Neural Network Introduction

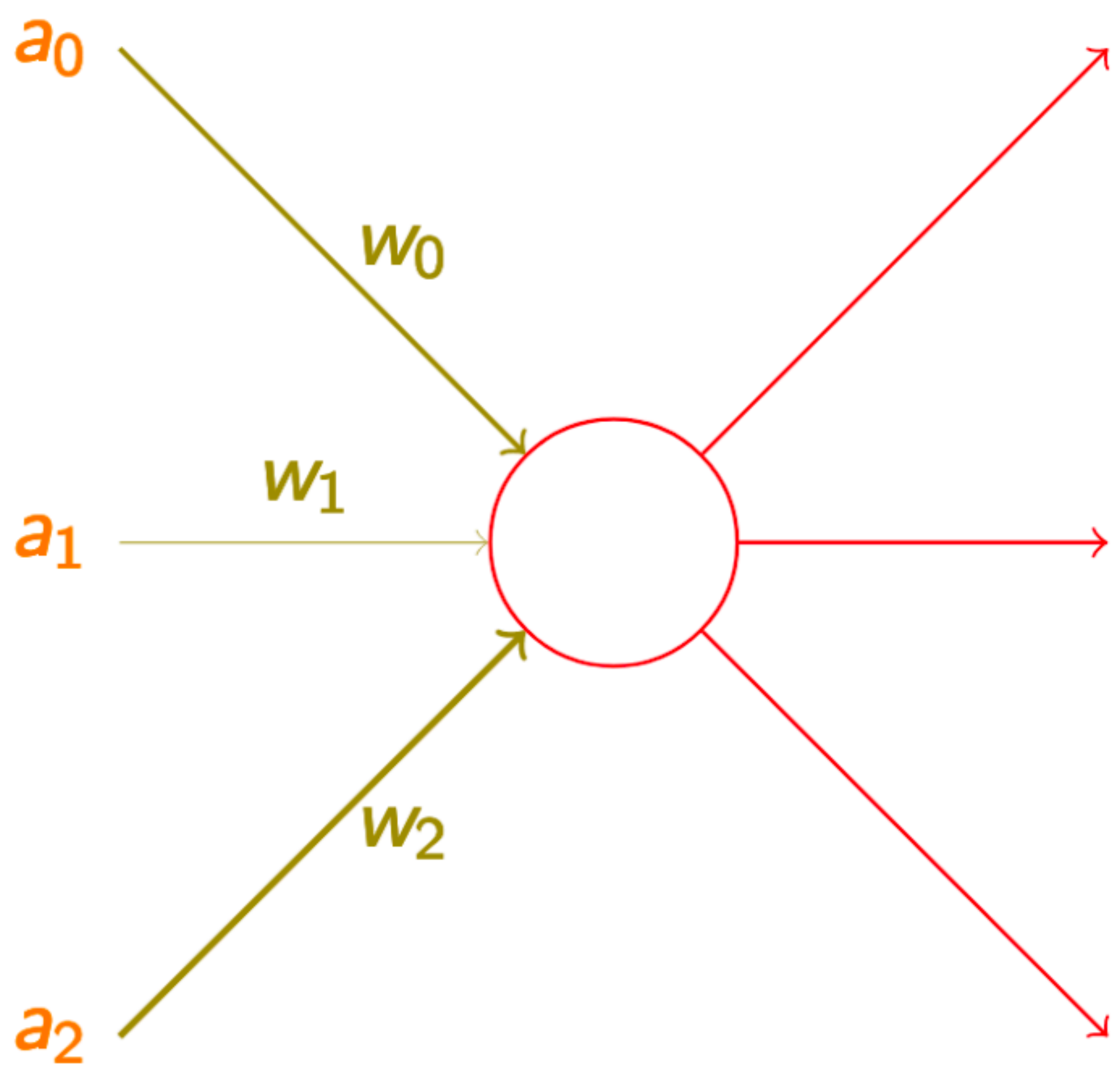
Ling 575j: Deep Learning for NLP
C.M. Downey
Spring 2023

