

Neural Network Introduction

LING 574 Deep Learning for NLP

Shane Steinert-Threlkeld

Announcements

- HW1 due tomorrow night, upload readme and hw1.tar.gz to Canvas
 - NB: two separate files!
 - Do not put readme inside of tar.gz; no “nested” structure inside tarball either
 - Run `check_hw1.sh`
- `indices_to_tokens` (and in general): 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

```
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

```
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}")

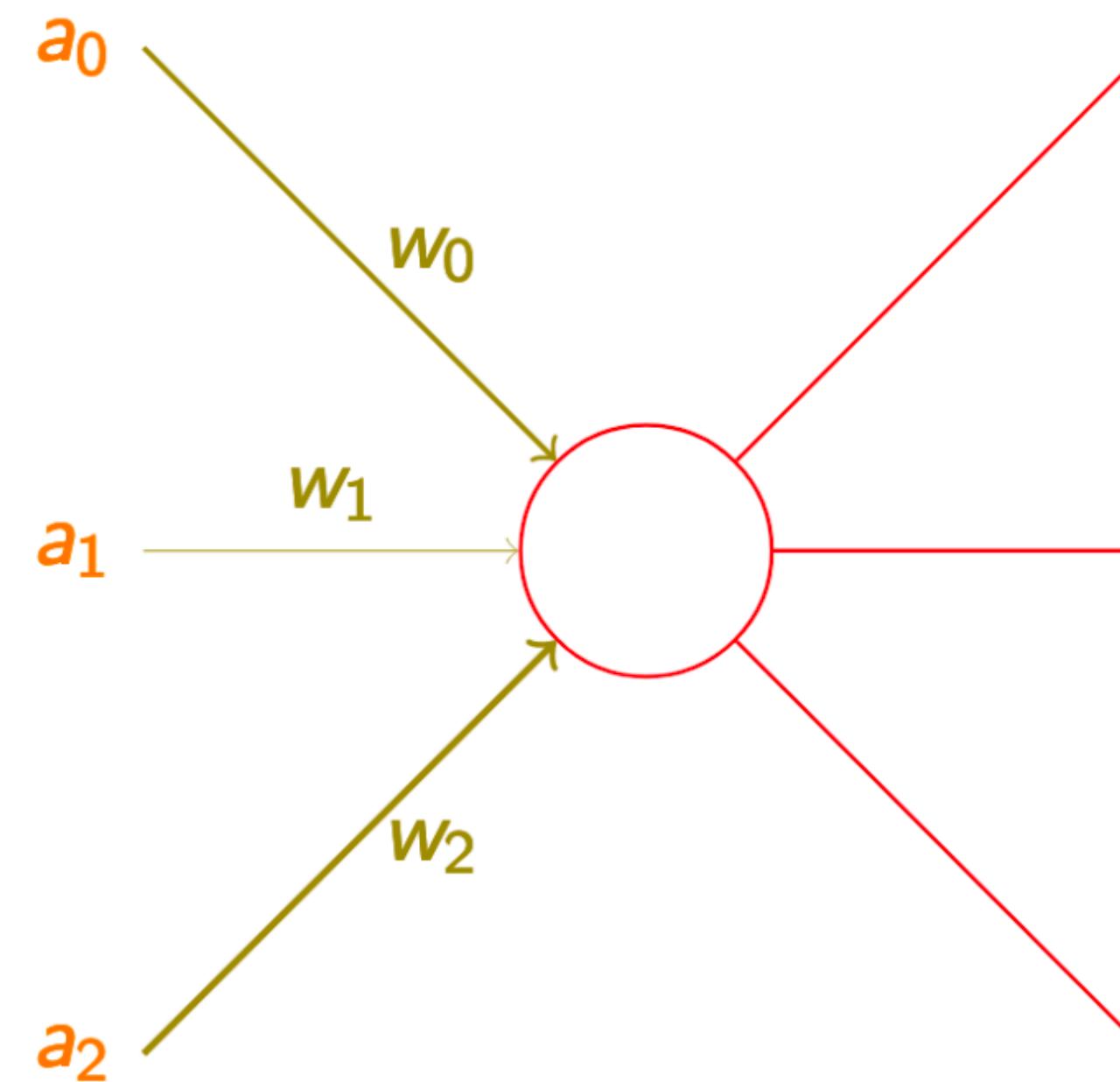
keywords_any(name="Shane", course="575k")
keywords_any(name="Shane", course="575k", foo="bar")
keywords_any(**{"name": "Shane", "course": "575k"})
```

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

