1}^1 \end{bmatrix}$$

Shape: (n_0, n_1)

n_0: number of neurons in layer 0 (input)

n_1: number of neurons in layer 1

Mini-batch Gradient Descent (from lecture 2)

```
initialize parameters / build model

for each epoch:

 data = shuffle(data)
 batches = make_batches(data)

 for each batch in batches:

  outputs = model(batch)
  loss = loss_fn(outputs, true_outputs)
  compute gradients
  update parameters
```

Computing with Mini-batches

- Bad idea:

```
for each batch in batches:
 for each datum in batch:
  outputs = model(datum)
  loss = loss_fn(outputs, true_outputs)
  compute gradients
 update parameters
```

Computing with a Batch of Inputs

Computing with a Batch of Inputs

$$\hat{y} = f_n\left(f_{n-1}\left(\cdots f_2\left(f_1\left(XW^1 + b^1\right)W^2 + b^2\right)\cdots\right)W^n + b^n\right)$$

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Shape: (n, n_0)
n: batch_size

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Shape: $(1, n_1)$

Added to each row of XW^1

Note on mini-batches and shape

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- Most modern neural net libraries (e.g. PyTorch) expect the *first* dimension of matrices/tensors to be a batch size
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- Two comments:
  - In your code, **annotate every tensor** with a comment saying intended shape
  - When debugging, look at shapes early on!!

Homework 2

Next Time

- Further abstraction: *computation graph*
- Backpropagation algorithm for computing gradients
  - Using forward/backward API for nodes in a comp graph