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

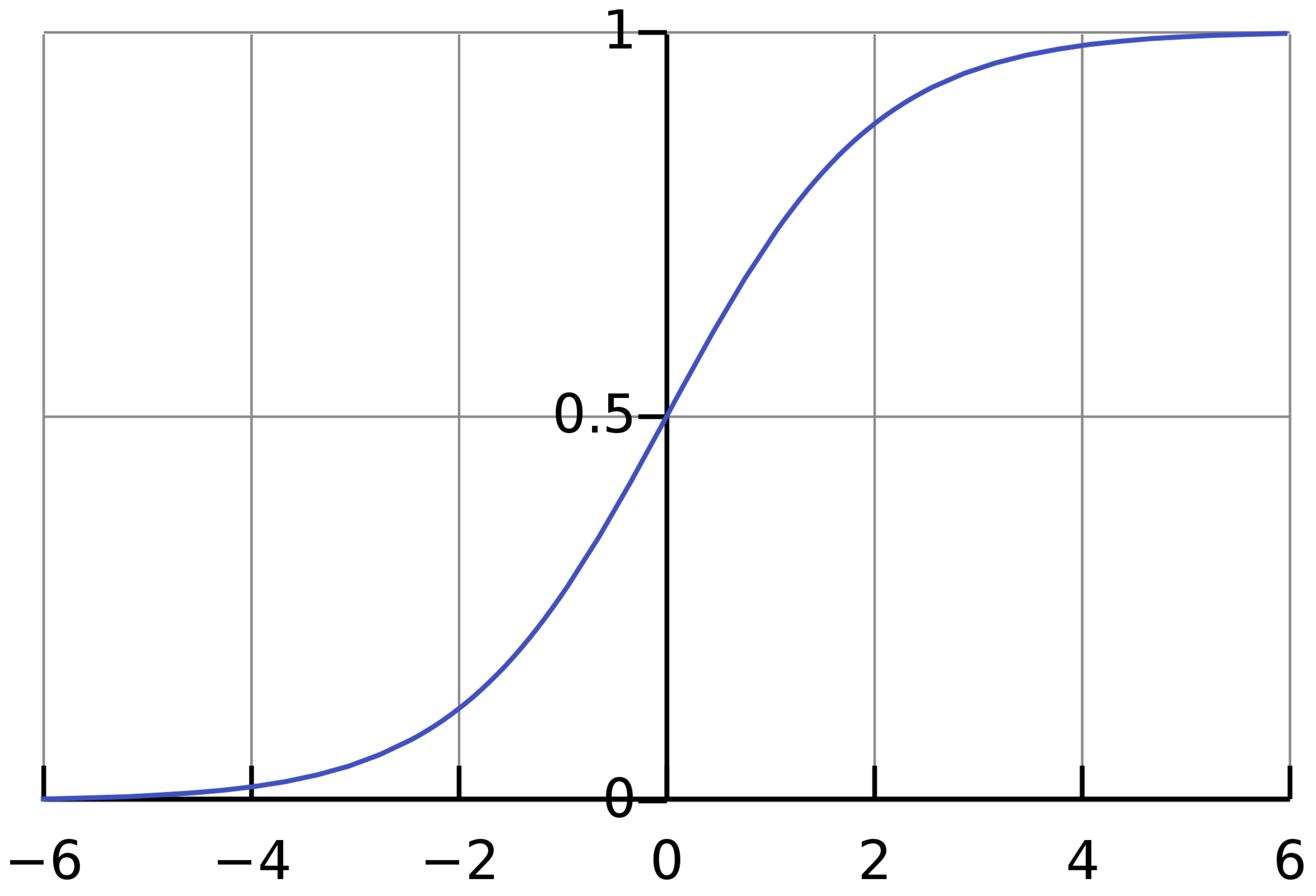
Artificial Neuron



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

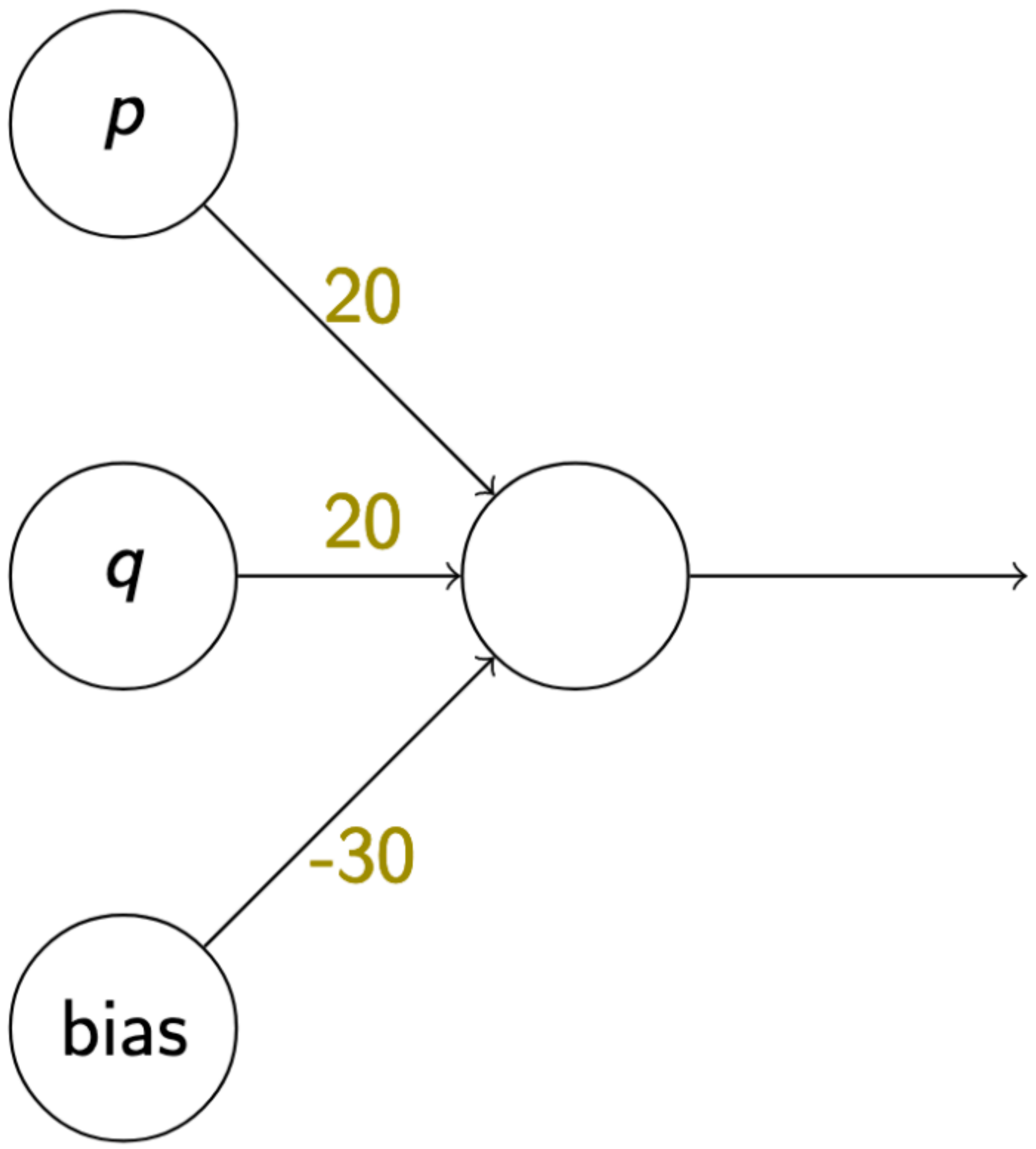
https://github.com/shanest/nn-tutorial

Activation Function: Sigmoid



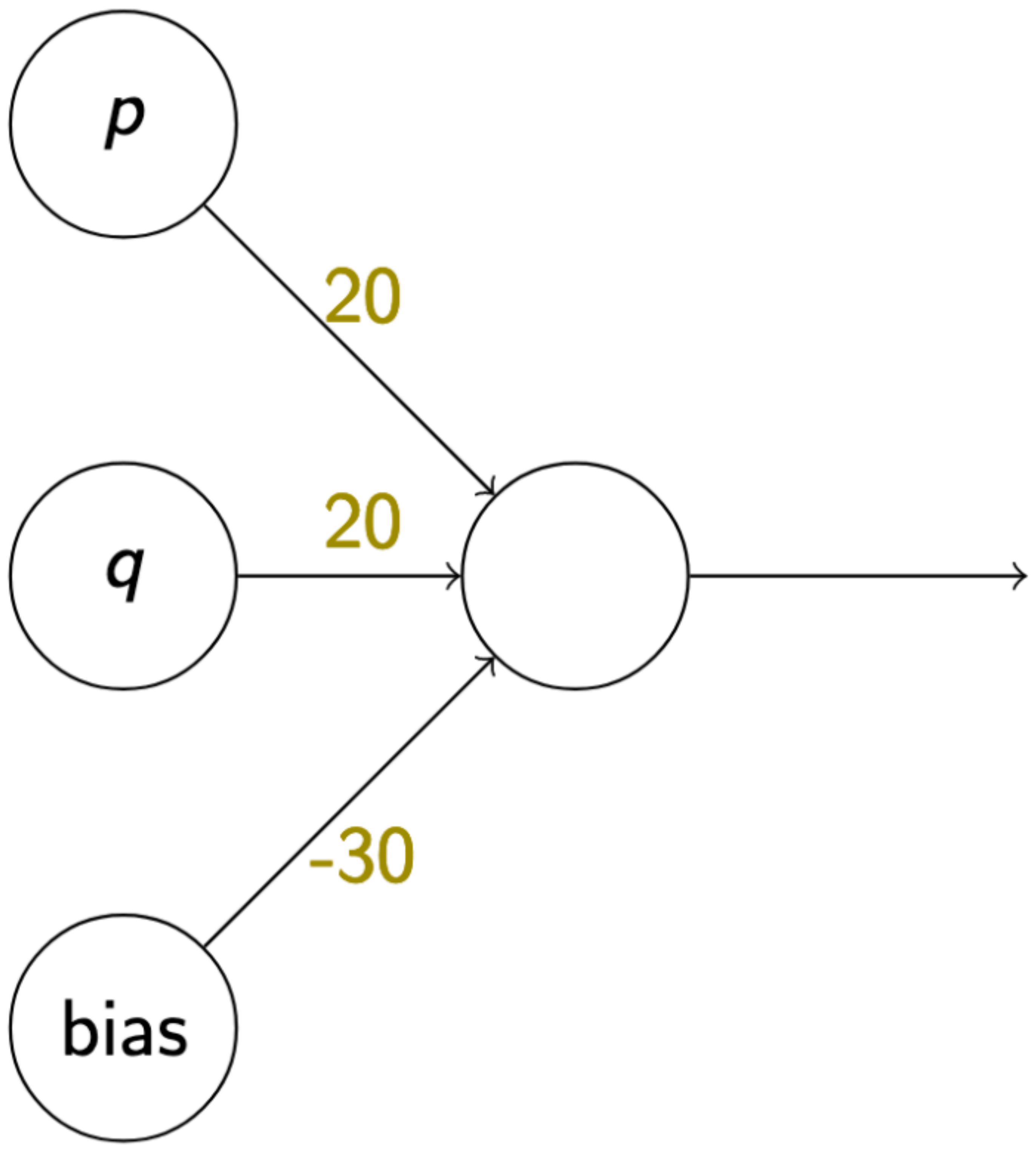
$$\sigma(x) = \frac{1}{1 + e^{-x}} = \frac{e^x}{e^x + 1}$$