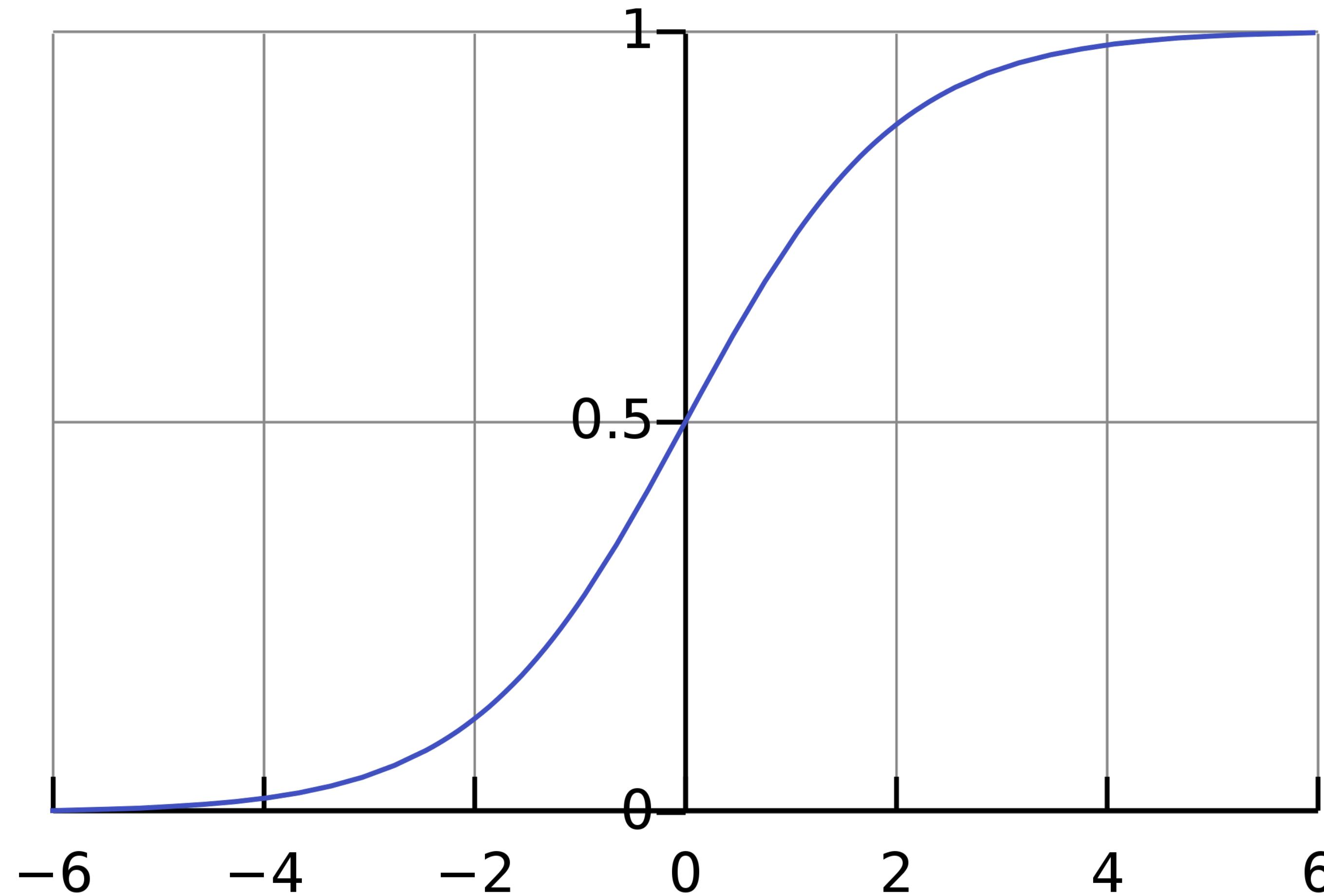
Artificial Neuron



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

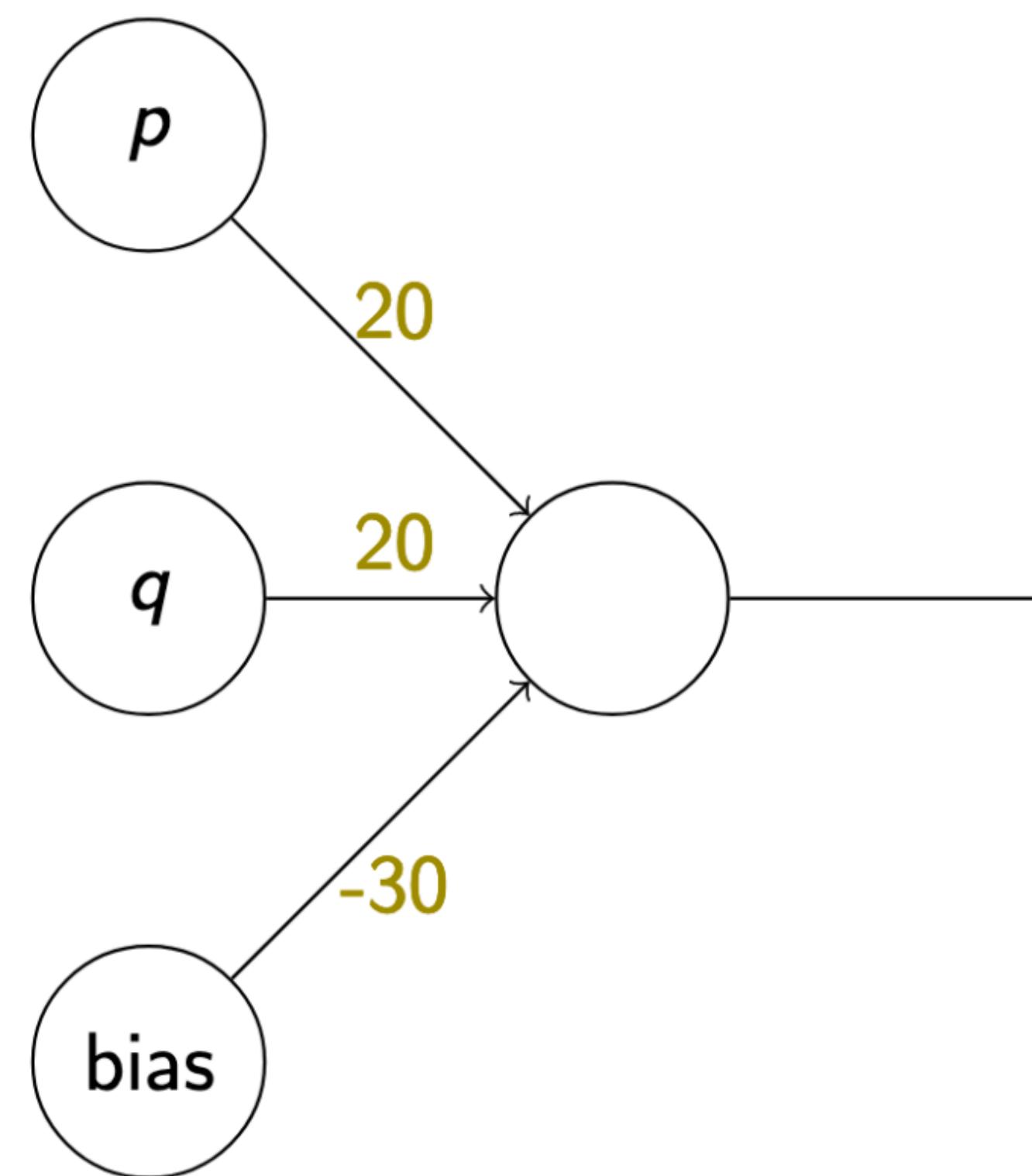
<https://github.com/shanest/nn-tutorial>

Activation Function: Sigmoid



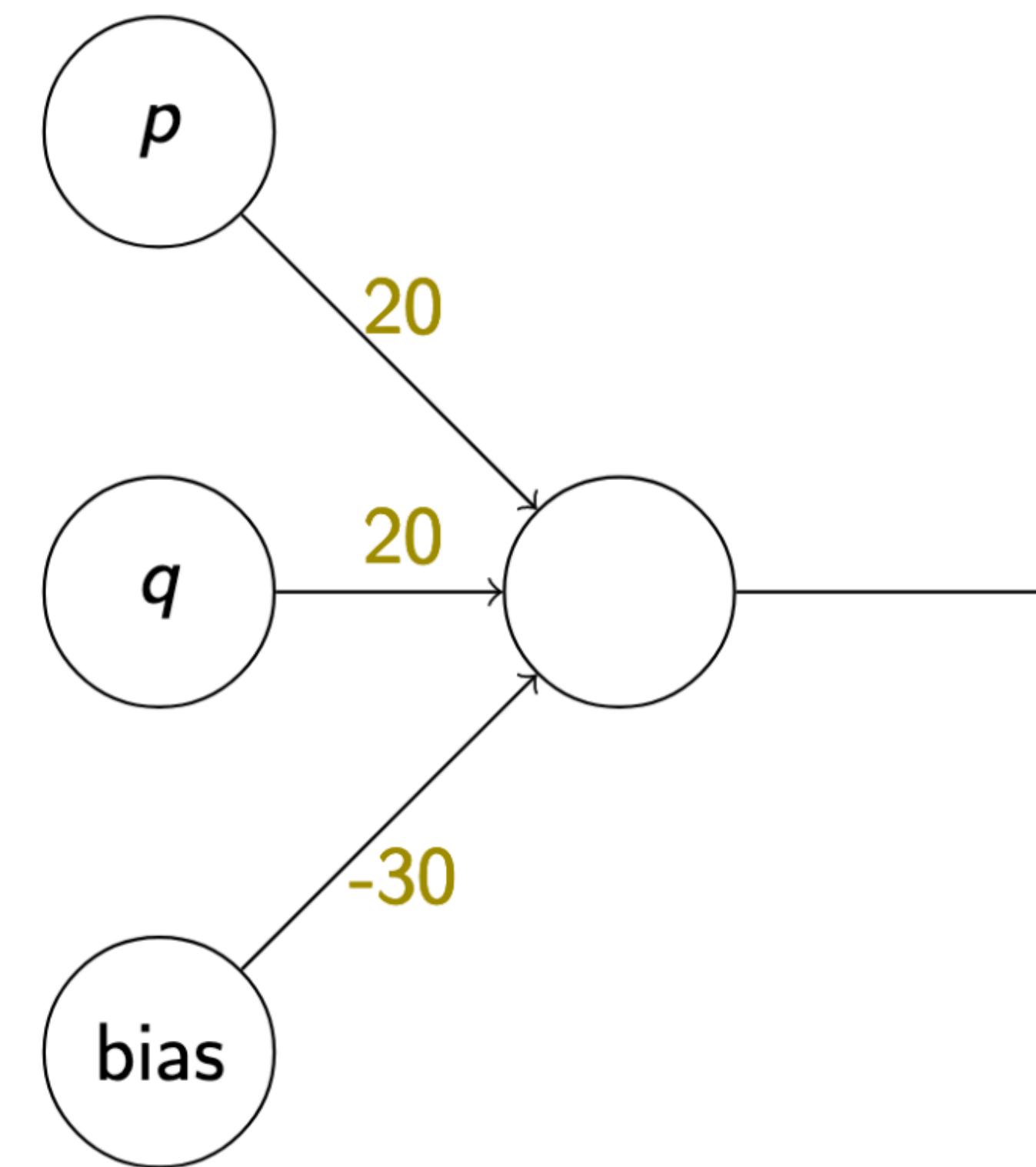
$$\sigma(x) = \frac{1}{1 + e^{-x}} = \frac{e^x}{e^x + 1}$$

Computing a Boolean function



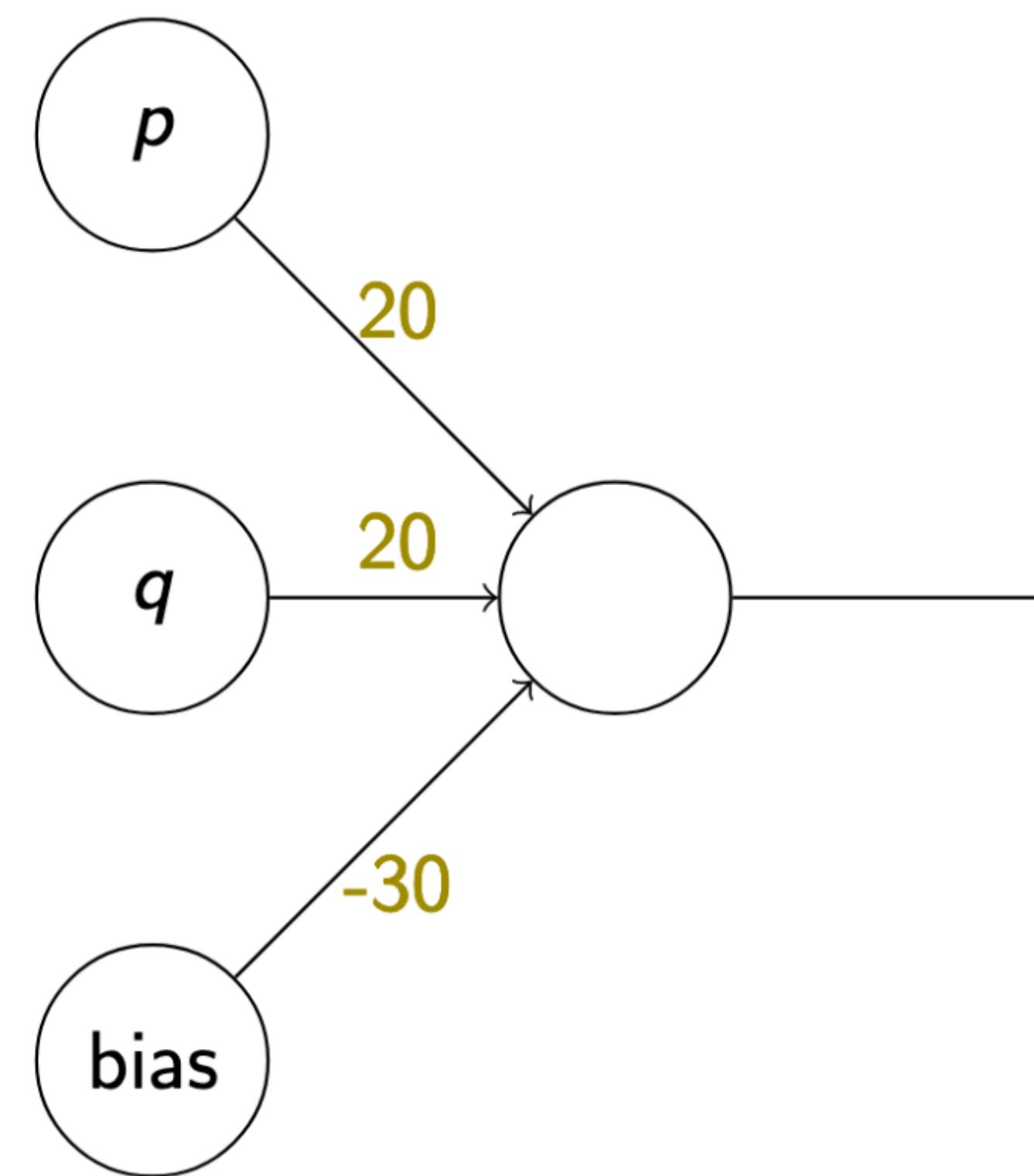
Computing a Boolean function

p	q	a
---	---	---



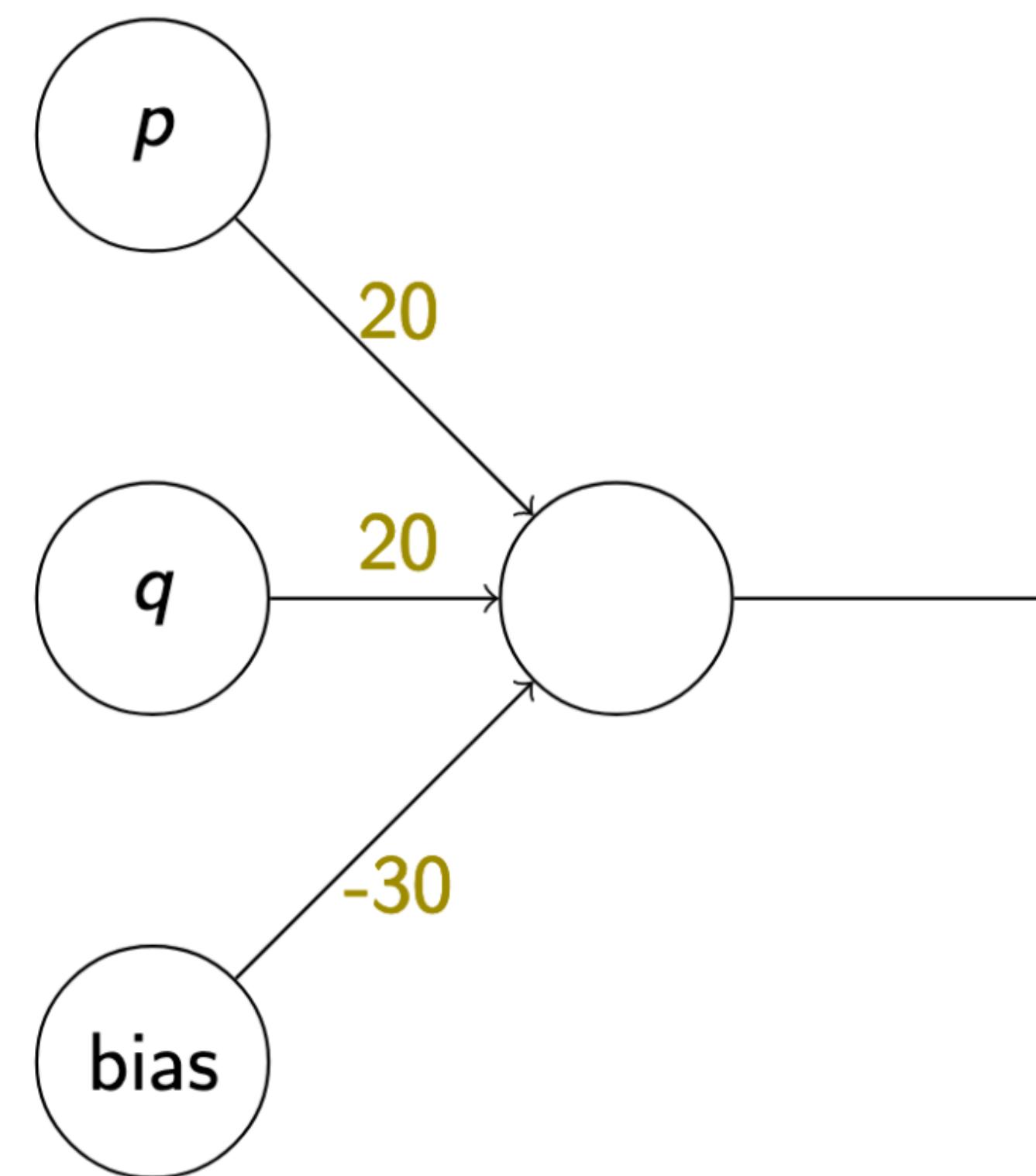
Computing a Boolean function

p	q	a
1	1	1



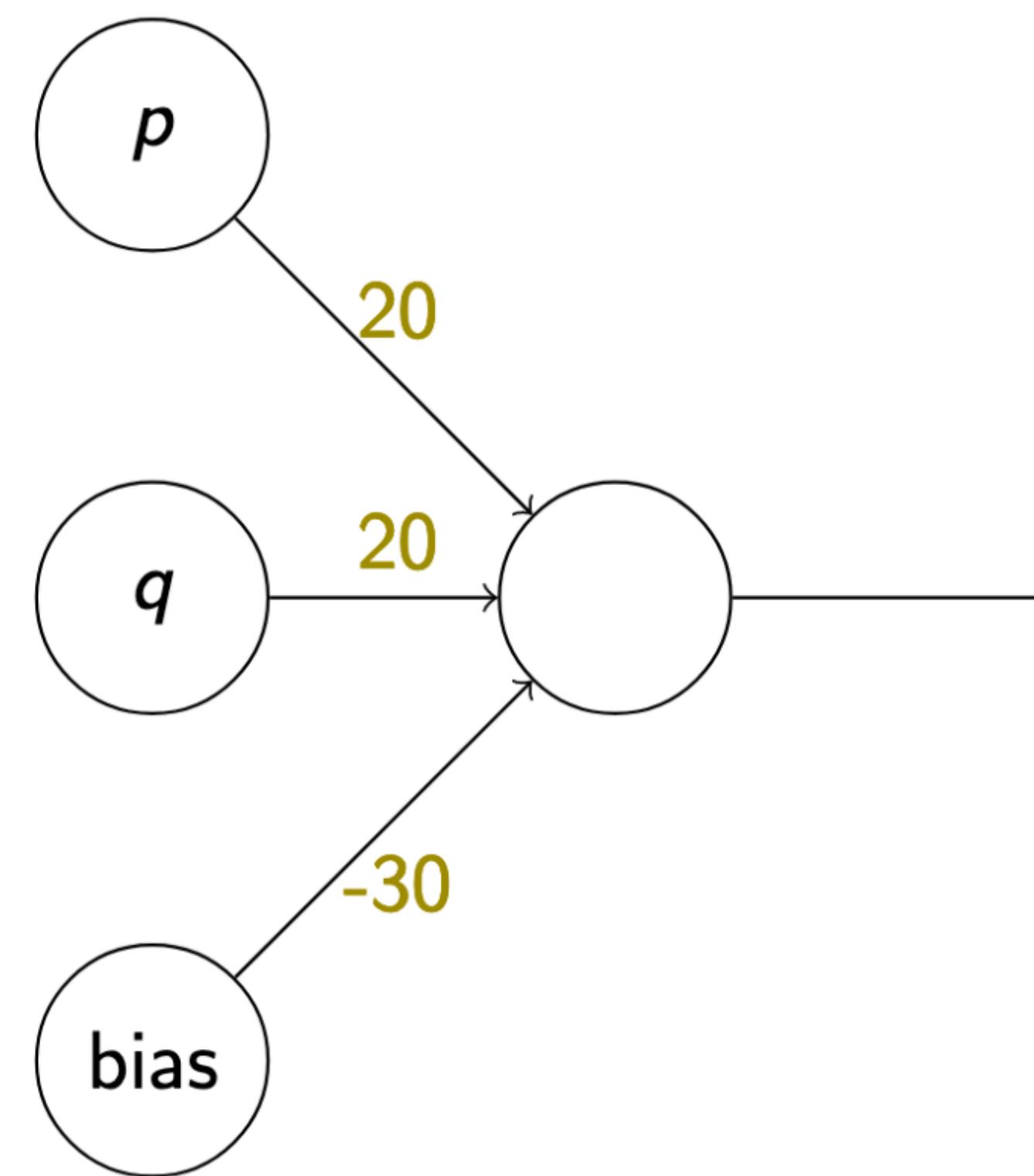
Computing a Boolean function

p	q	a
1	1	1
1	0	0



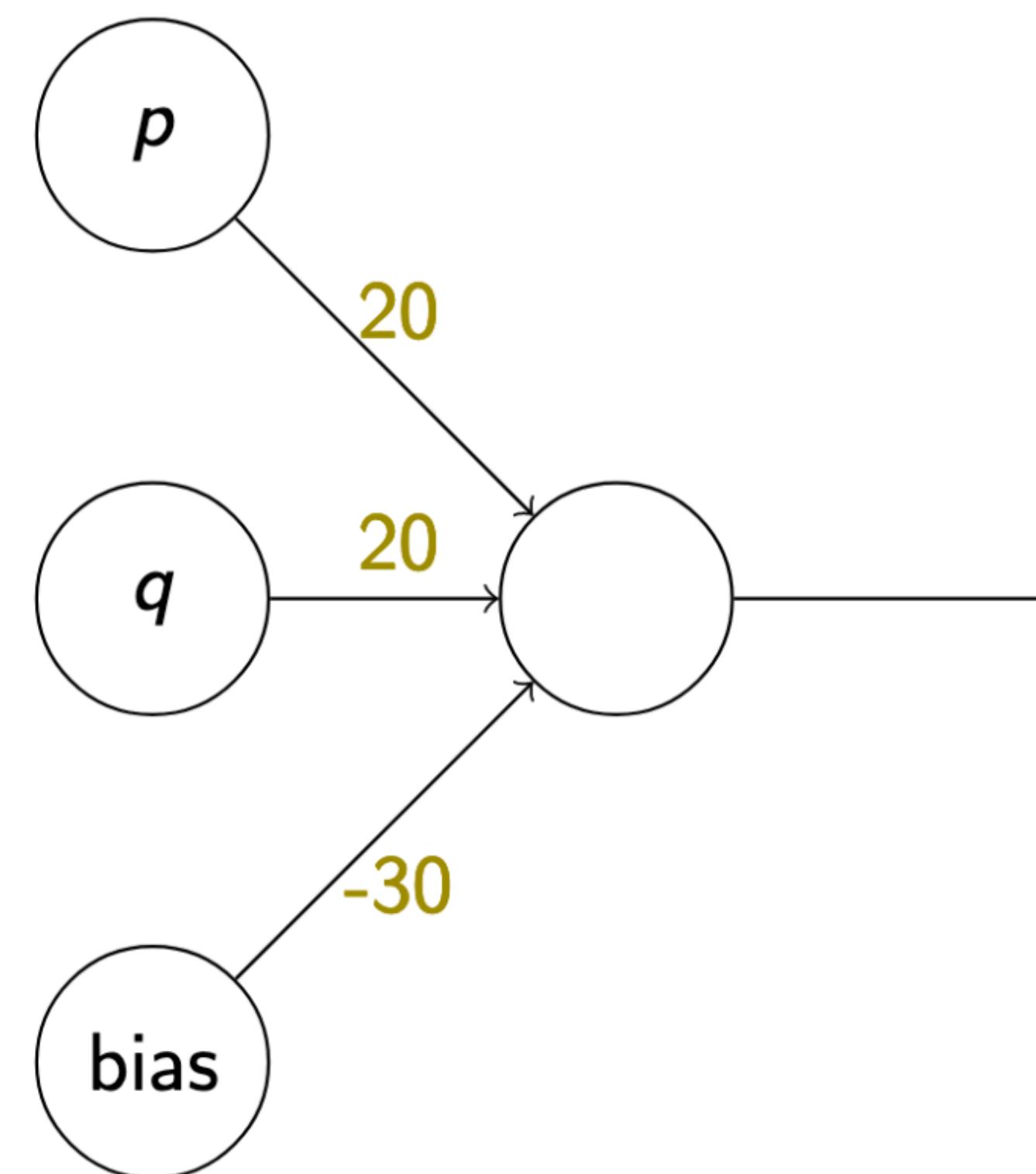
Computing a Boolean function

p	q	a
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1	0	0