Computing a Boolean function



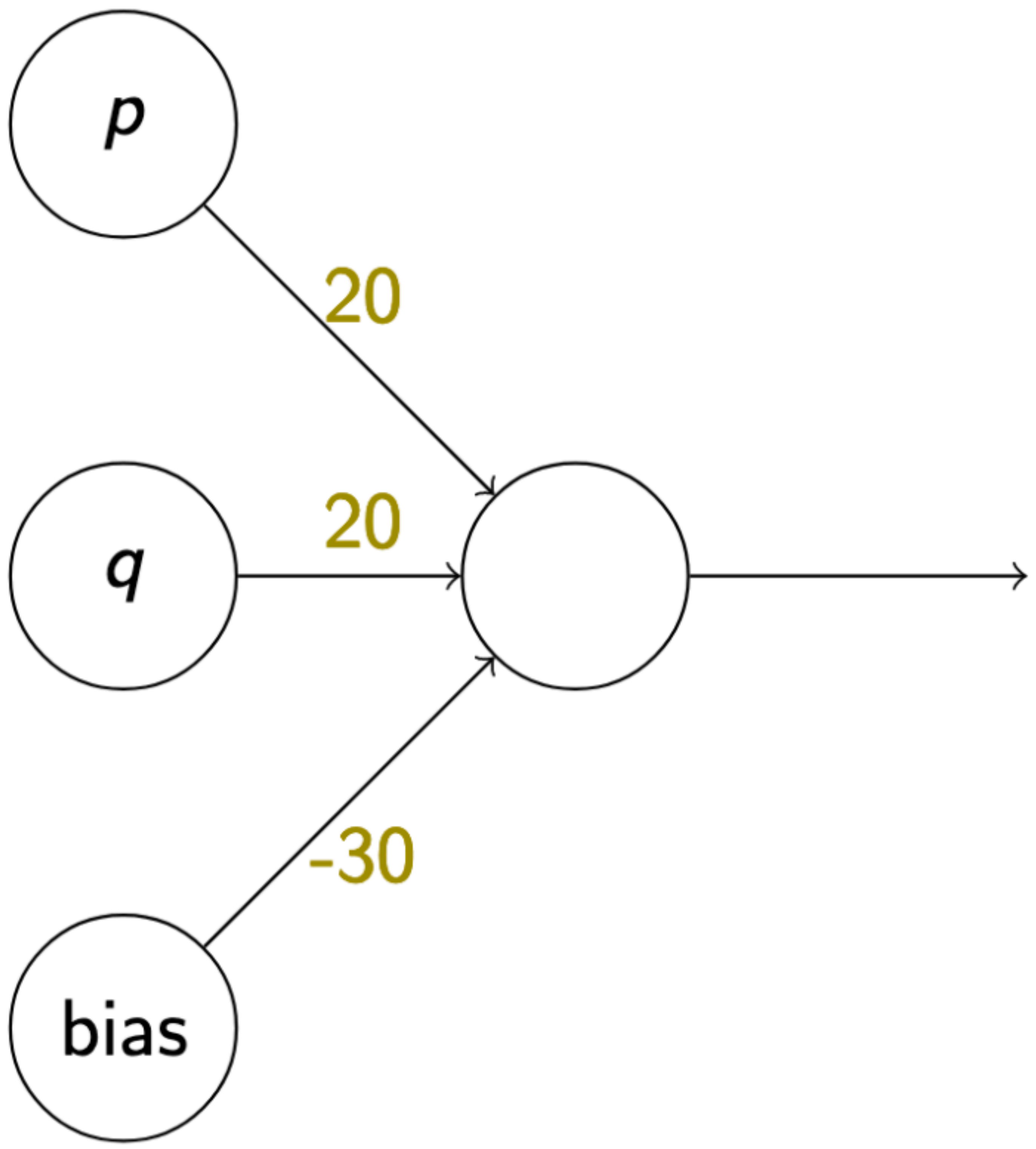
Computing a Boolean function

p	q	a



Computing a Boolean function

p	q	a
1	1	1



Computing a Boolean function

p	q	a
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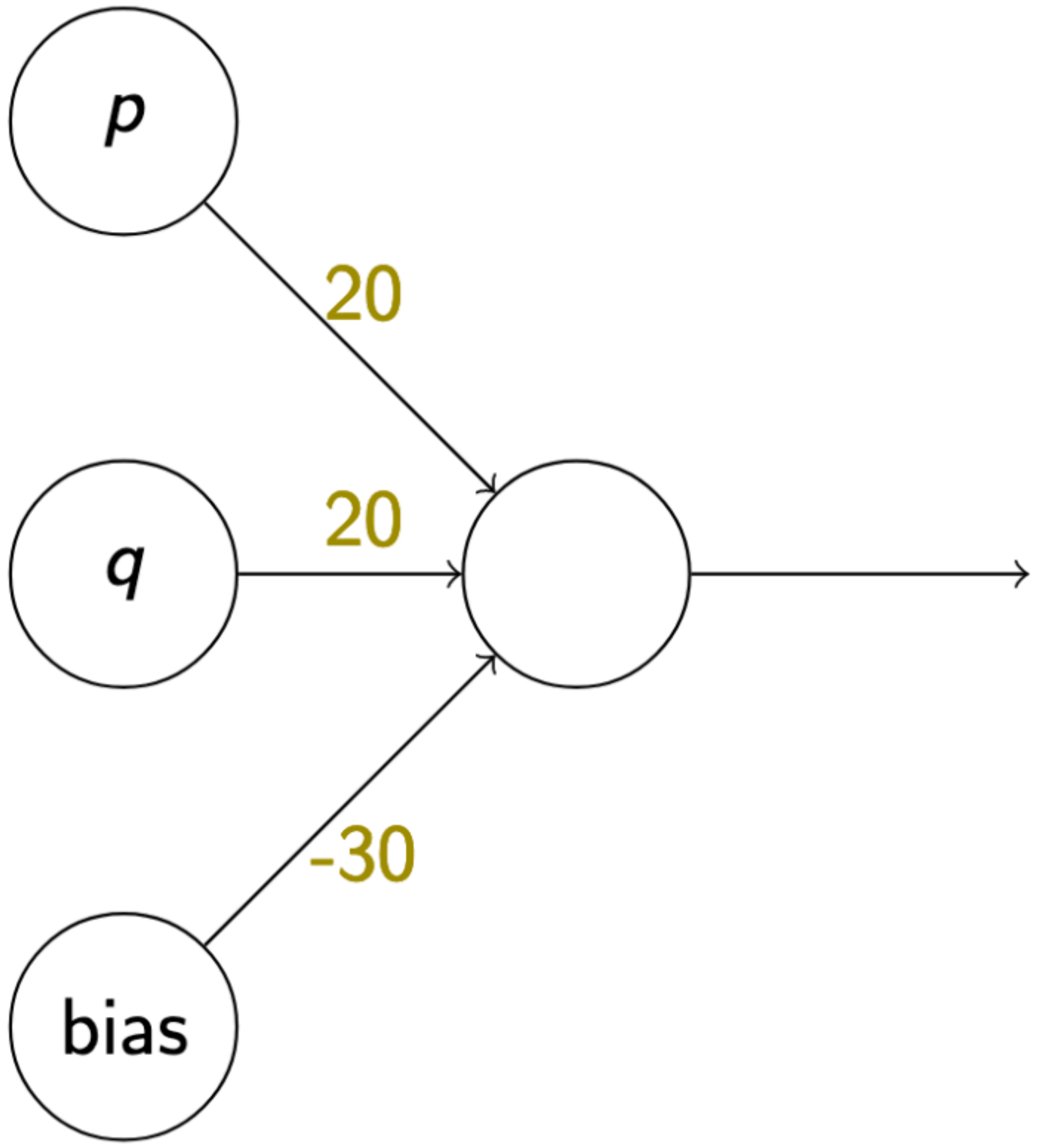
1	0	0



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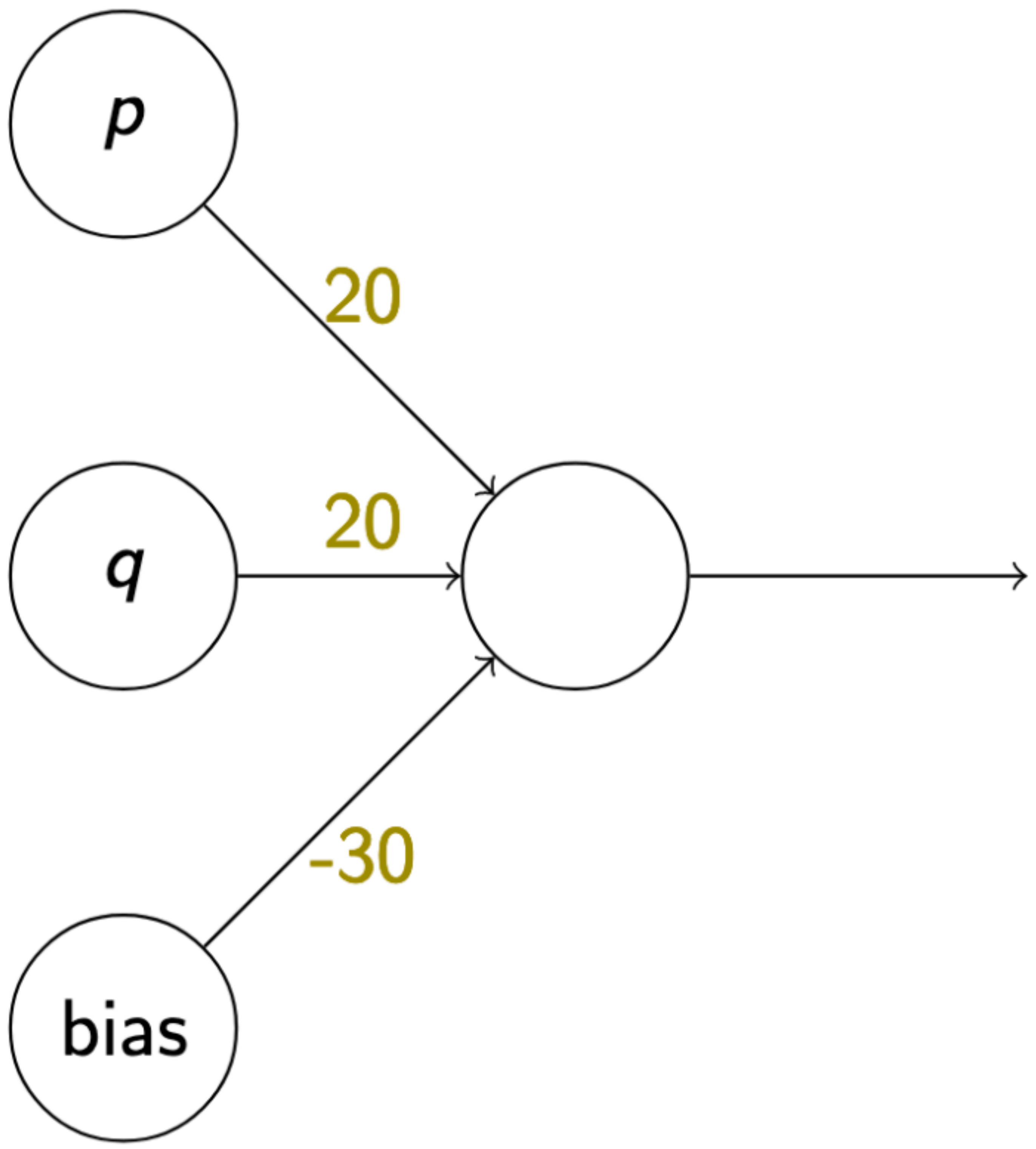