0	1	0

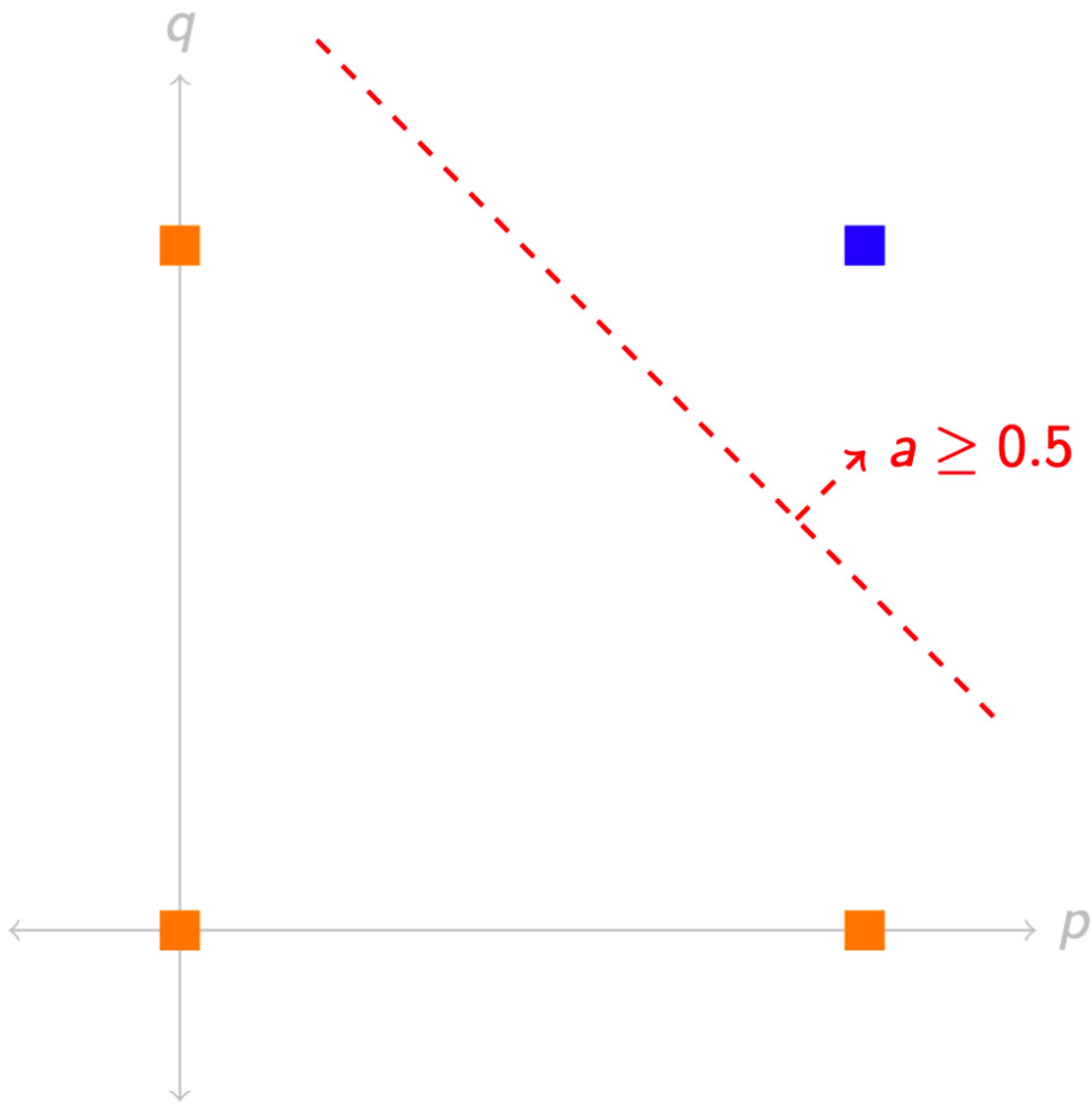


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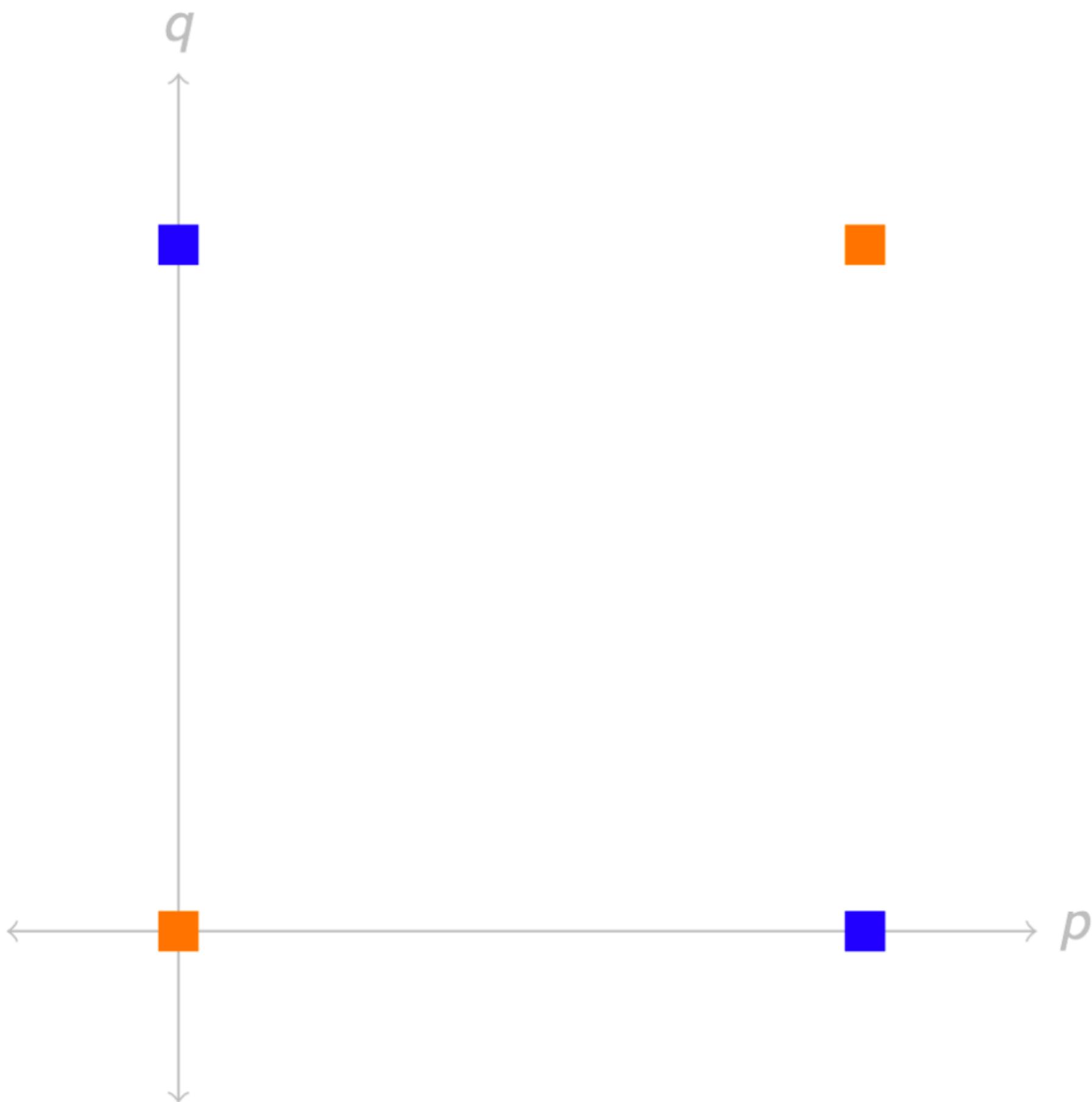
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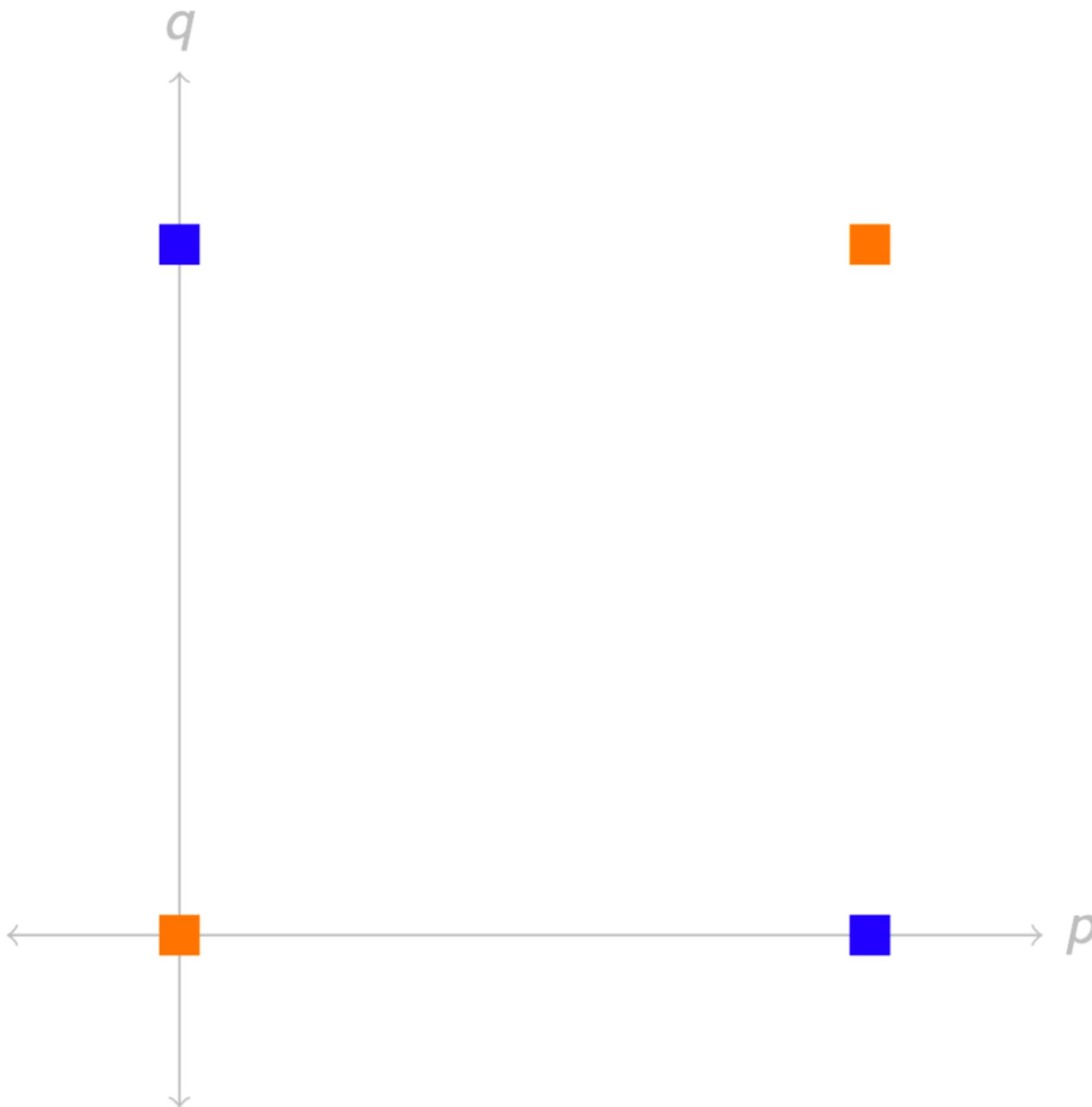
Computing ‘and’



The XOR problem

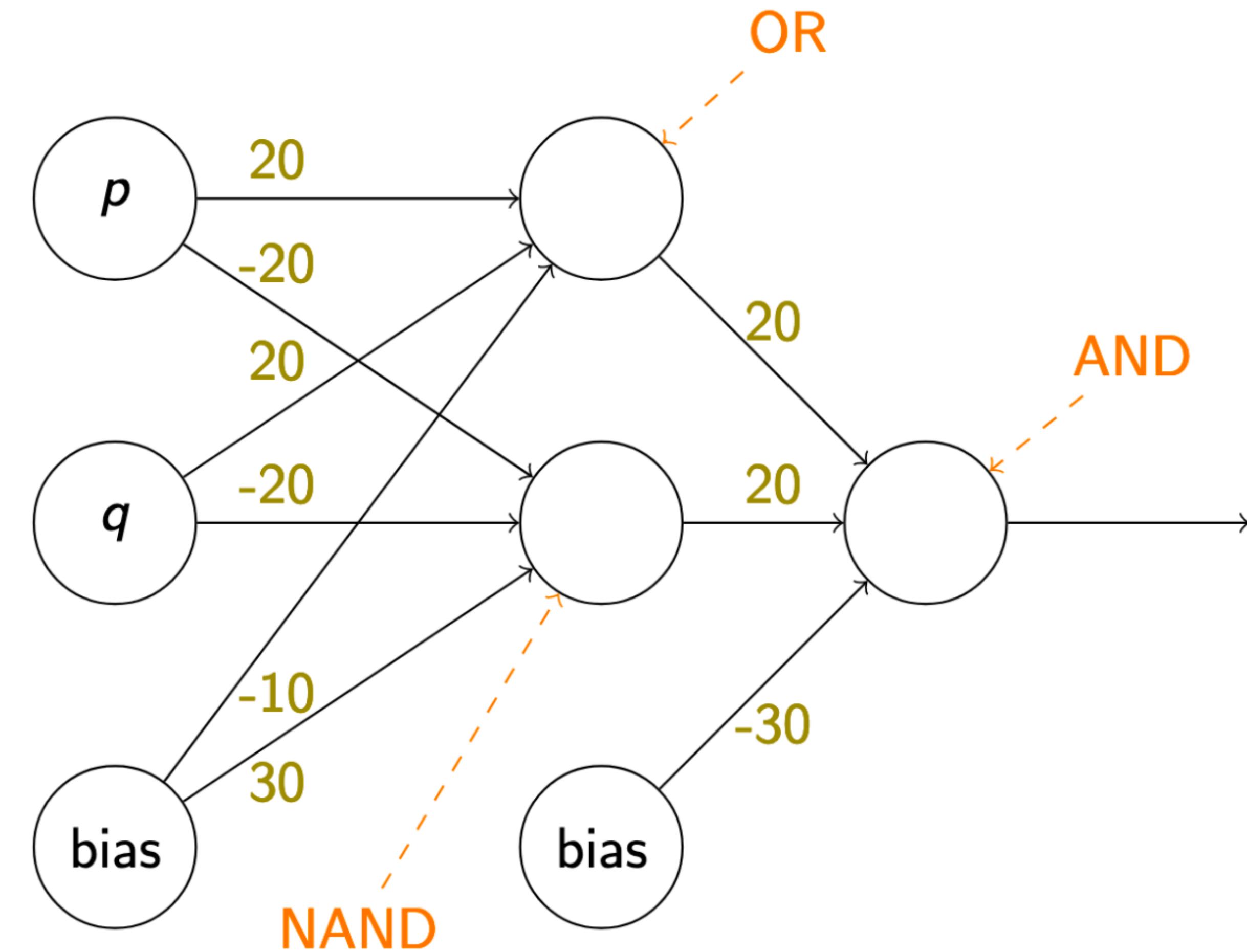


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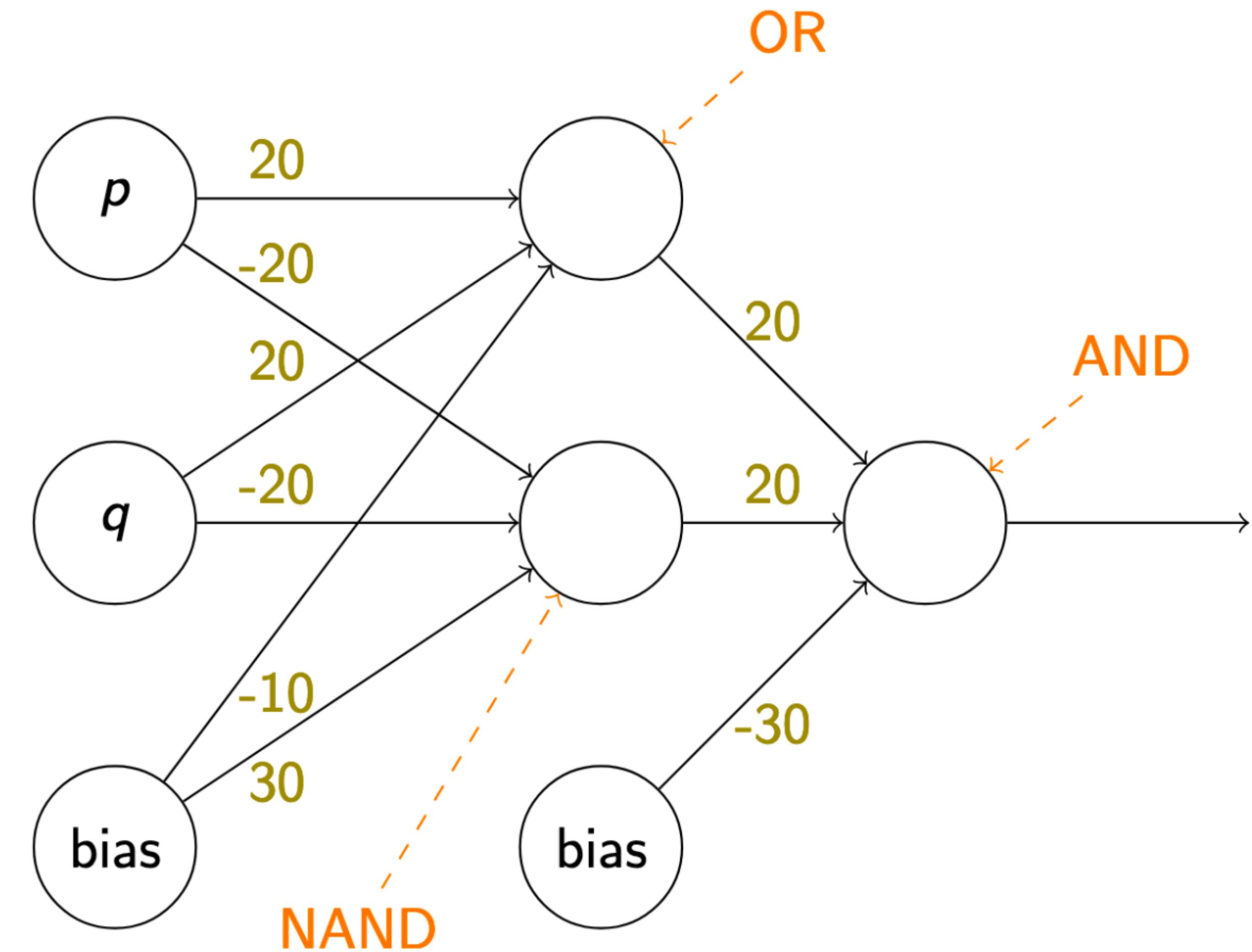


XOR is not linearly separable

Computing XOR

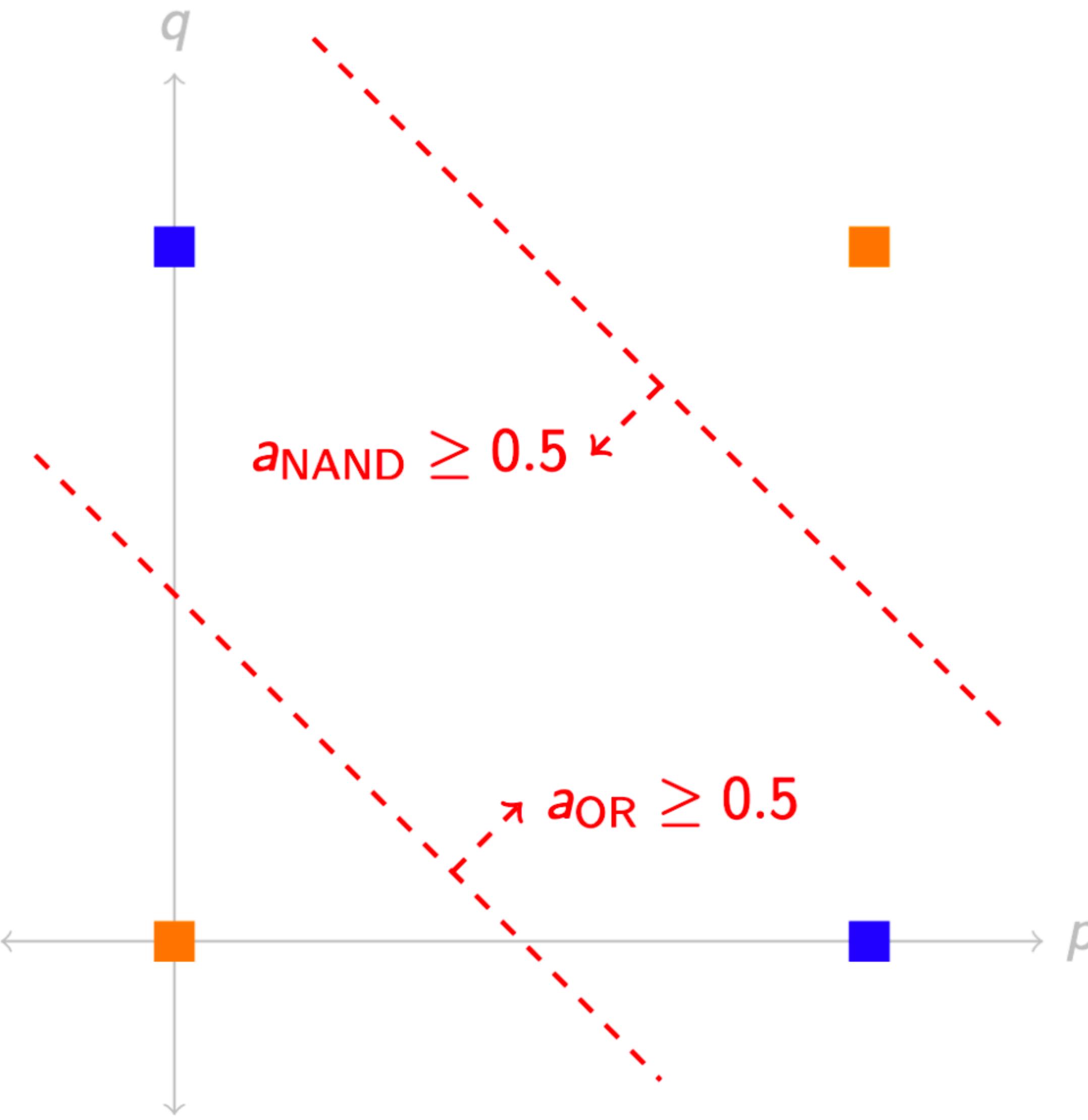


Computing XOR



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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 - Size of the hidden layer is *exponential* in m
 - How does one *find/learn* such a good approximation?

Expressive Power

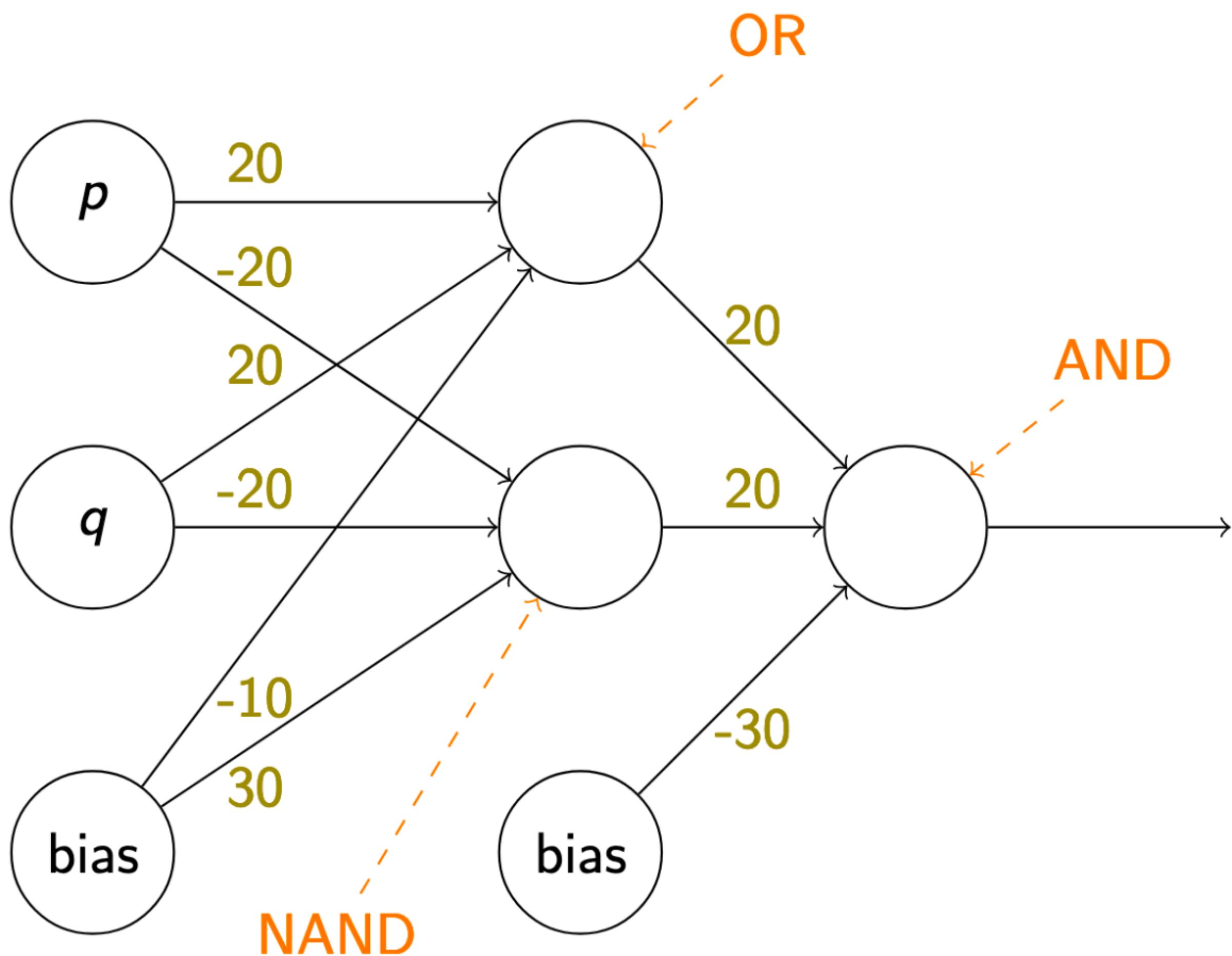
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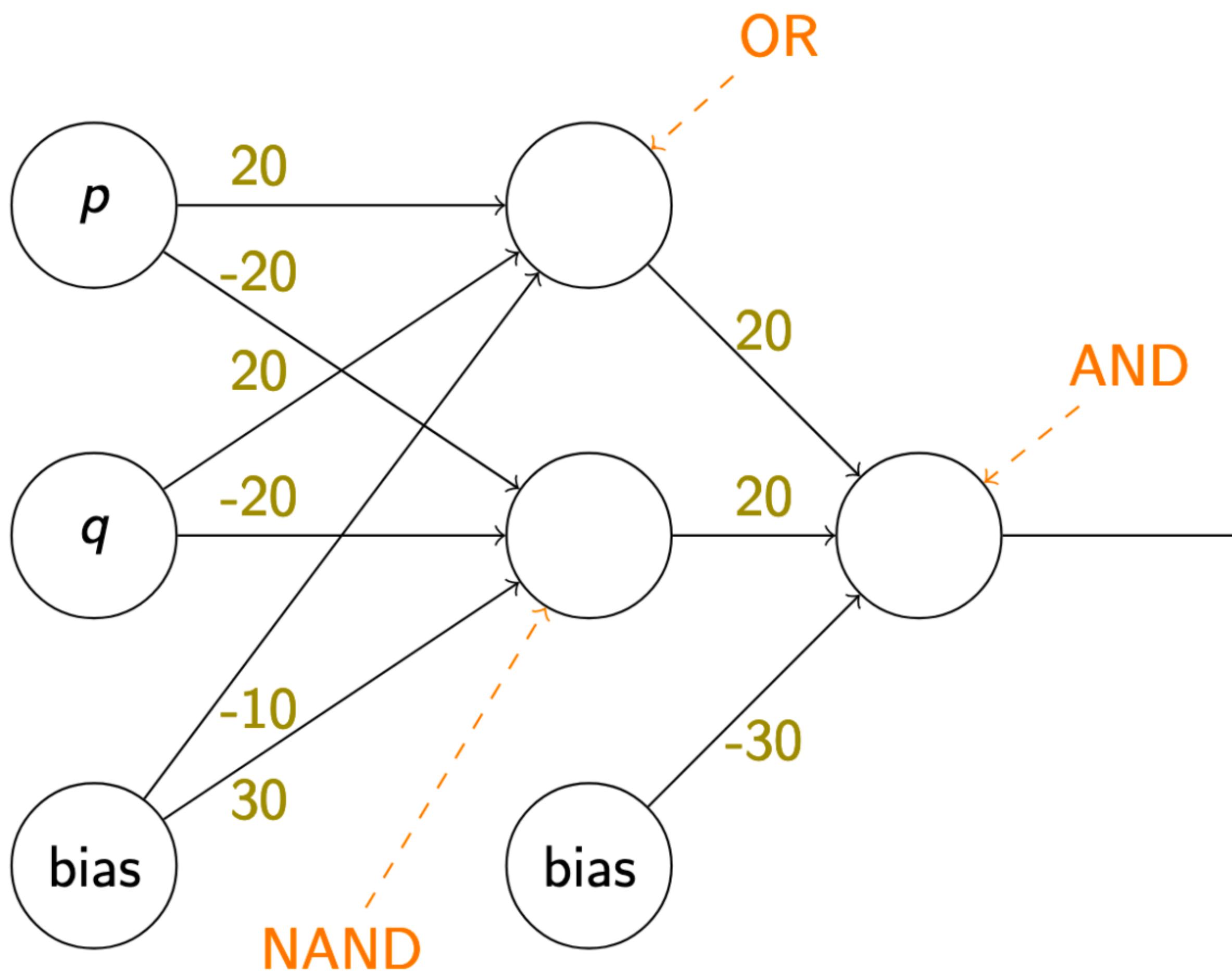
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- See also GBC 6.4.1 for more references, generalizations, discussion

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

XOR Network

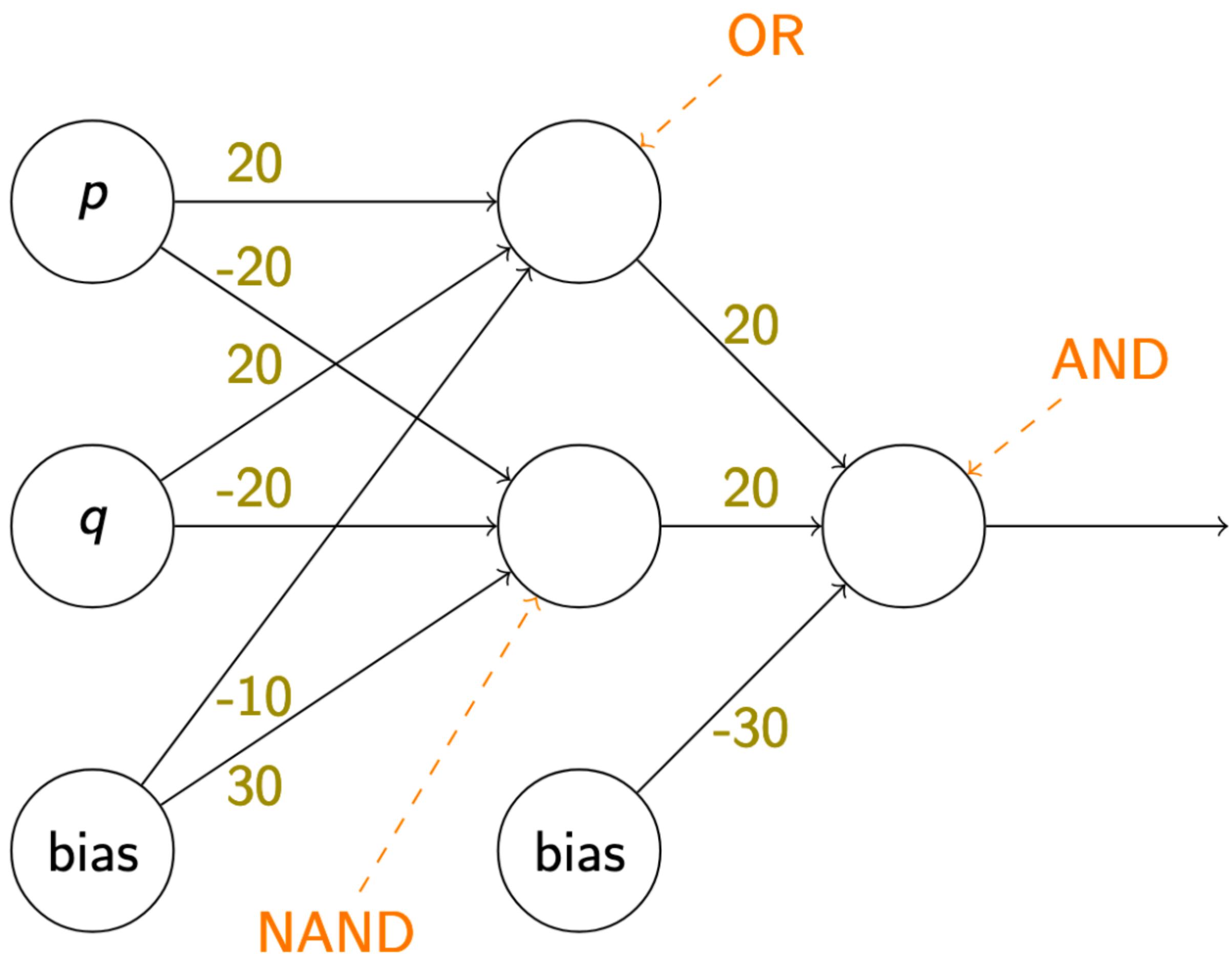


XOR Network



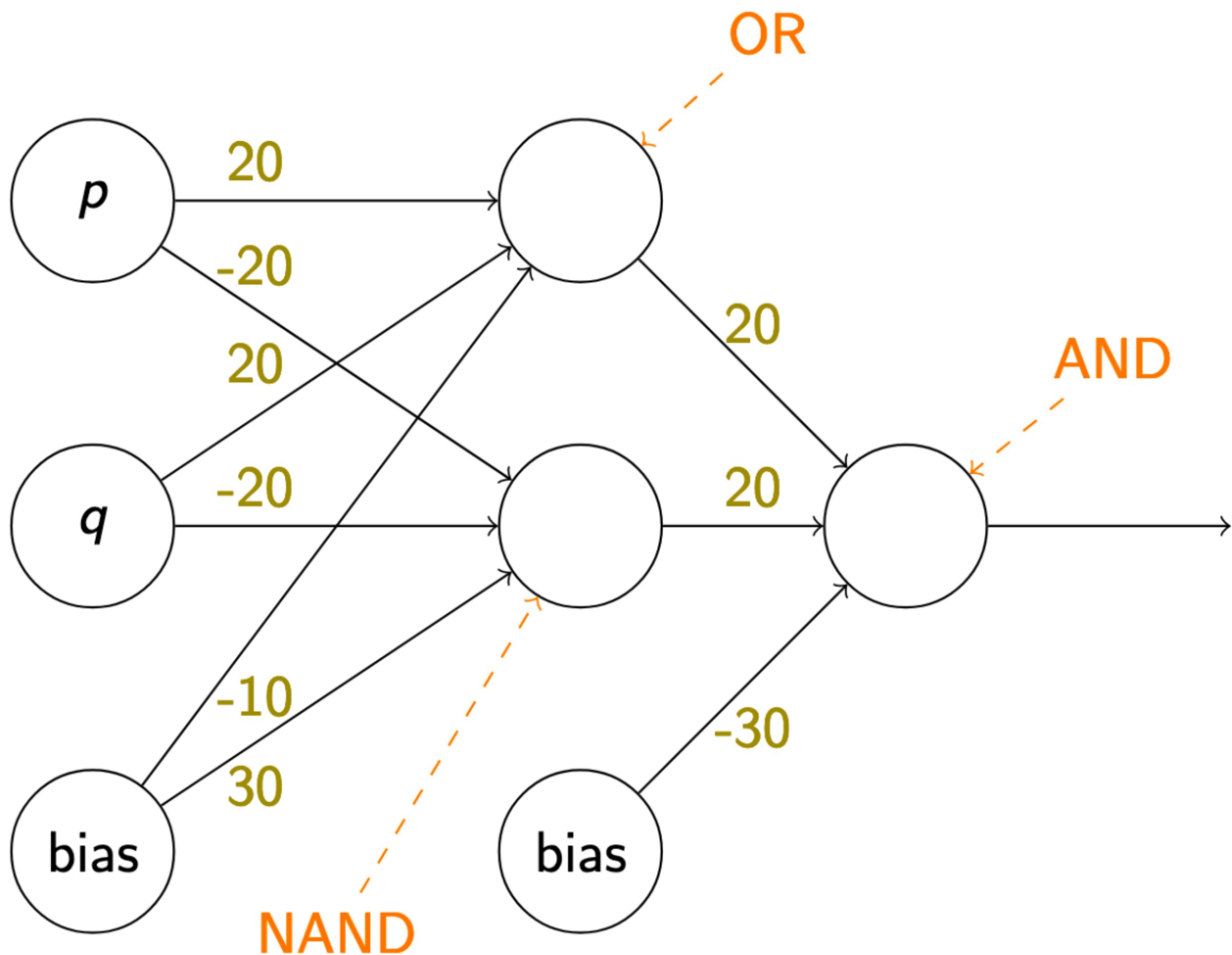
$$a_{\text{and}} = \sigma(w_{\text{or}}^{\text{and}} \cdot a_{\text{or}} + w_{\text{nand}}^{\text{and}} \cdot a_{\text{nand}} + b^{\text{and}})$$

XOR Network



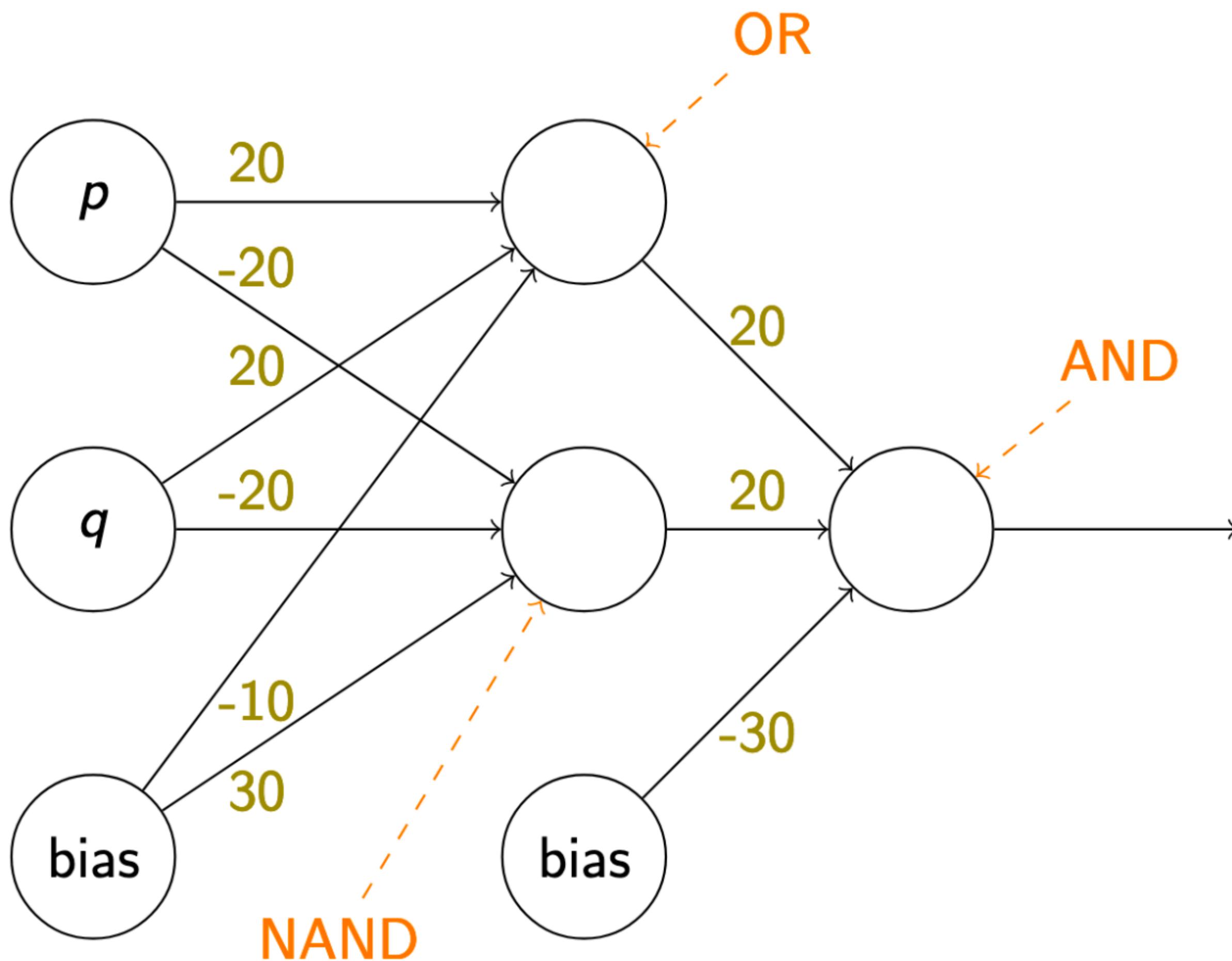
$$\begin{aligned}a_{\text{and}} &= \sigma \left(w_{\text{or}}^{\text{and}} \cdot a_{\text{or}} + w_{\text{nand}}^{\text{and}} \cdot a_{\text{nand}} + b^{\text{and}} \right) \\&= \sigma \left([a_{\text{or}} \quad a_{\text{nand}}] \begin{bmatrix} w_{\text{or}}^{\text{and}} \\ w_{\text{nand}}^{\text{and}} \end{bmatrix} + b^{\text{and}} \right)\end{aligned}$$

XOR Network



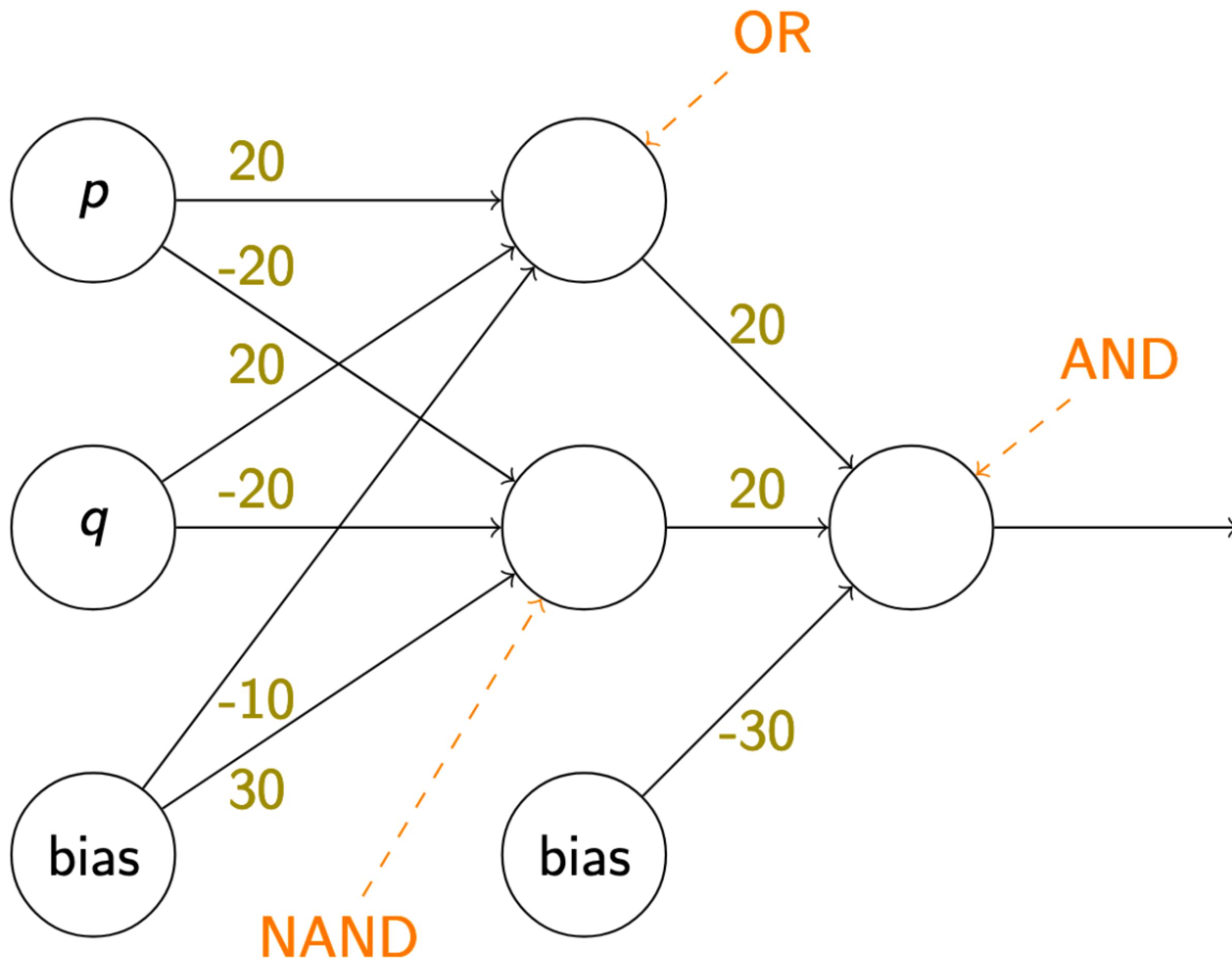
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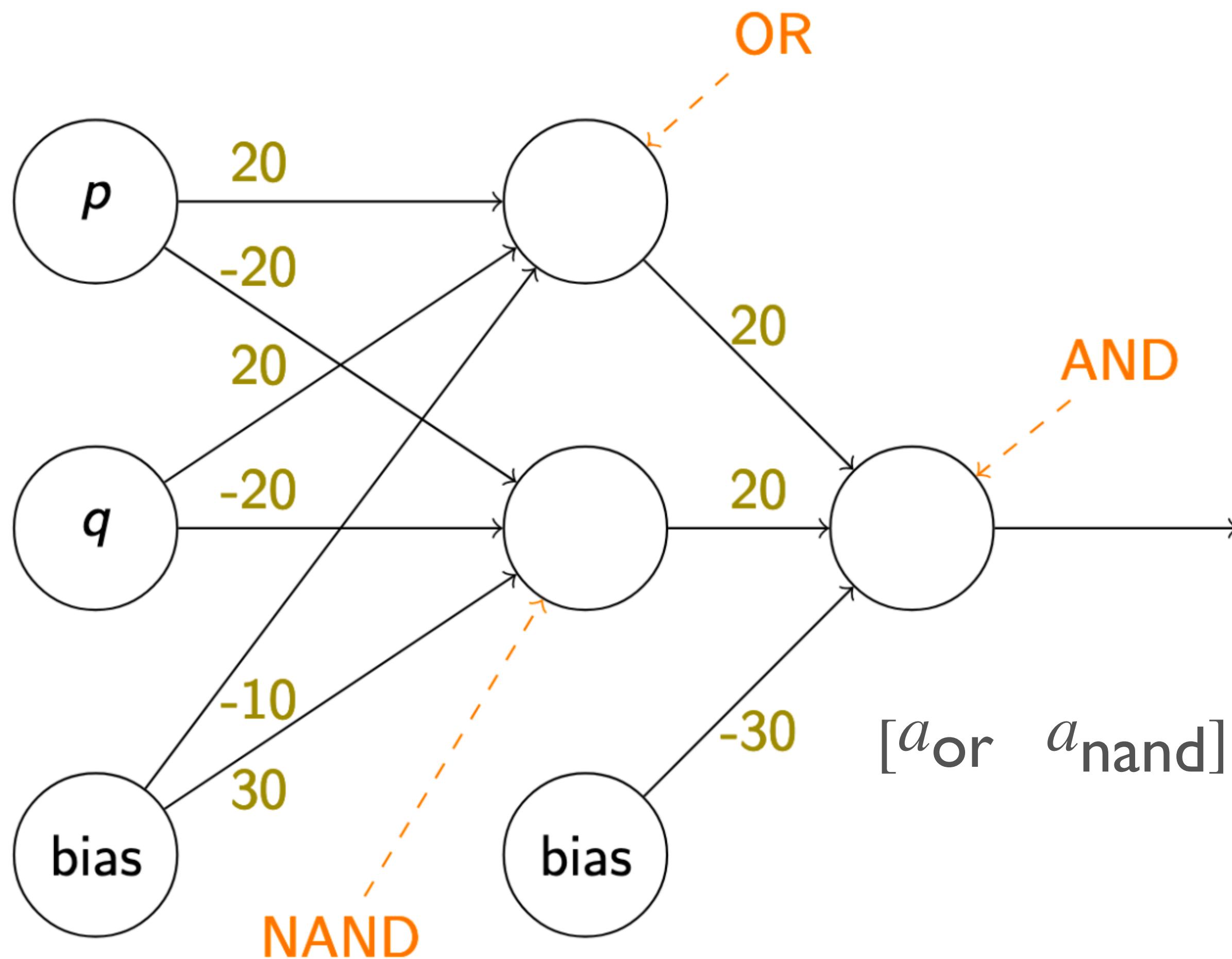
$$\begin{aligned}
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 &= \sigma \left([a_{\text{or}} \quad a_{\text{nand}}] \begin{bmatrix} w_{\text{or}}^{\text{and}} \\ w_{\text{nand}}^{\text{and}} \end{bmatrix} + b^{\text{and}} \right) \\