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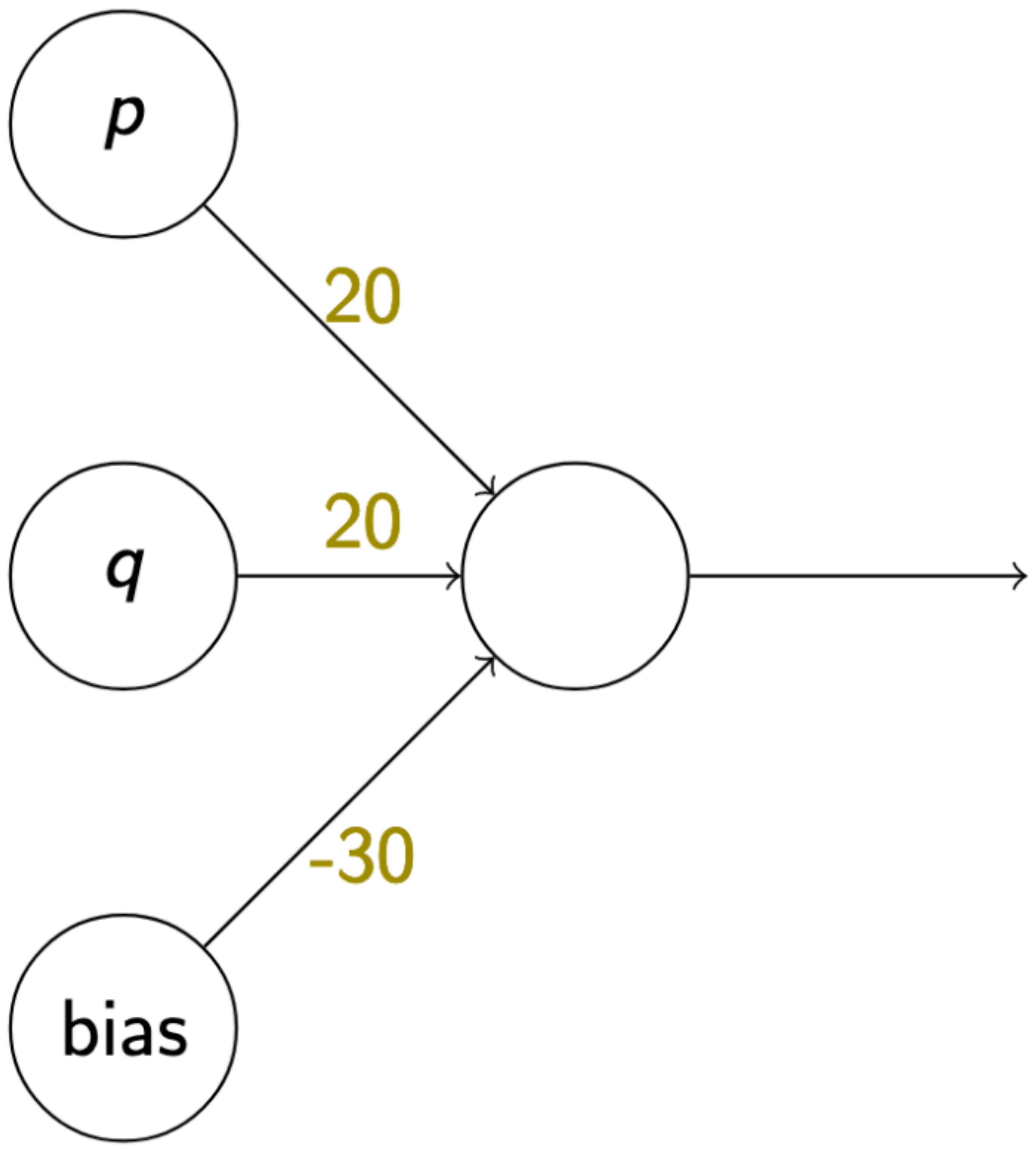
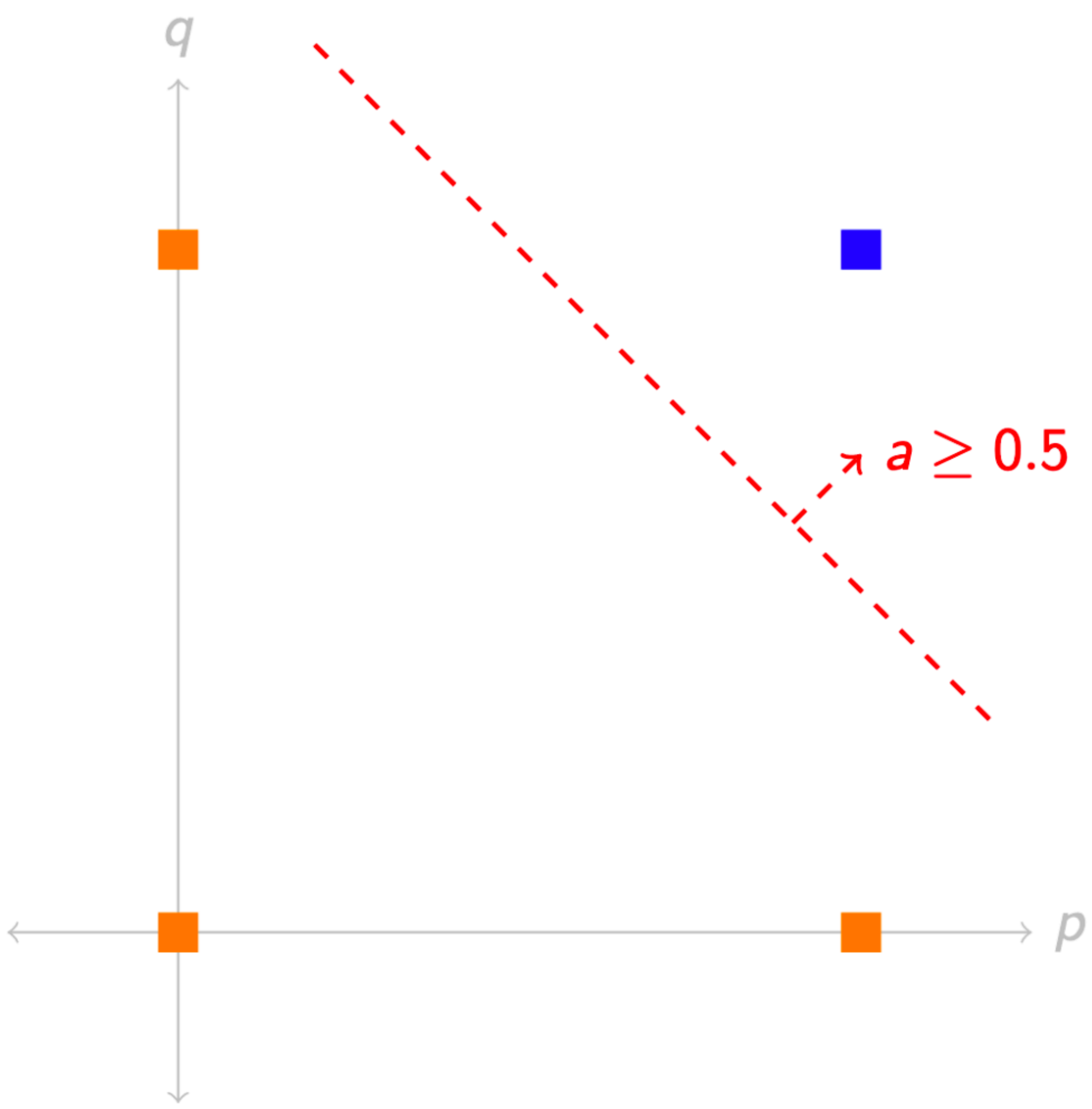
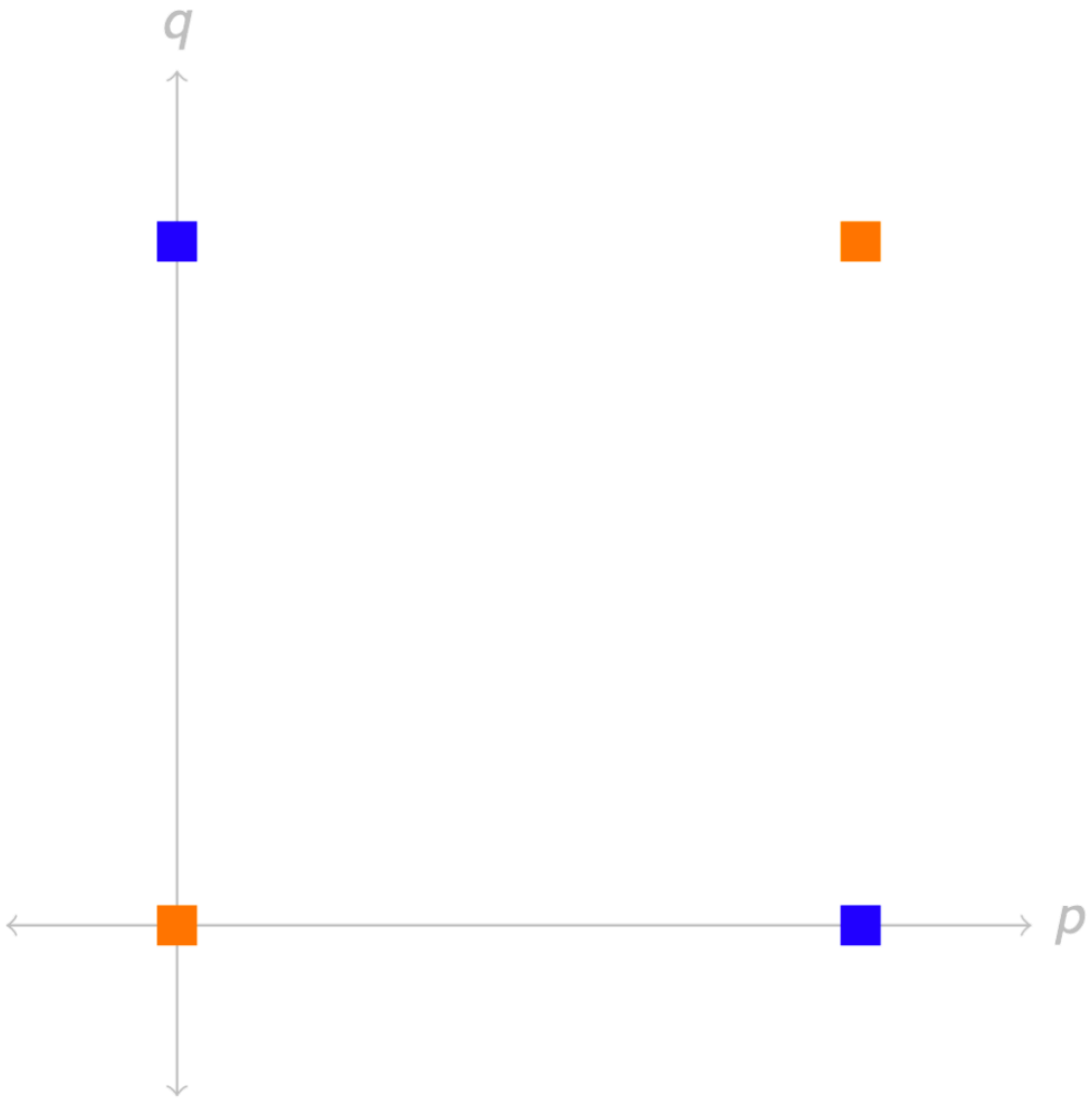


Computing ‘and’