 a_{\text{or}} &= \sigma(w_p^{\text{or}} \cdot a_p + w_q^{\text{or}}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

XOR Network



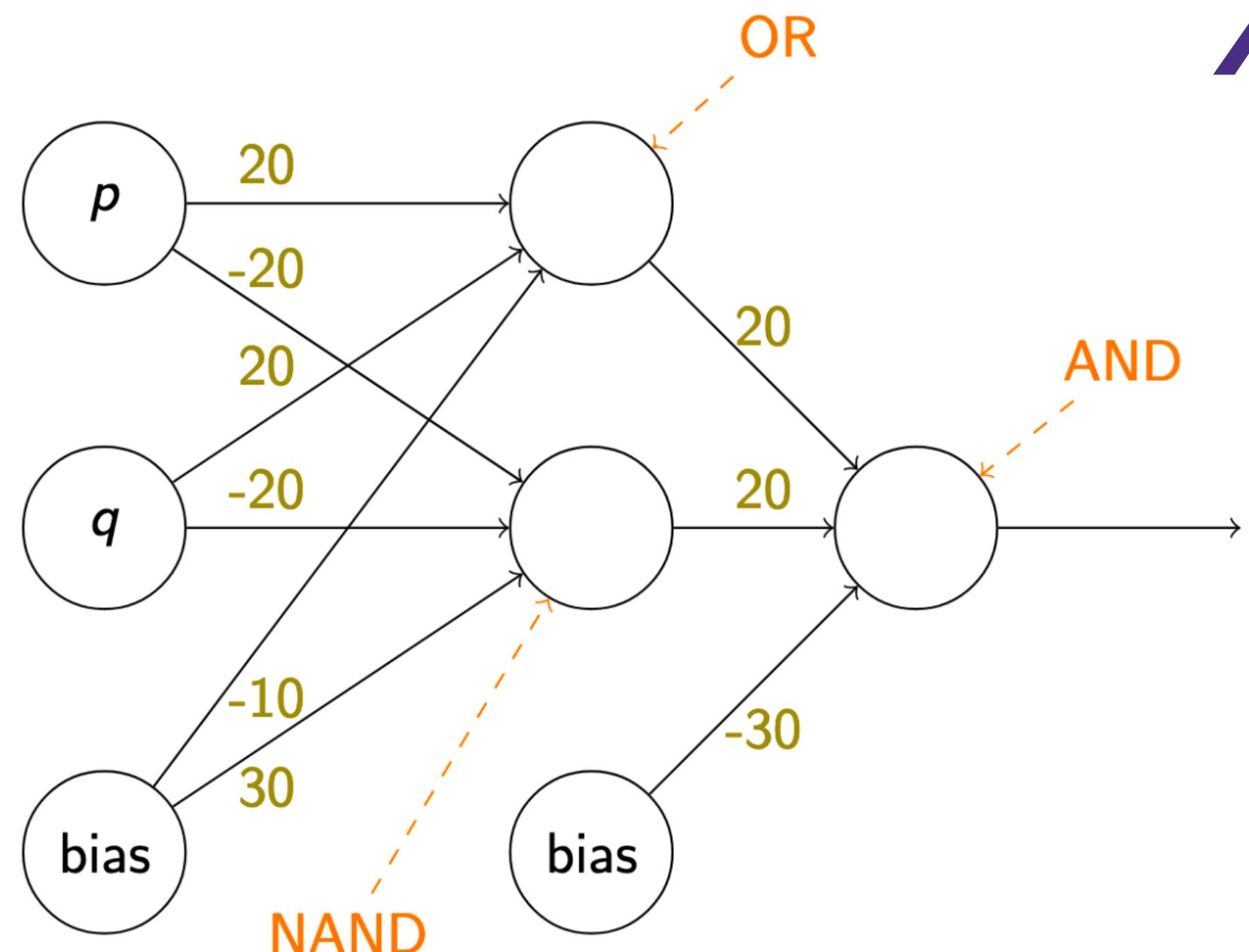
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 a_{\text{nand}} &= \sigma(w_p^{\text{nand}} \cdot a_p + w_q^{\text{nand}} \cdot a_q + b^{\text{nand}})
 \end{aligned}$$

XOR Network



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

XOR Network



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

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

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

Generalizing

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

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

Generalizing

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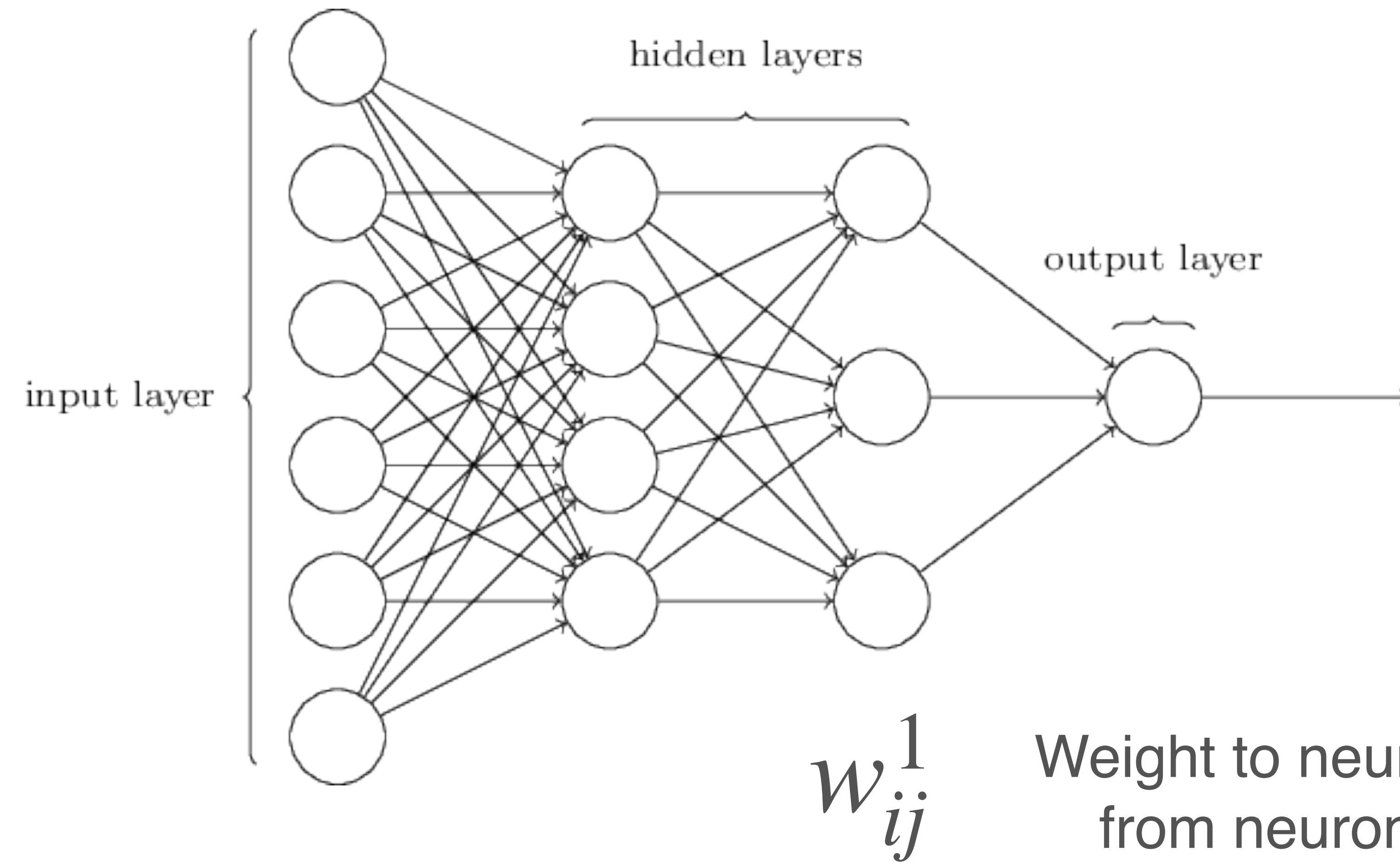
$$\hat{y} = f_2 \left(f_1 \left(xW^1 + b^1 \right) W^2 + b^2 \right)$$

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

Some terminology

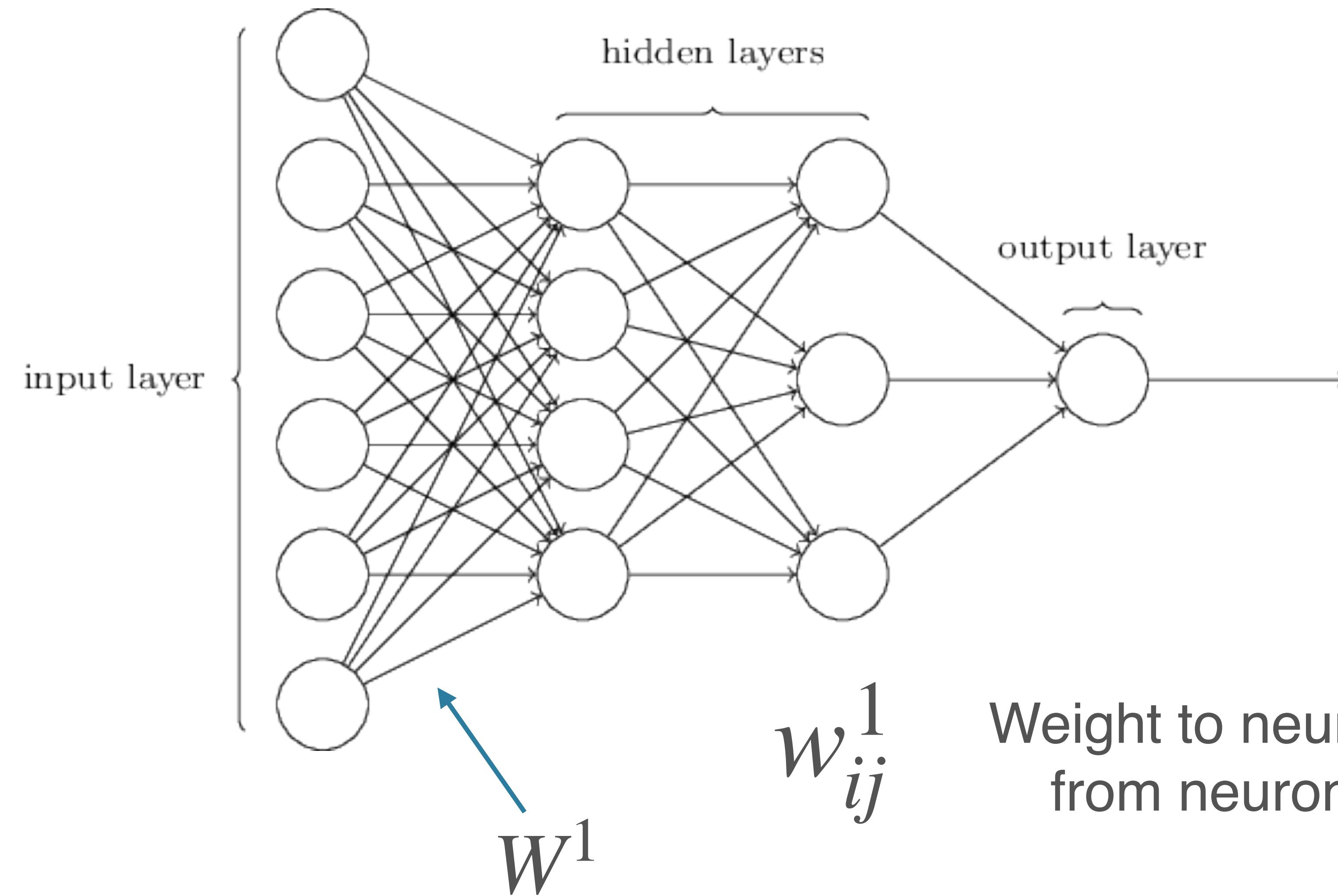
- Our XOR network is a *feed-forward neural network* with *one hidden layer*
 - Aka a multi-layer perceptron (MLP)
 - Input nodes: 2; output nodes: 1
 - Activation function: sigmoid

General MLP



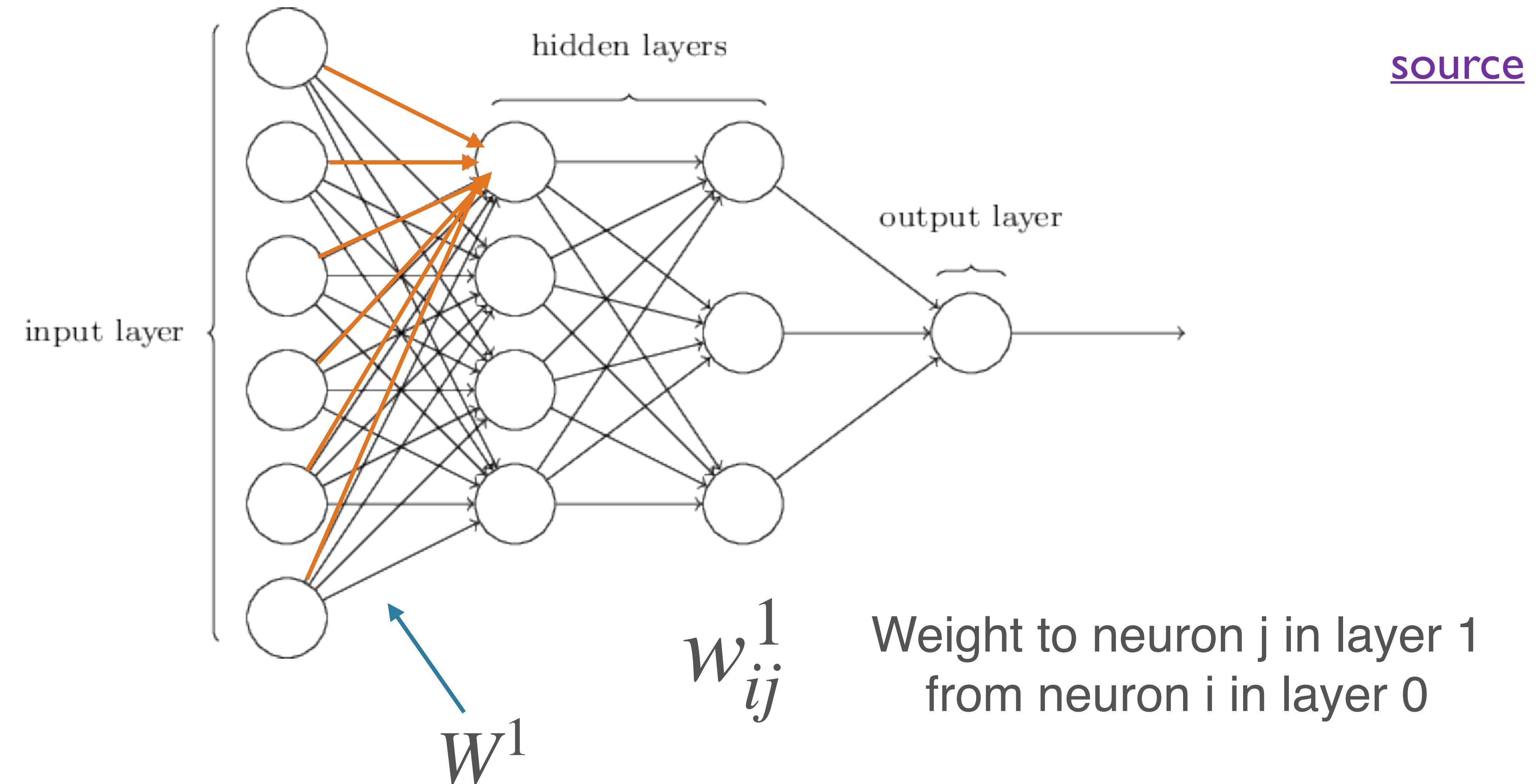
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General MLP



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$$x = [x_0 \quad x_1 \quad \cdots \quad x_{n_0}]$$

Shape: $(1, n_0)$

General MLP

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

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Shape: (n_0, n_1)

n_0 : number of neurons in layer 0 (input)

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$$x = [x_0 \ x_1 \ \cdots \ x_{n_0}]$$

Shape: $(1, n_0)$

$$b^1 = [b_0^1 \ b_1^1 \ \cdots \ b_{n_1}^1]$$

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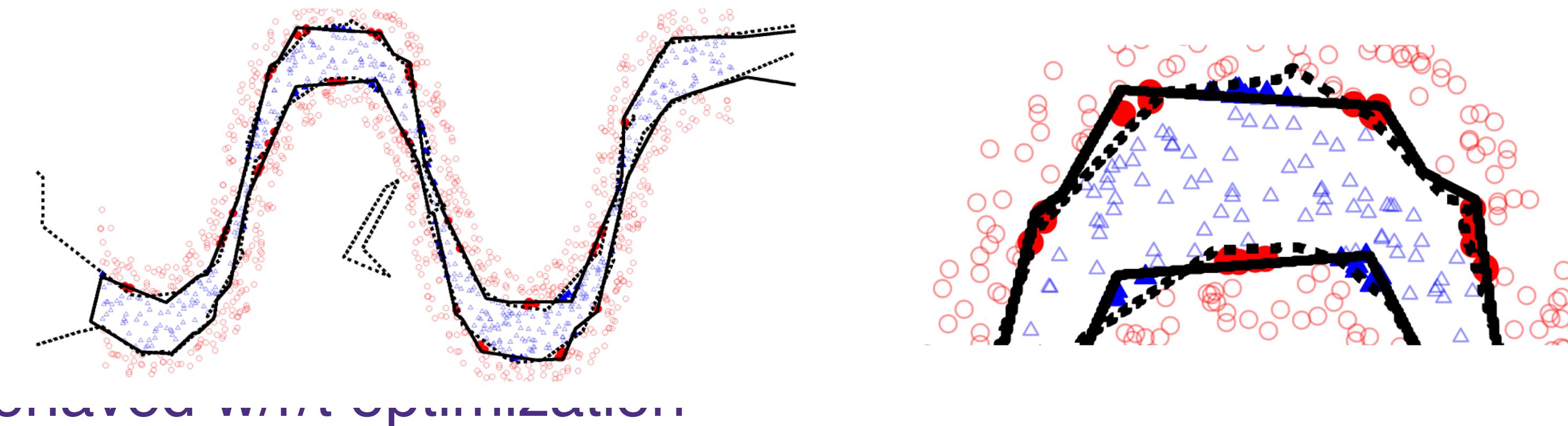
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- Others: initialization, regularization (and associated values), learning rate / training, ...

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” (some theoretical analysis)
 - In principle allows hierarchical features to be learned
 - More well-behaved w/r/t optimization

The Deep in Deep Learning

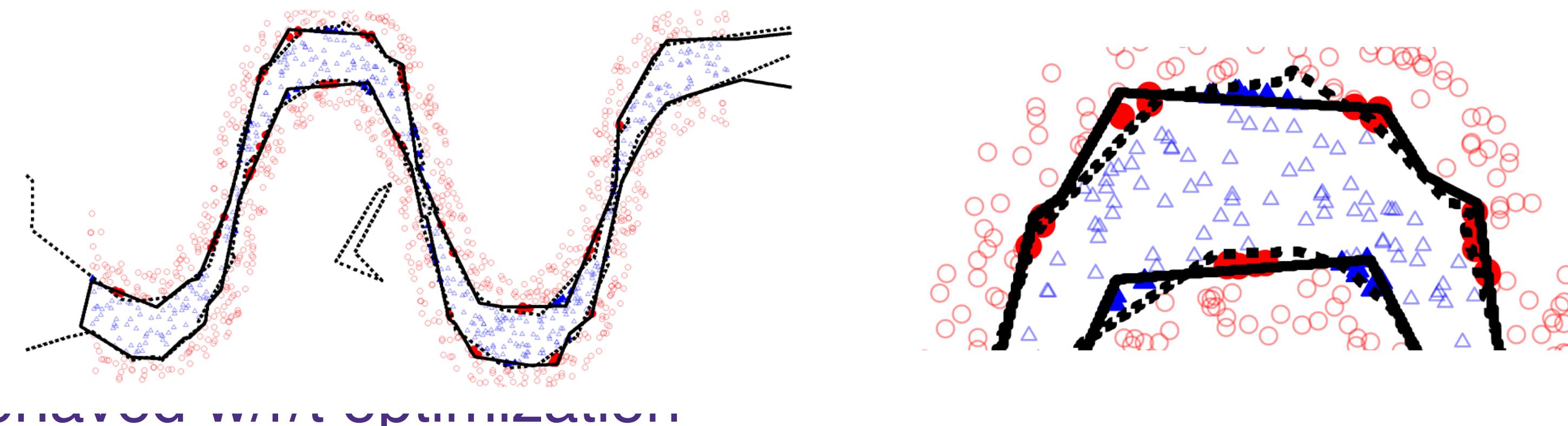
- The Universal Approximation Theorem says that one hidden layer suffices for arbitrarily-closely approximating a given function
- Empirical demonstration
- “Deep and narrow” vs “shallow and wide”
- In principle, “deep and narrow” is better
- More well-tuned optimization



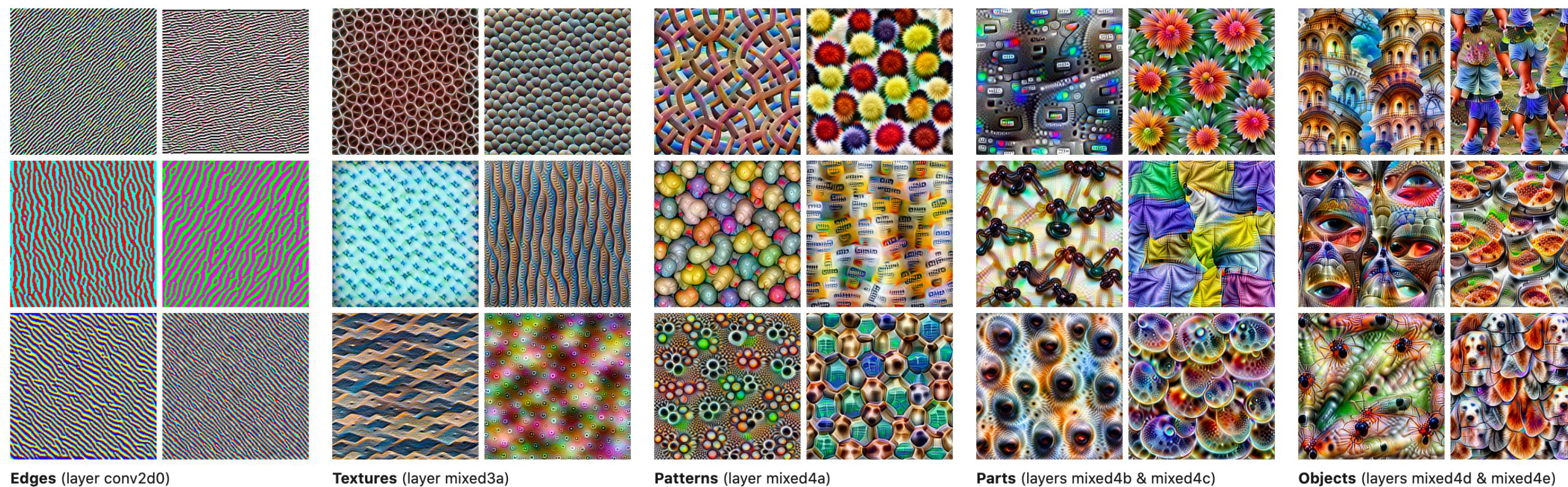
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Activation Functions

- 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
 - Composition of linear transformations is *also* linear!

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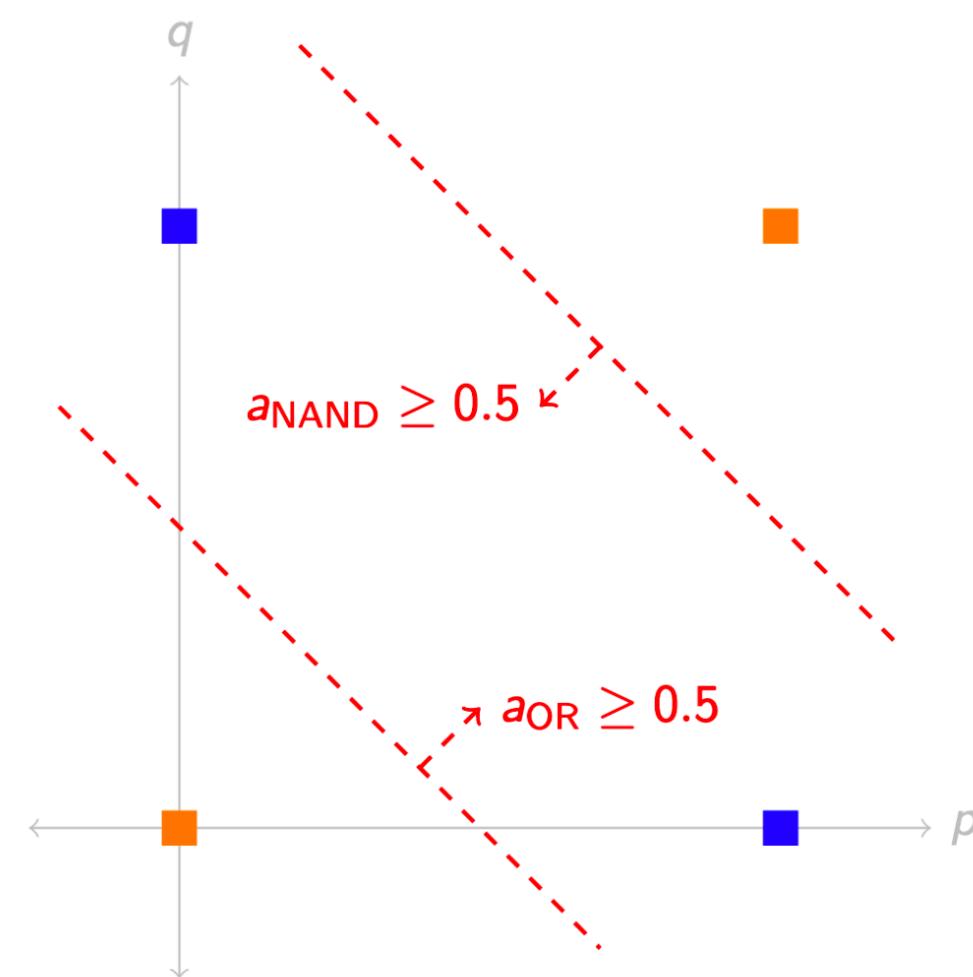
Non-linearity, cont.