The XOR problem



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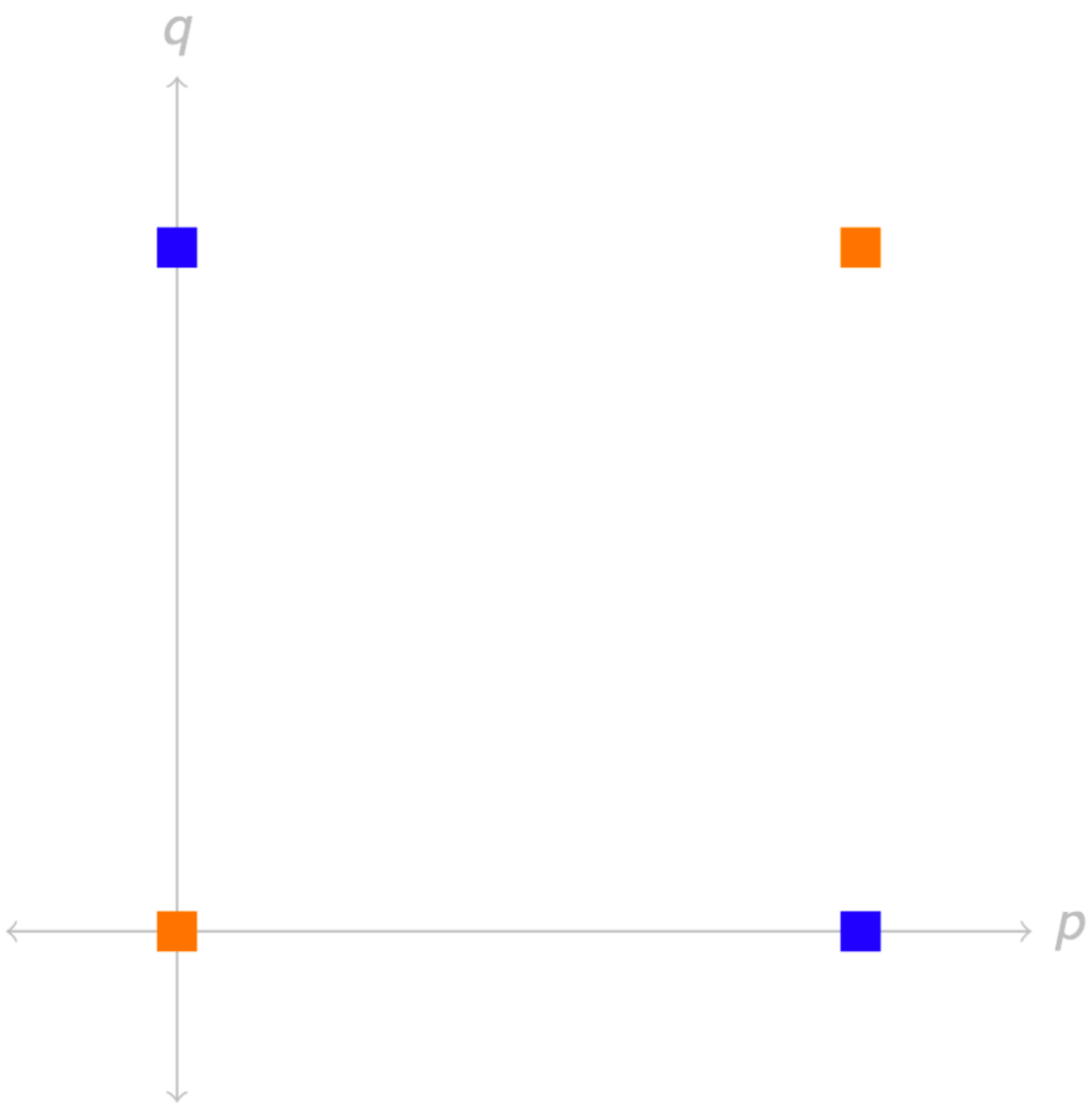
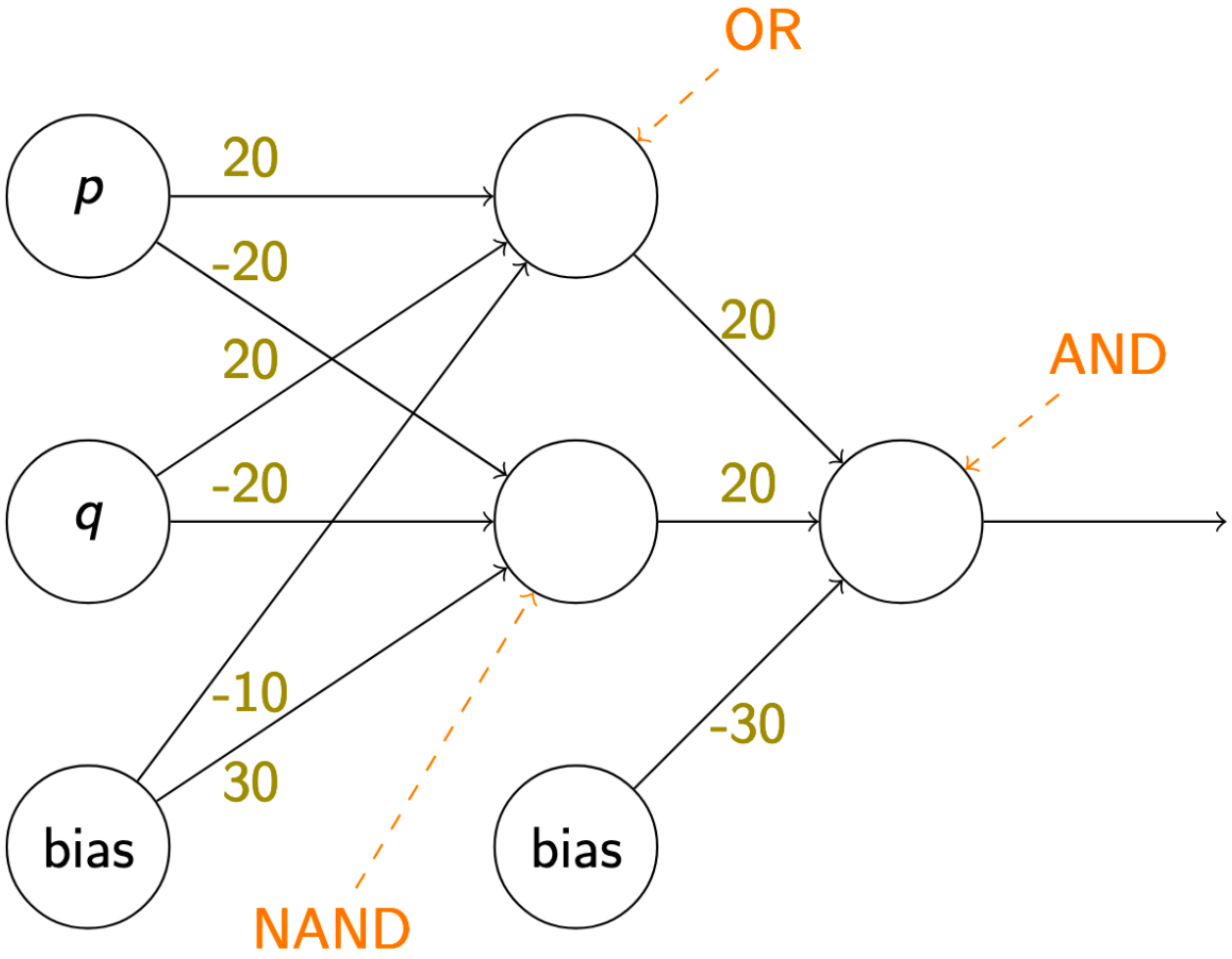


XOR is not linearly separable

Computing XOR



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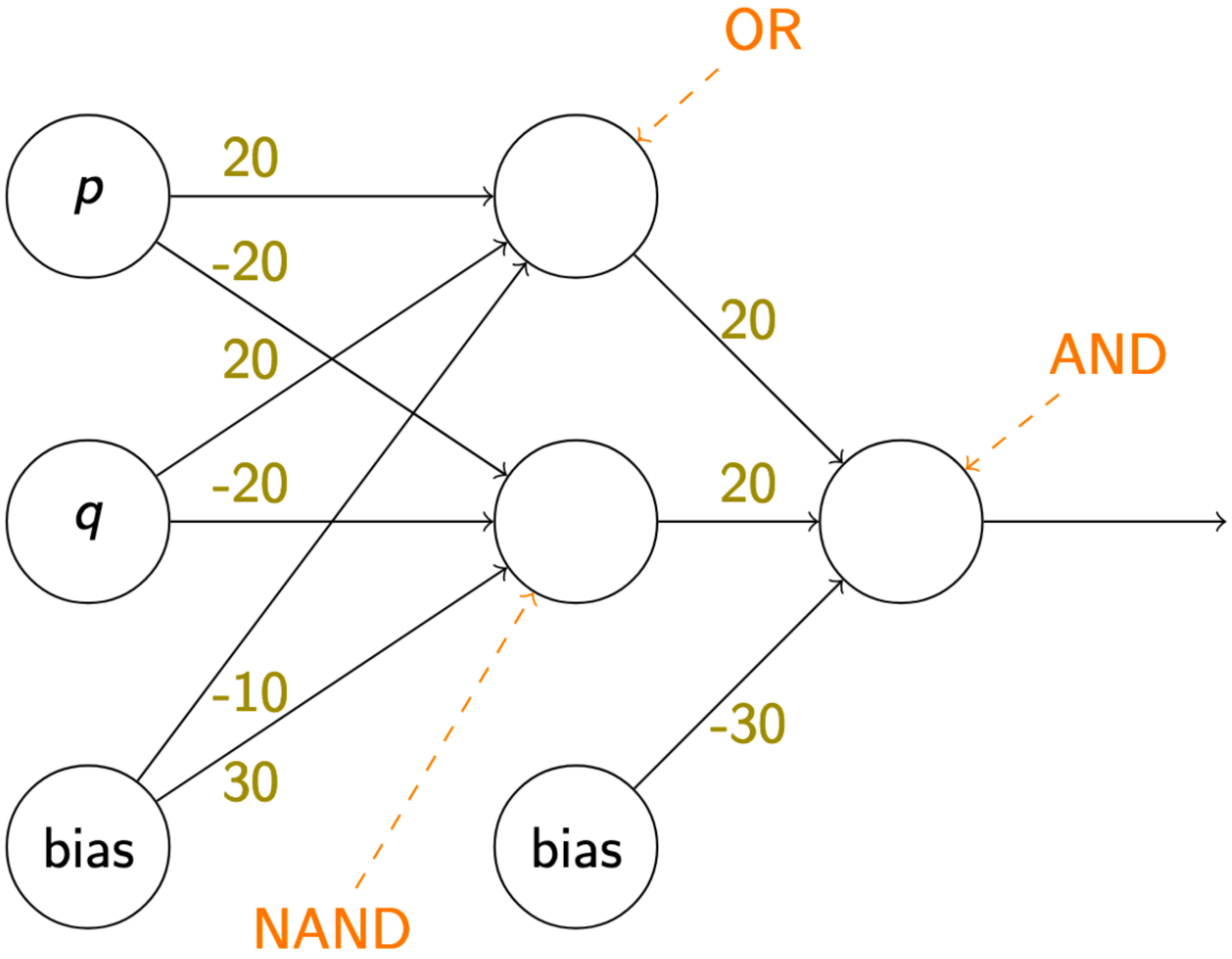
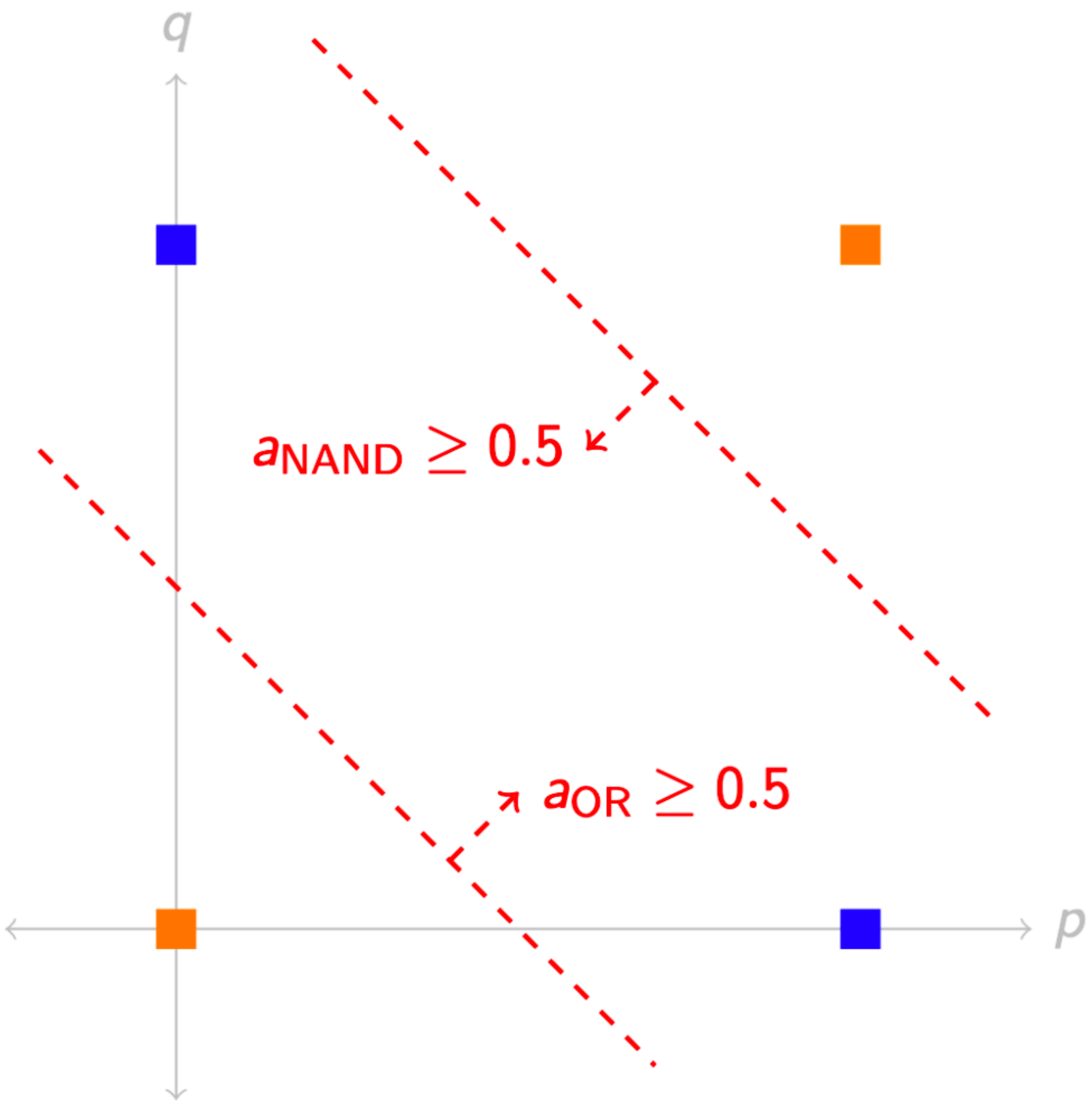