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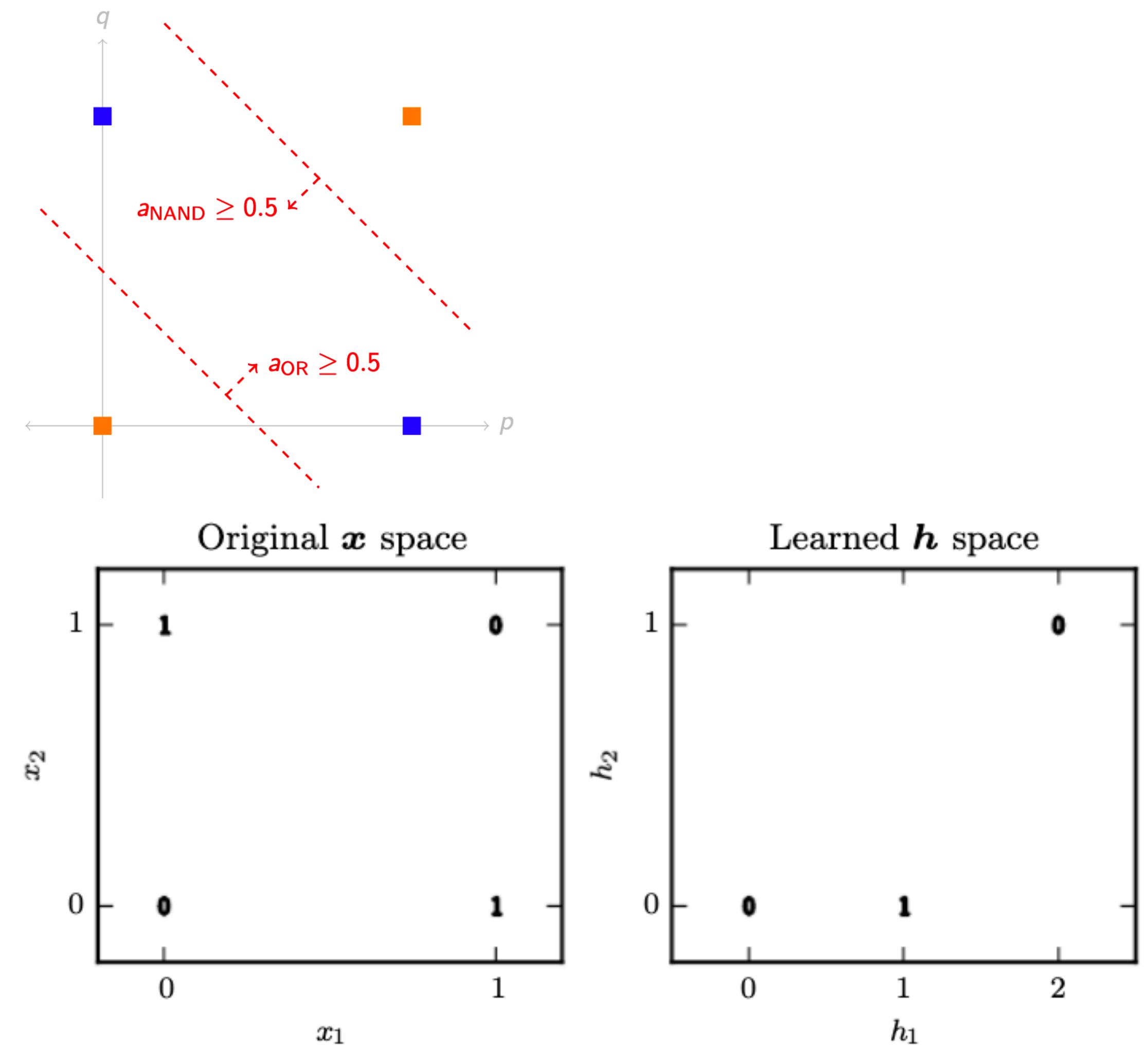
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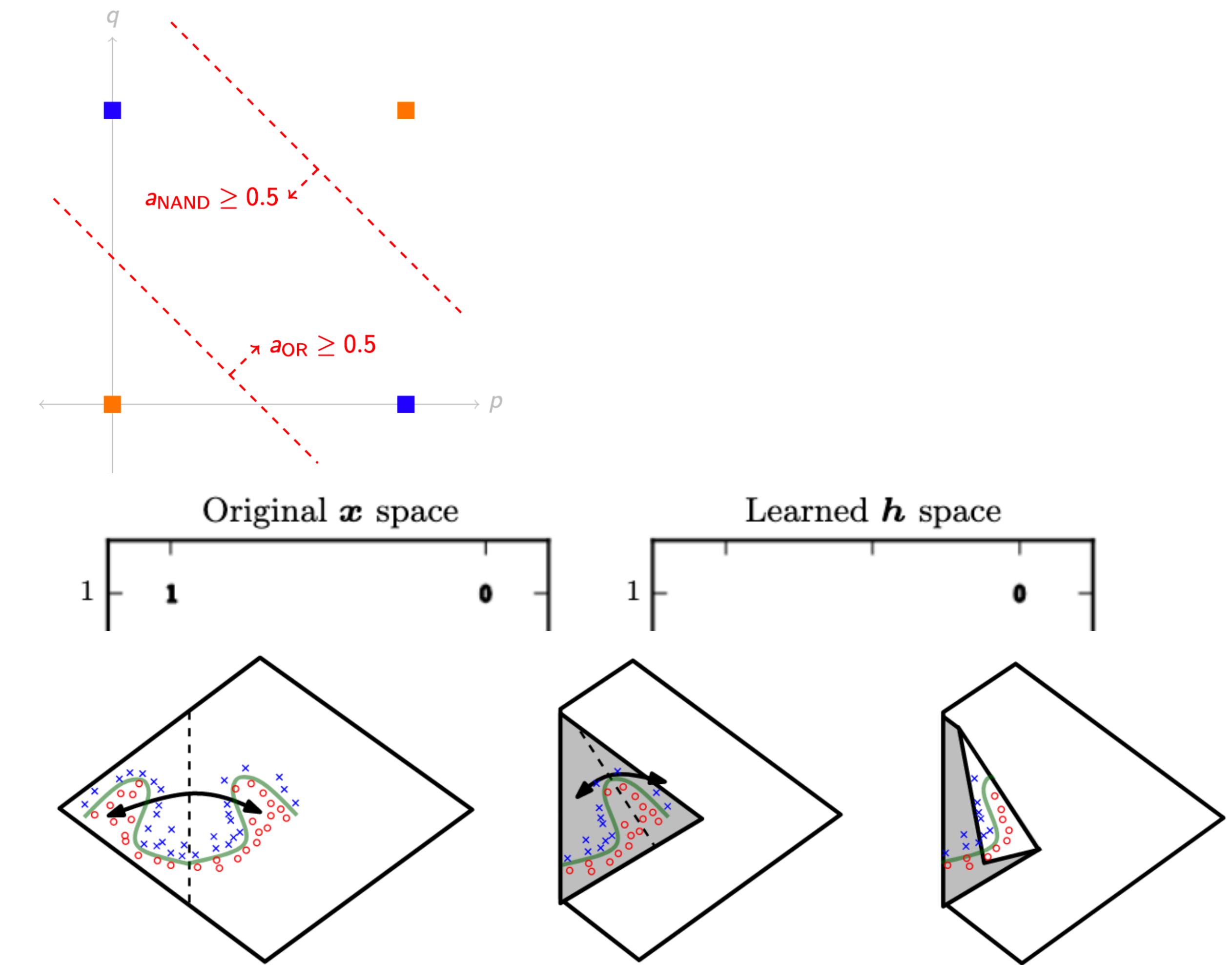
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- An equivalent perspective:
 - Transforming the input space ([source](#); p. 169)
 - This is a *non-linear* transformation
 - Space folding intuition more generally (also GBC sec 6.4.1)



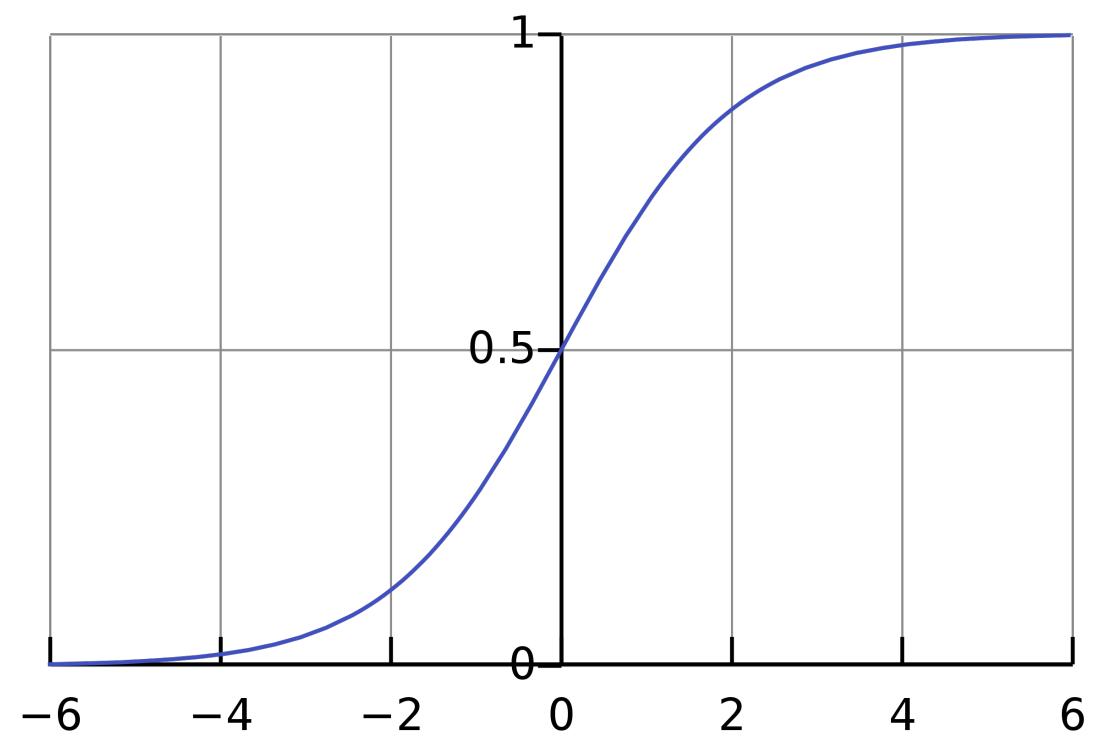
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Activation Functions: Hidden Layer

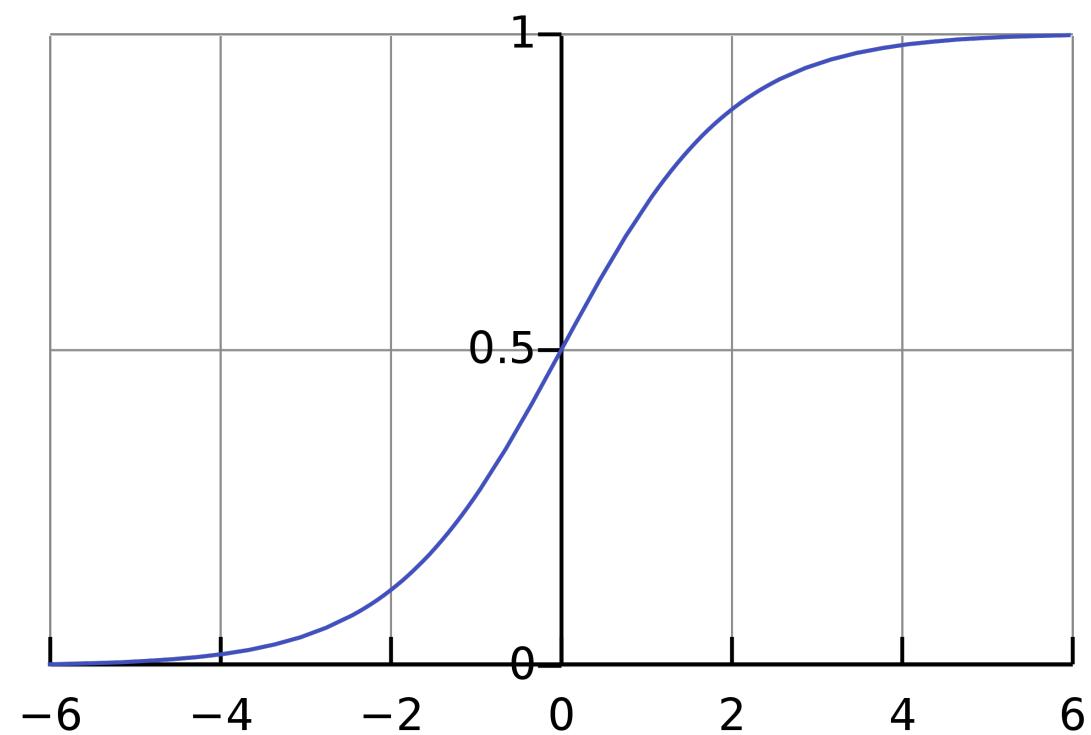
sigmoid



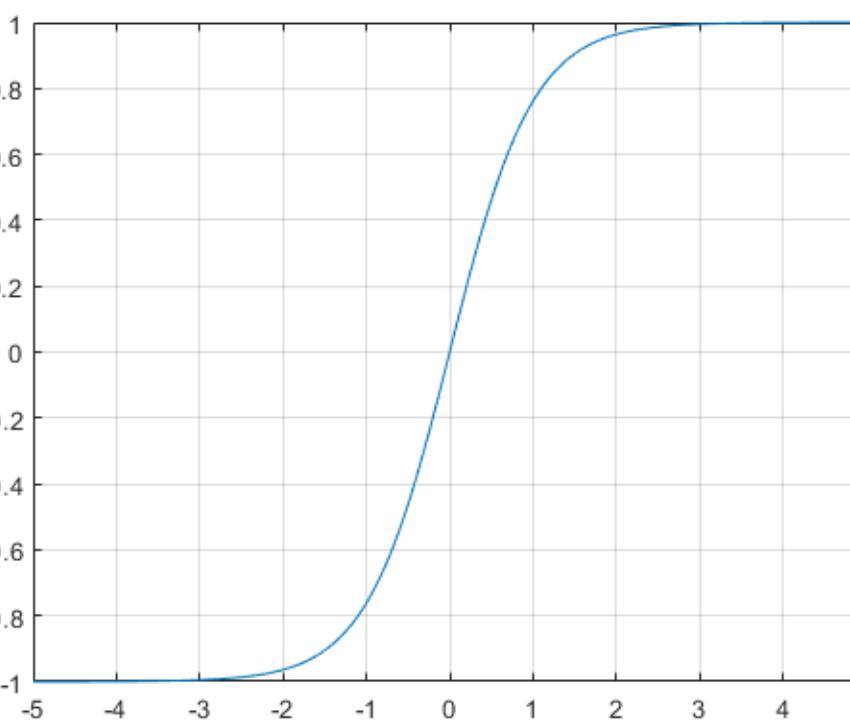
$$\sigma(x) = \frac{1}{1 + e^{-x}} = \frac{e^x}{e^x + 1}$$

Activation Functions: Hidden Layer

sigmoid



tanh

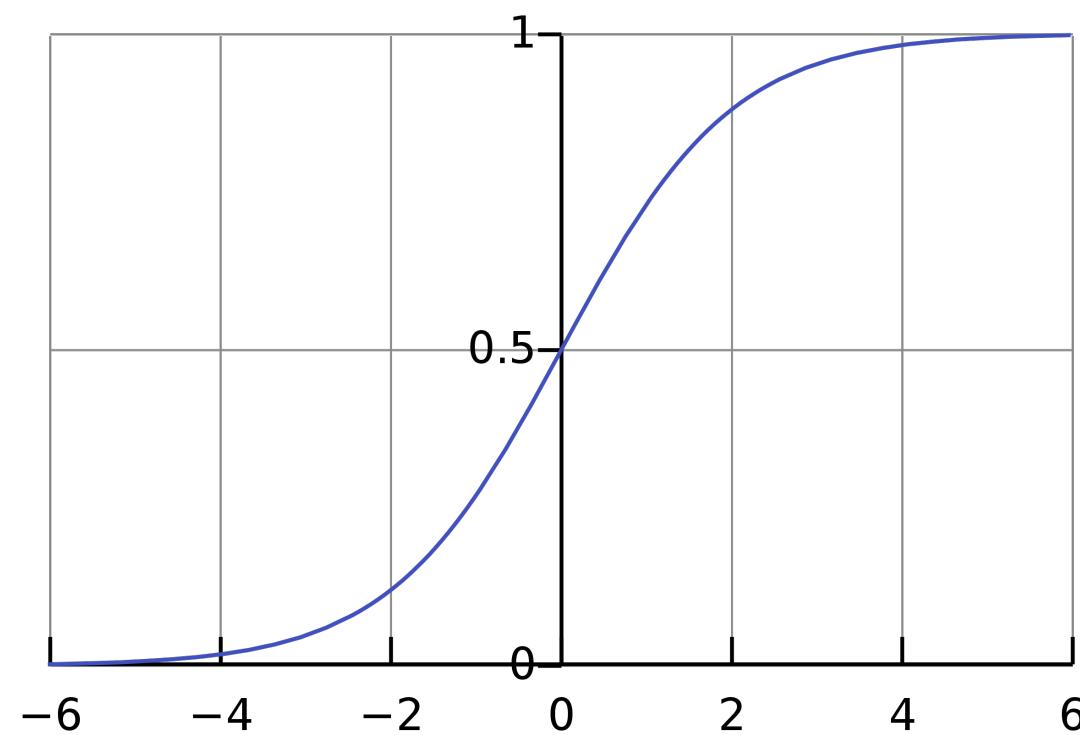


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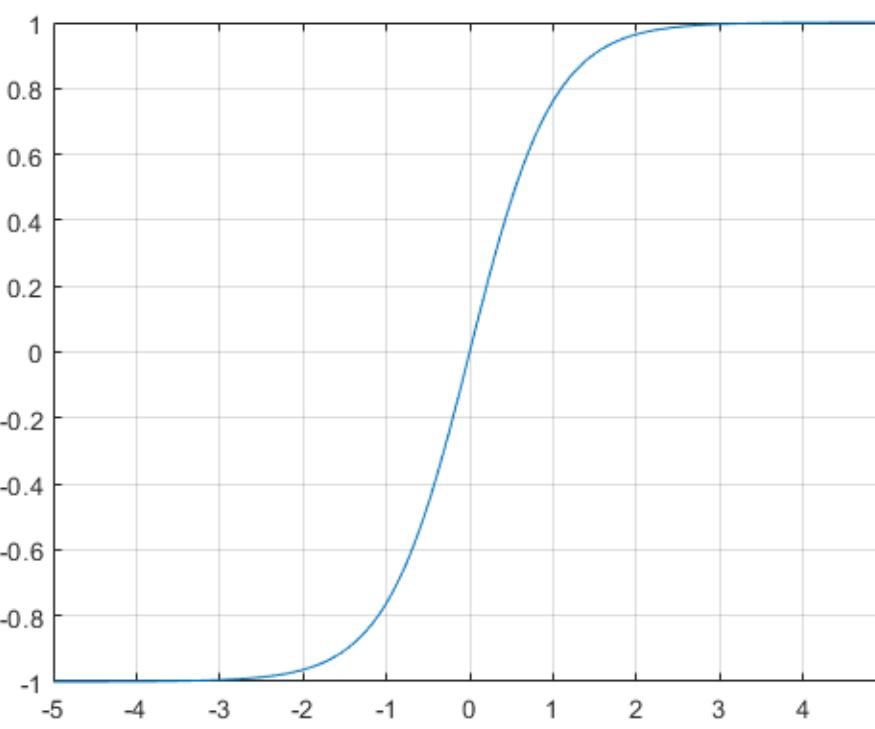
$$\tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}} = 2\sigma(2x) - 1$$

Activation Functions: Hidden Layer

sigmoid



tanh



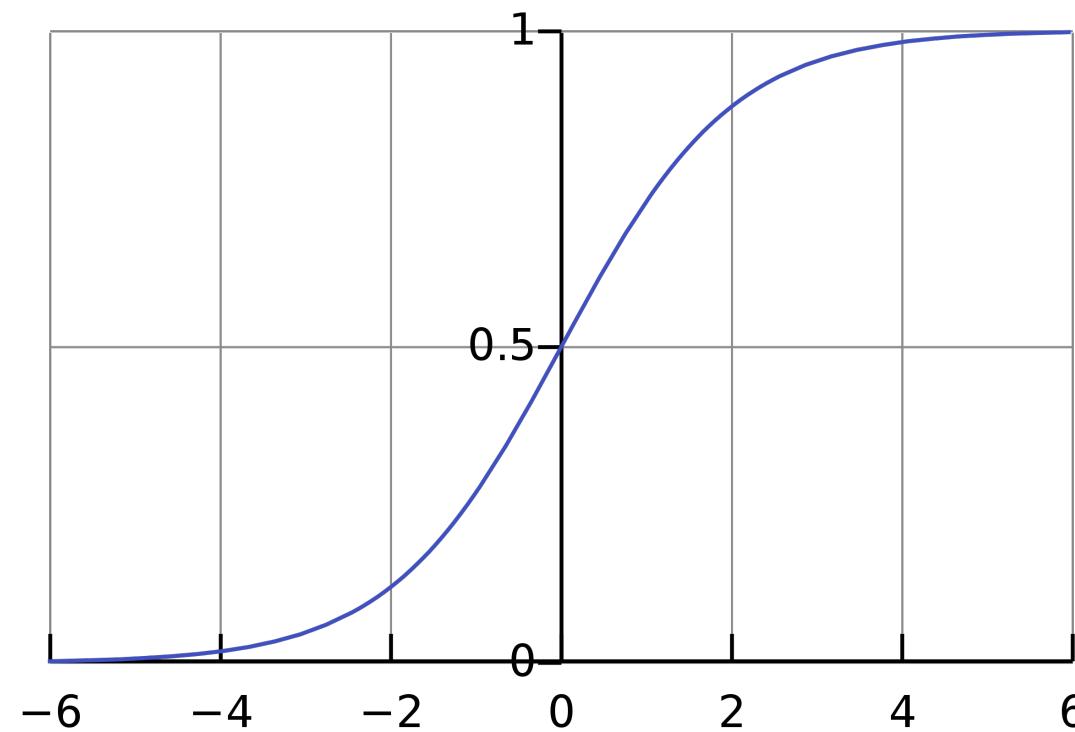
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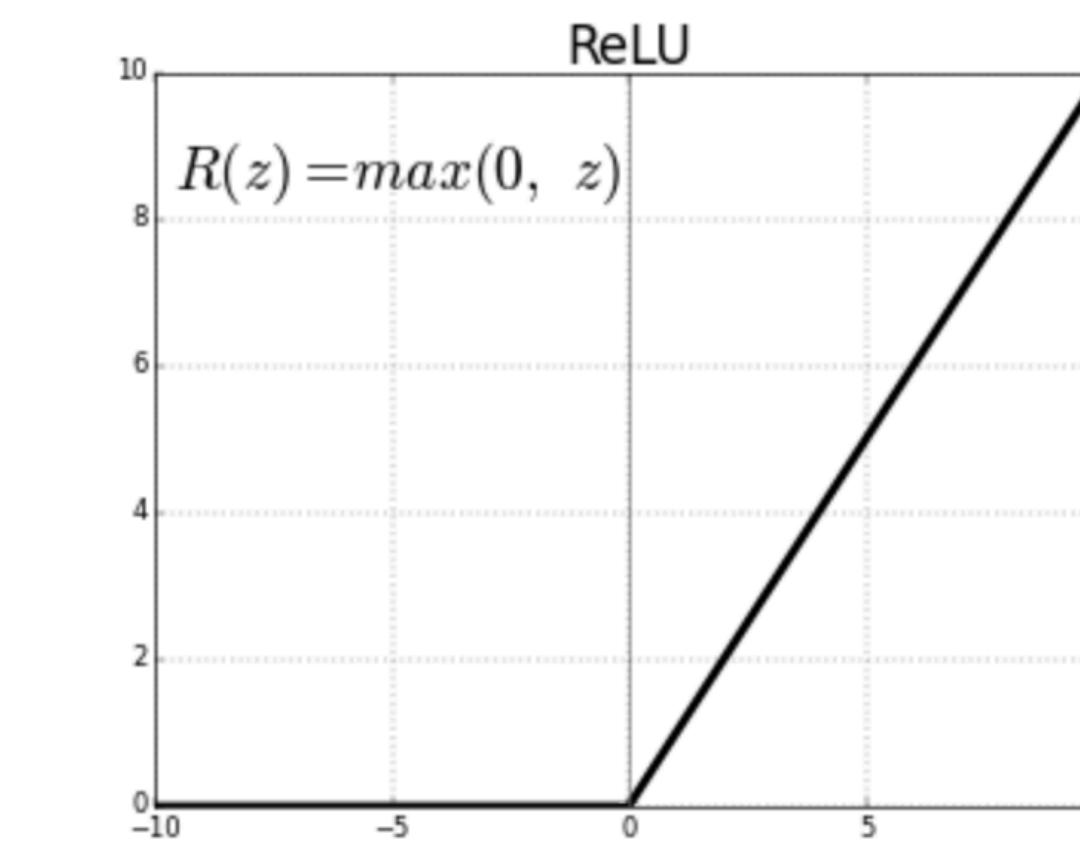
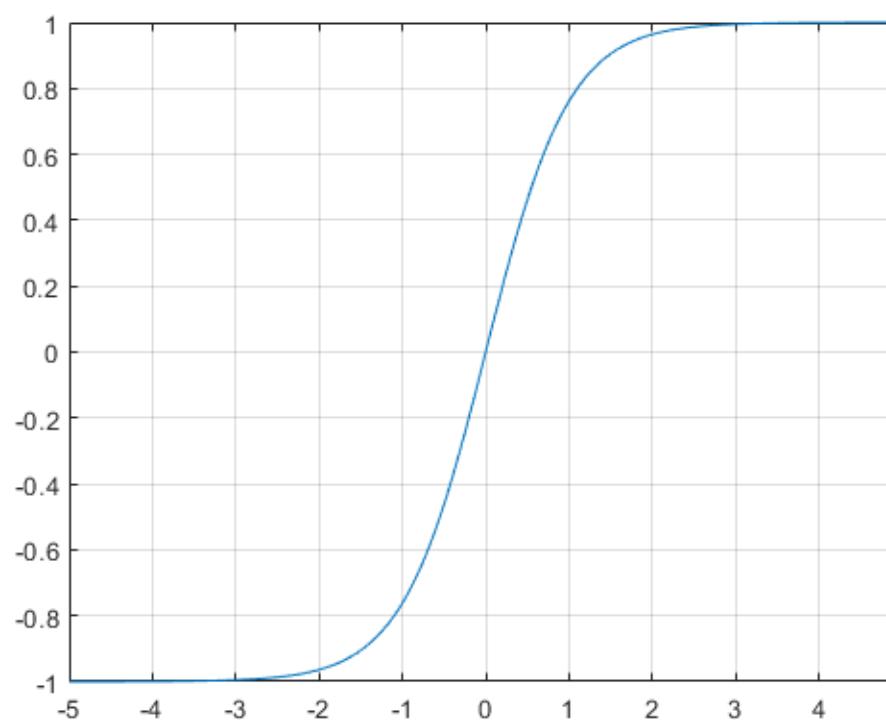
Problem: derivative “saturates” (nearly 0)
everywhere except near origin

Activation Functions: Hidden Layer

sigmoid



tanh



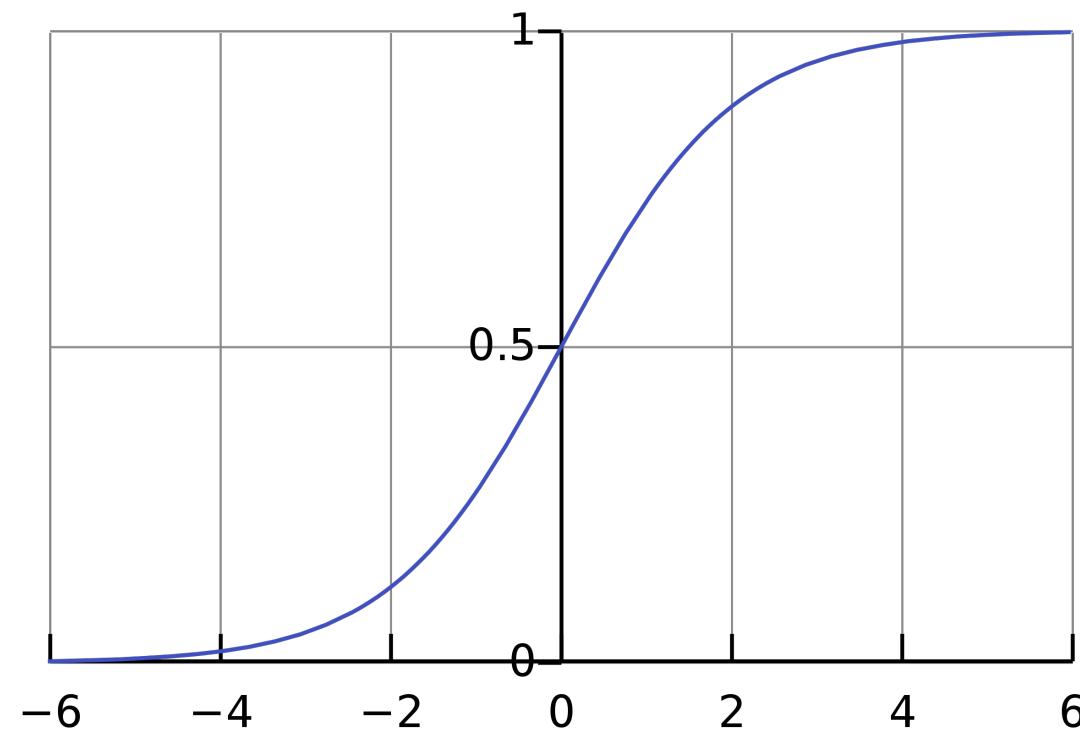
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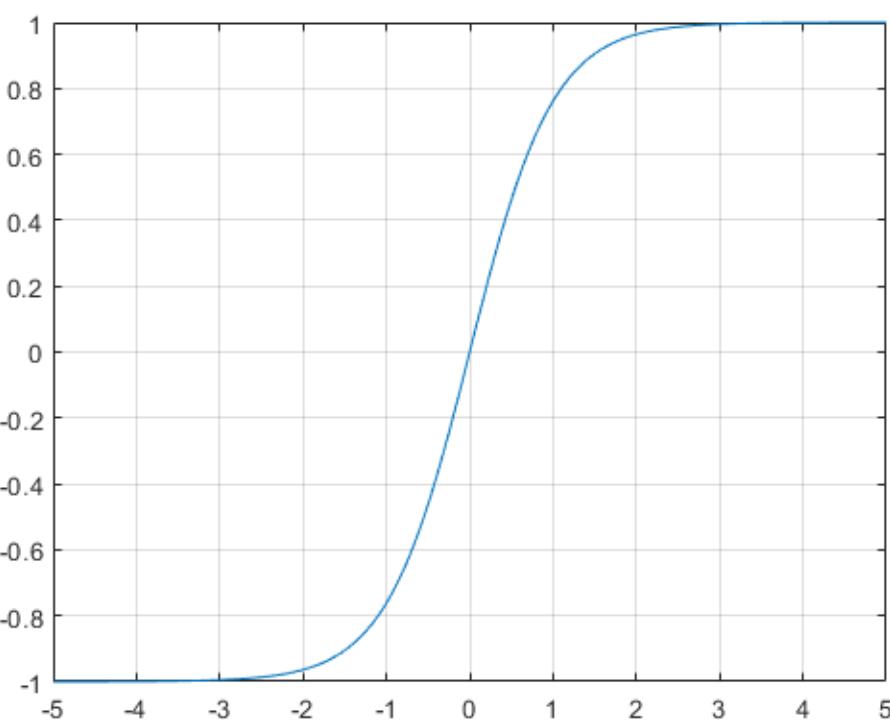
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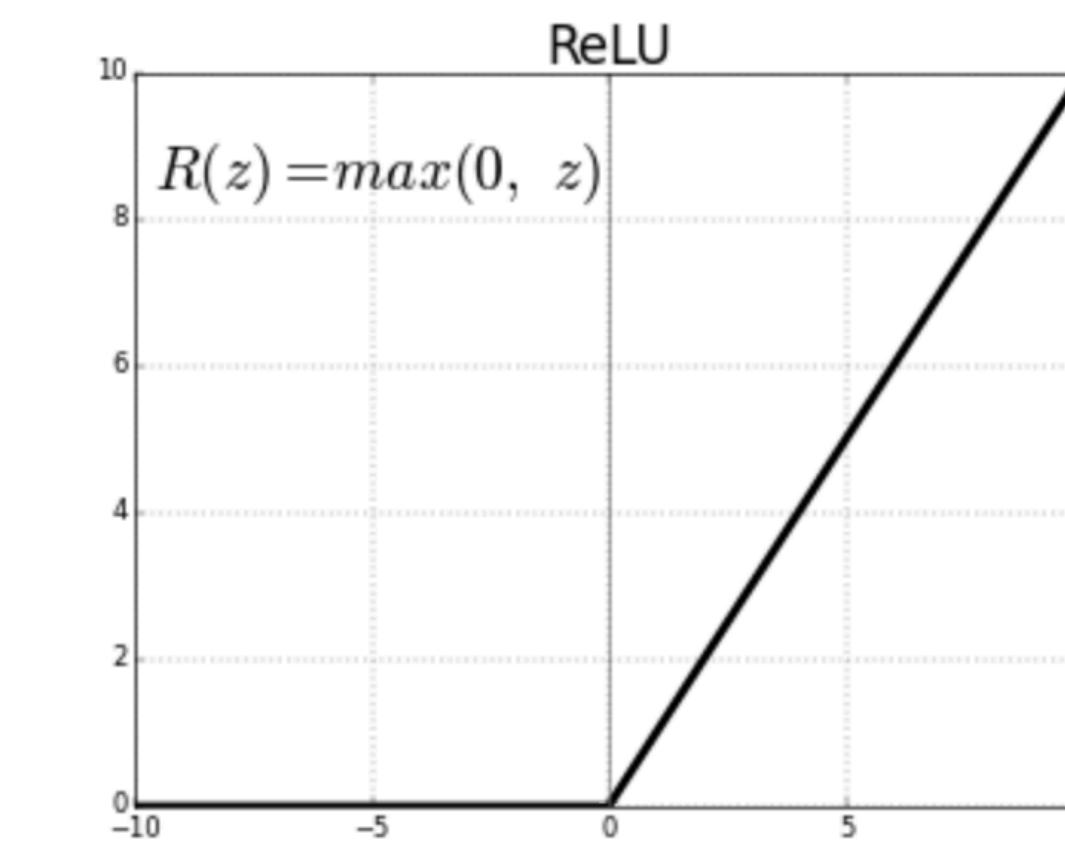
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Problem: derivative “saturates” (nearly 0)
everywhere except near origin



- Use ReLU by default
- Generalizations:
 - Leaky
 - ELU
 - GELU
 - 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

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

$$x = [x_0 \ x_1 \ \cdots \ x_{n_0}]$$

Shape: $(1, n_0)$

$$b^1 = [b_0^1 \ b_1^1 \ \cdots \ b_{n_1}^1]$$

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

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

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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
 - Produce a sequence of representations, *for each item* in the batch
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 - Images: (batch_size, width, height, 3)
 - Sequences: (batch_size, seq_len, representation_size)
- Two comments:
 - In your code, **annotate every tensor** with a comment saying intended shape
 - When debugging, look at shapes early on!!

Next Time

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