Exercise: show that
NAND behaves as described.

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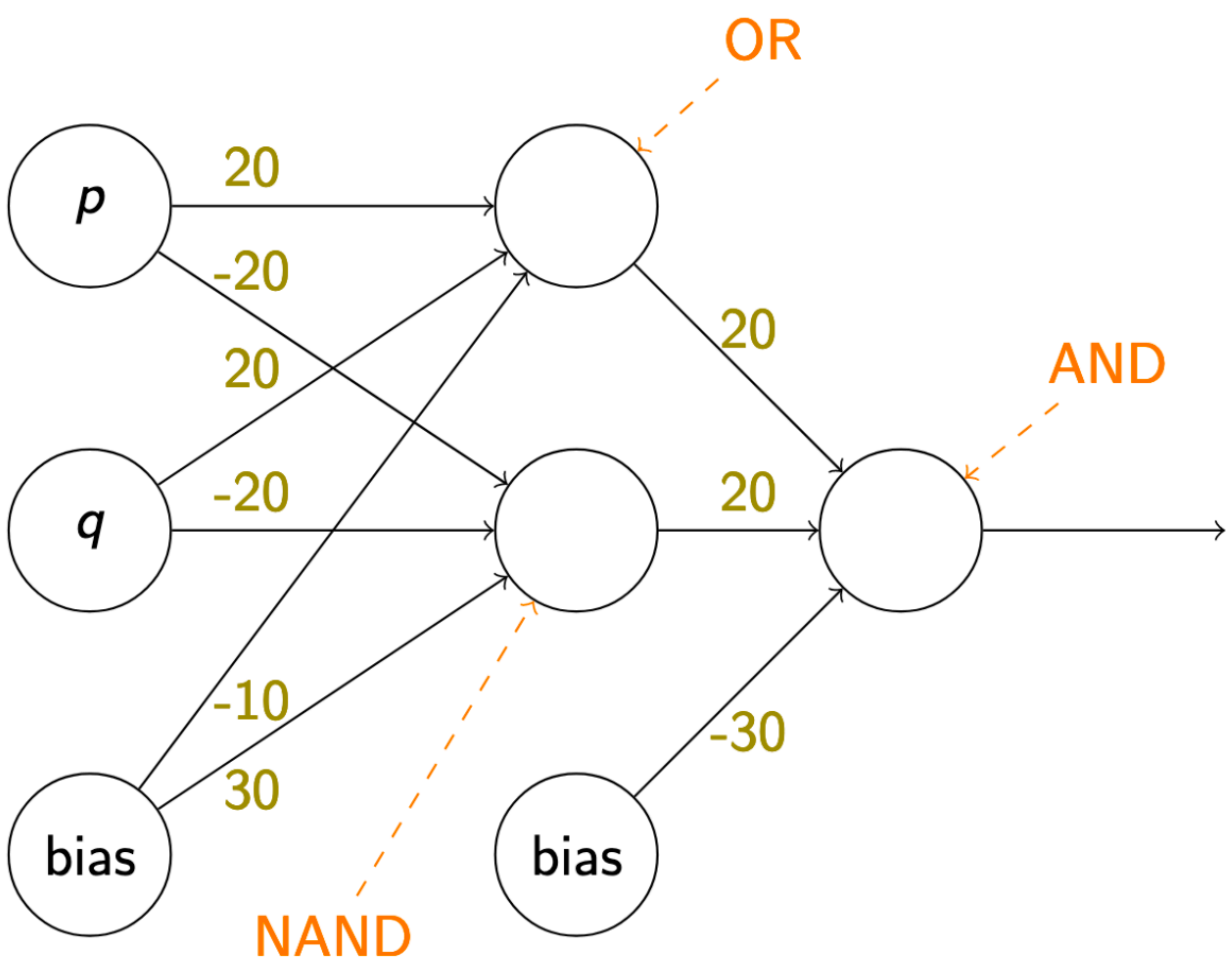
- See also GBC 6.4.1 for more references, generalizations, discussion

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

XOR Network



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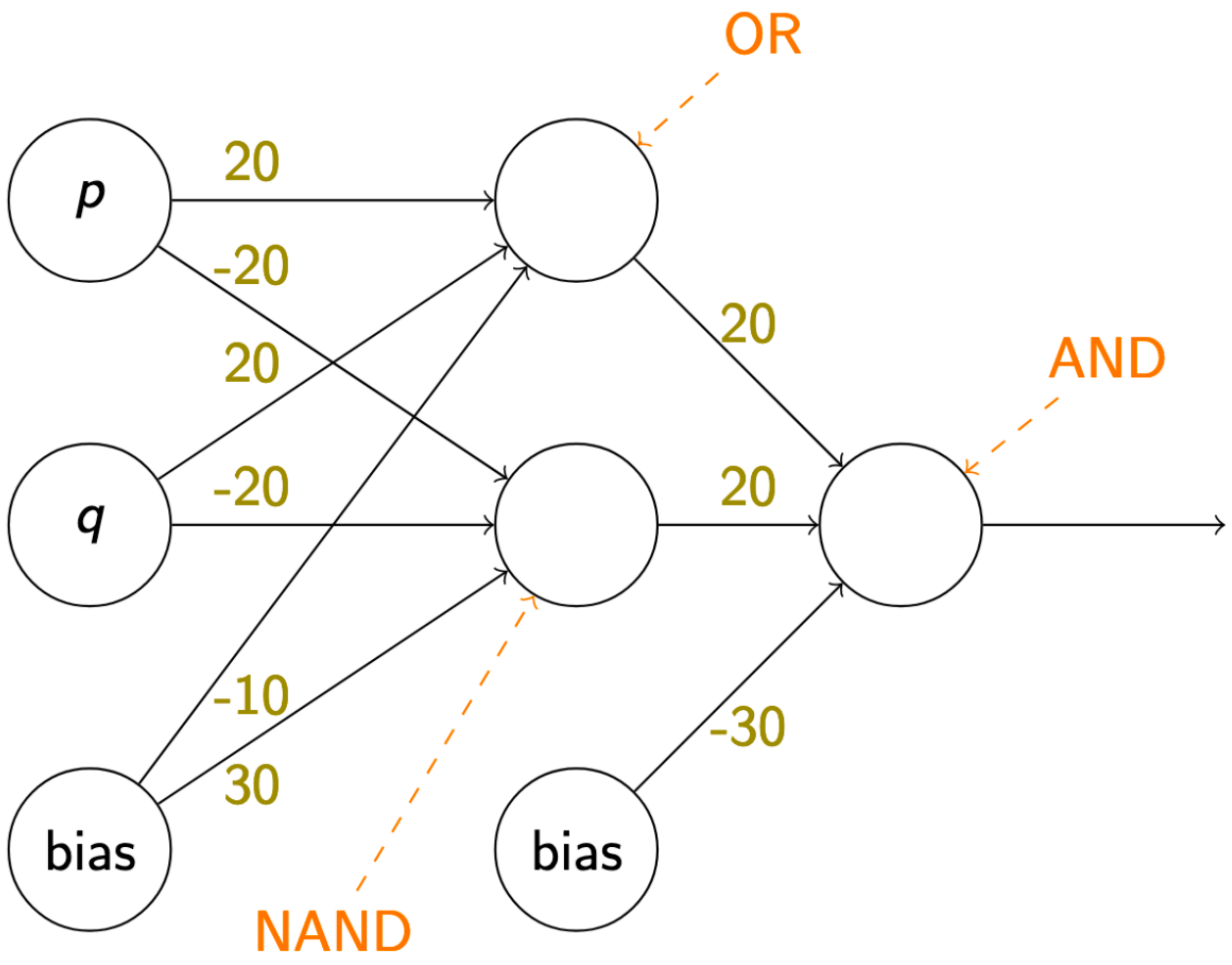

$$a_{\text{or}} = \sigma\left(\begin{bmatrix} w_p^{\text{or}} & w_q^{\text{or}} \end{bmatrix} \begin{bmatrix} a_p \\ a_q \end{bmatrix} + b^{\text{or}}\right)$$

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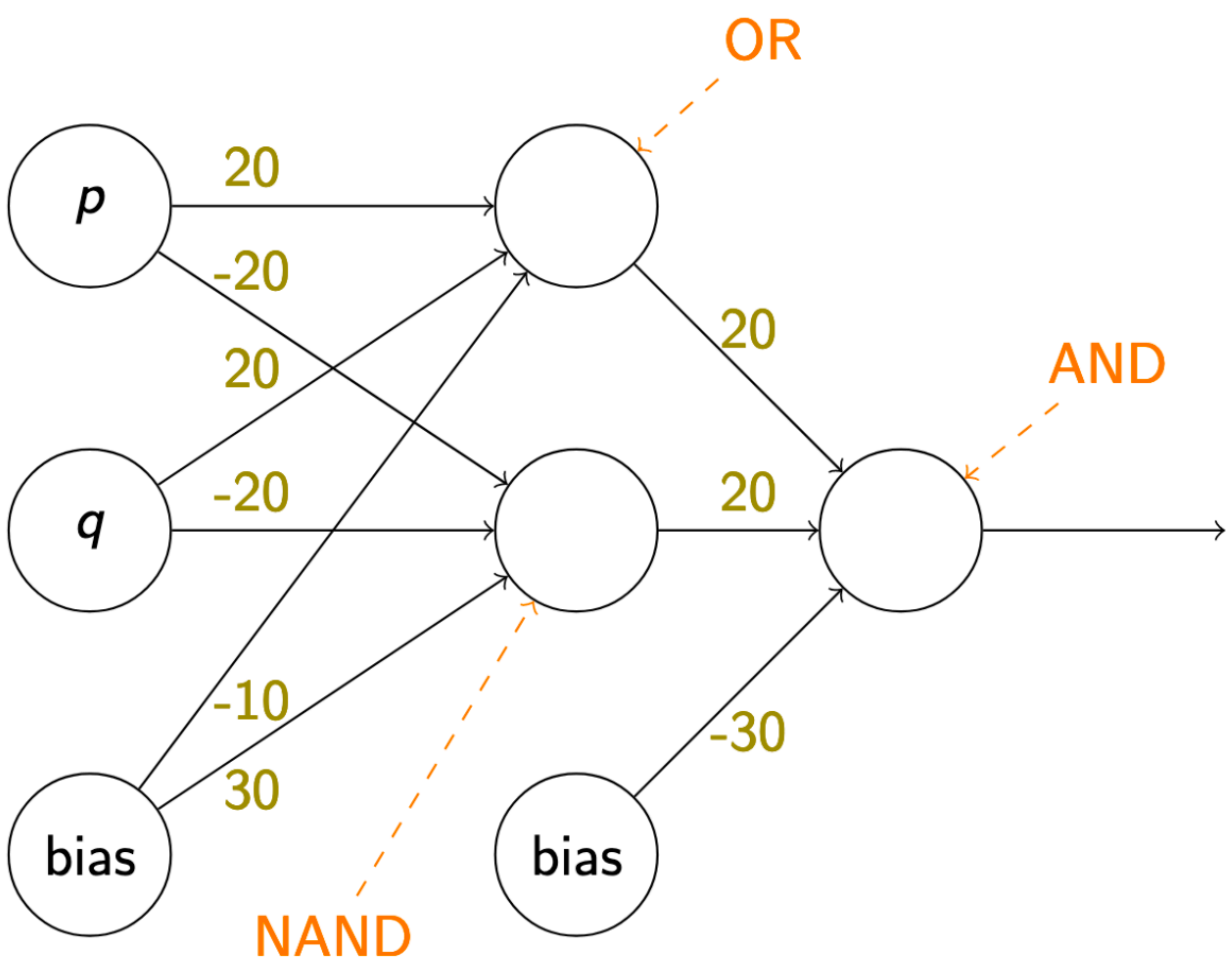

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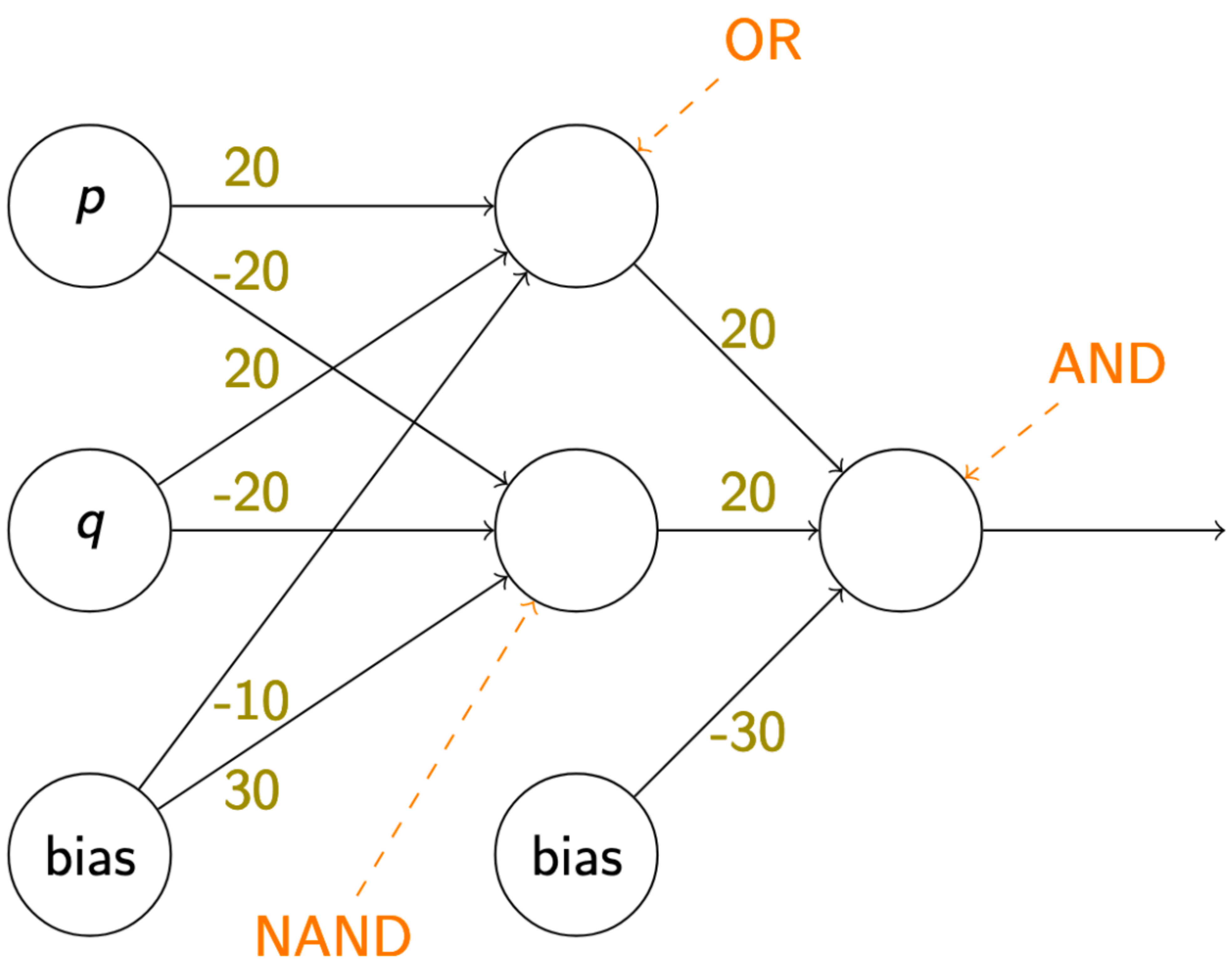
XOR Network



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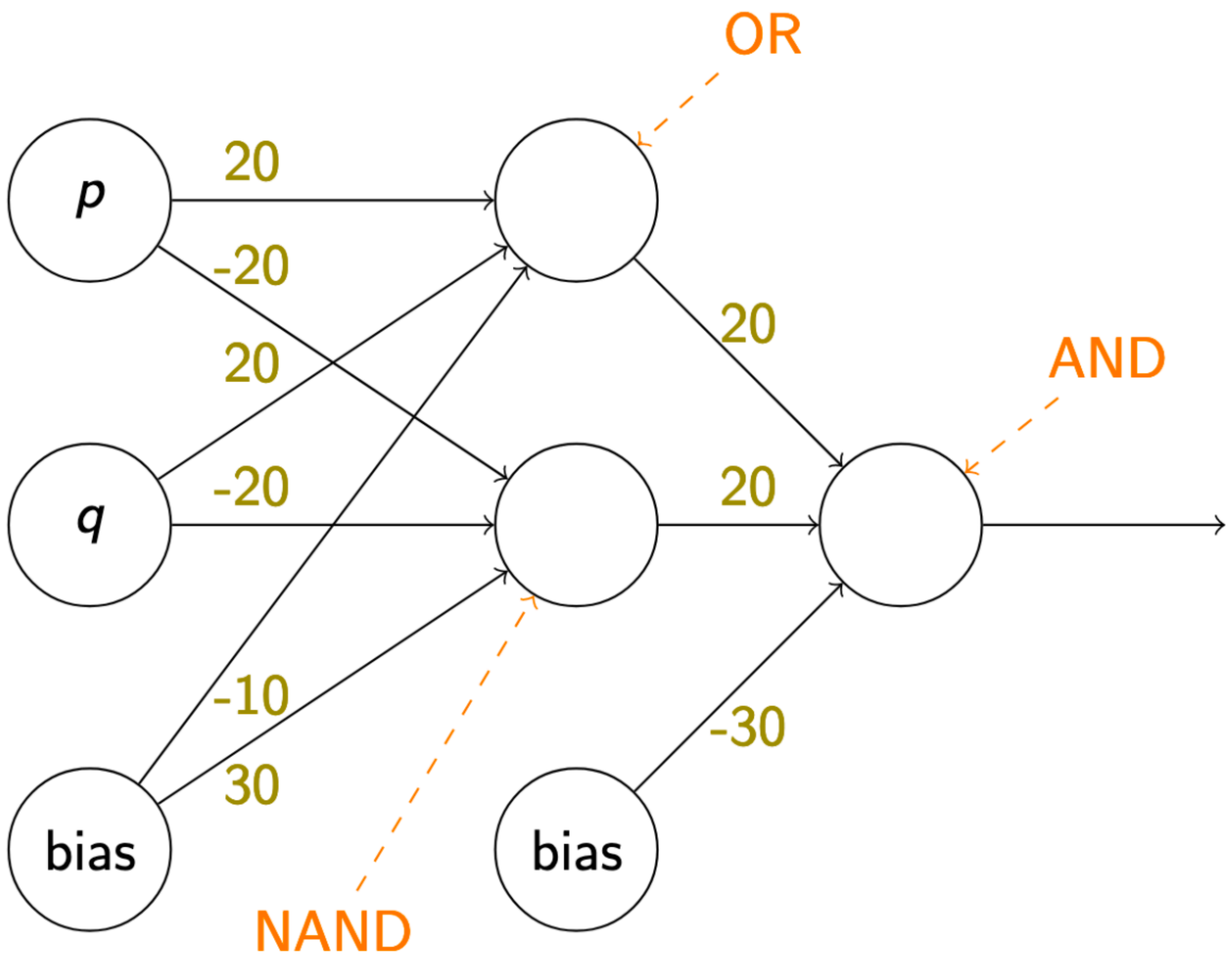
XOR Network



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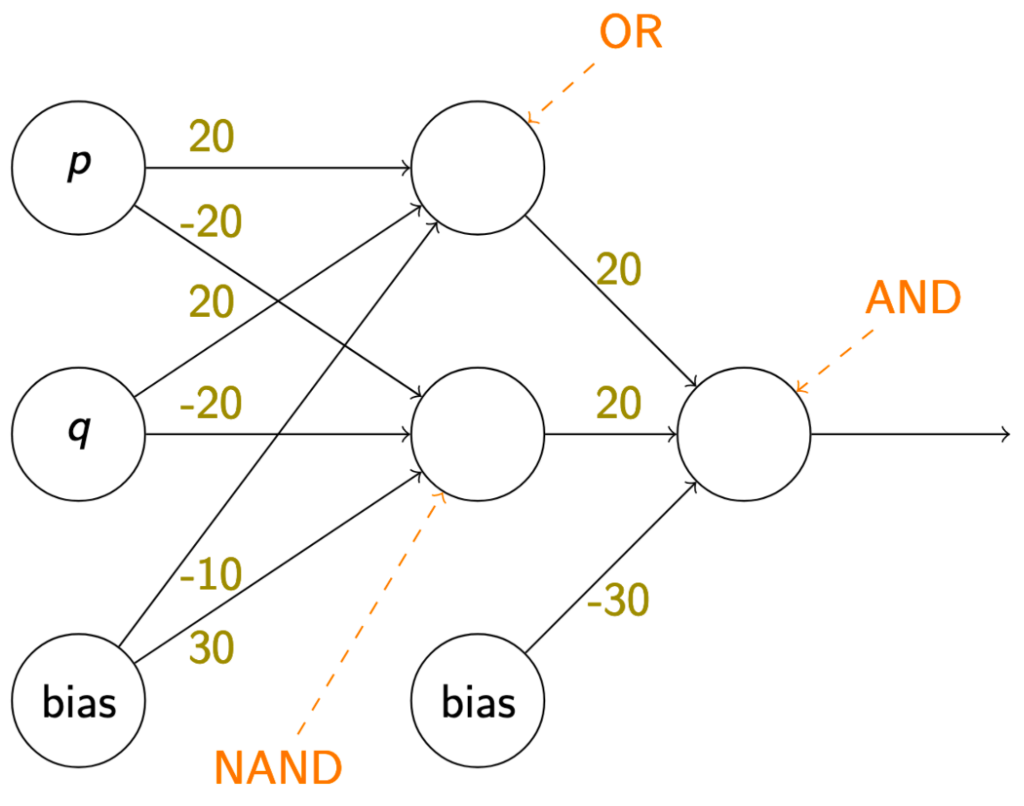

XOR Network

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Generalizing

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

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

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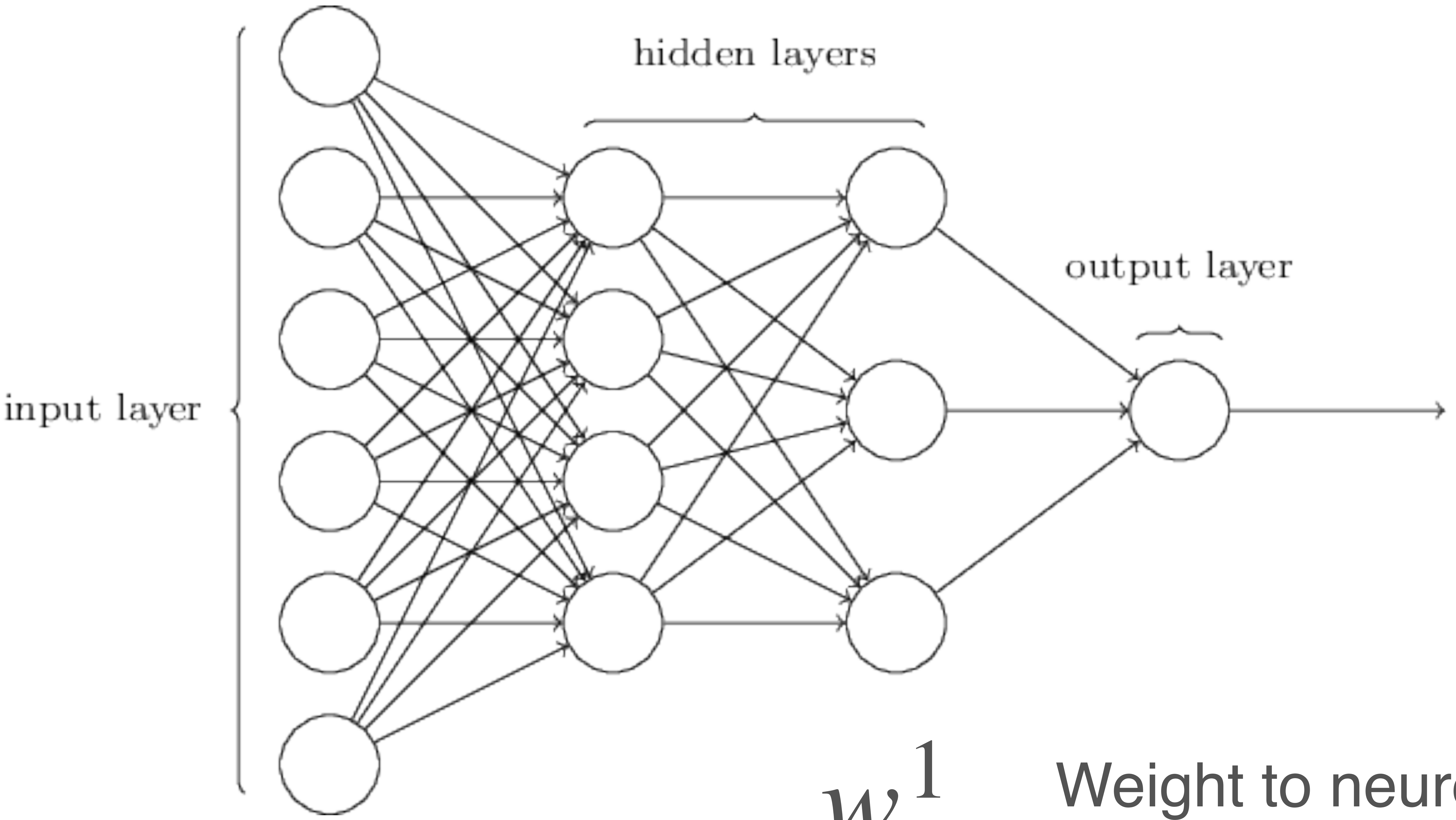
Some terminology

- 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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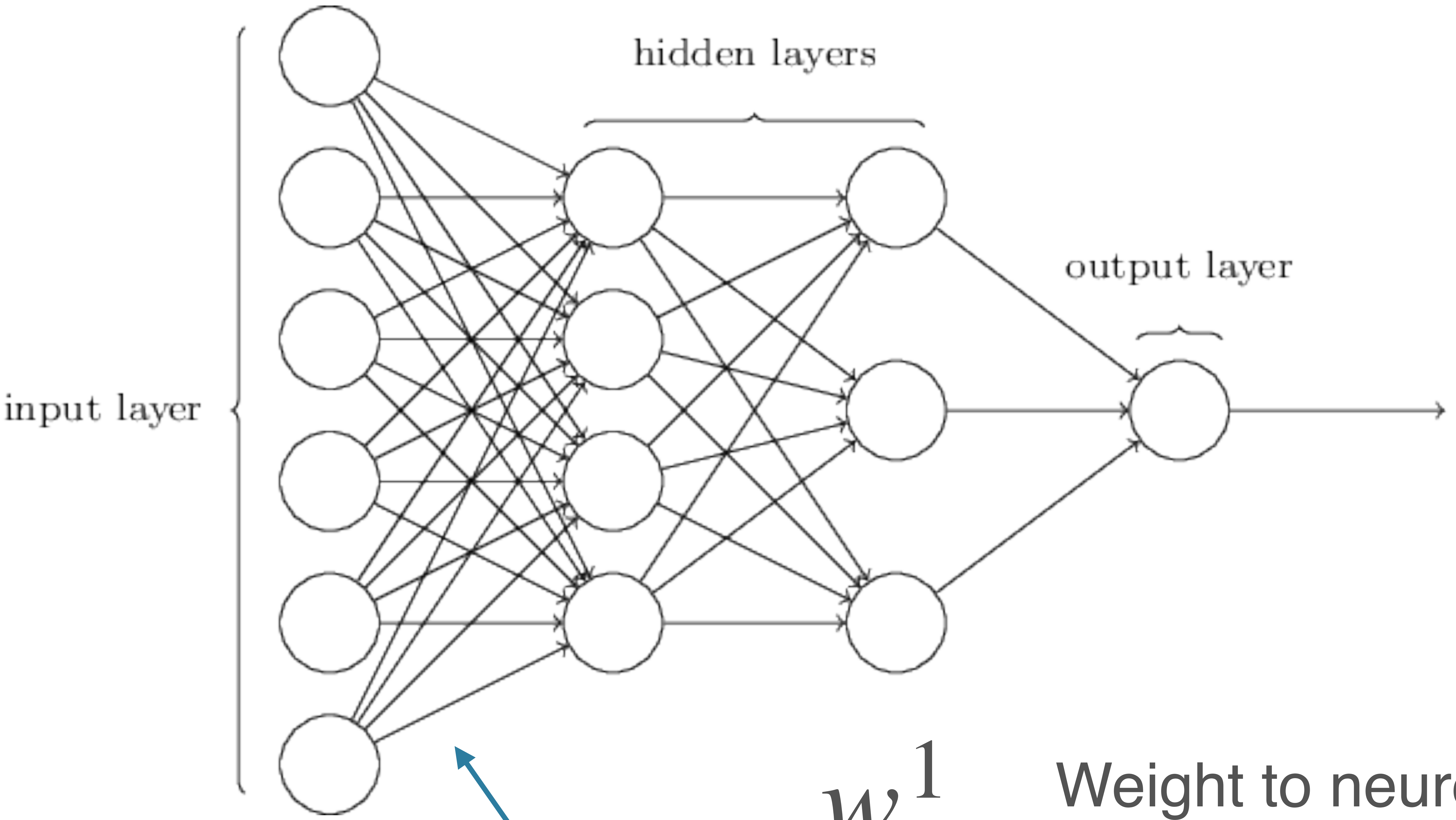
w_{ji}^{1} Weight to neuron j in layer 1 from neuron i in layer 0

General MLP



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W^1

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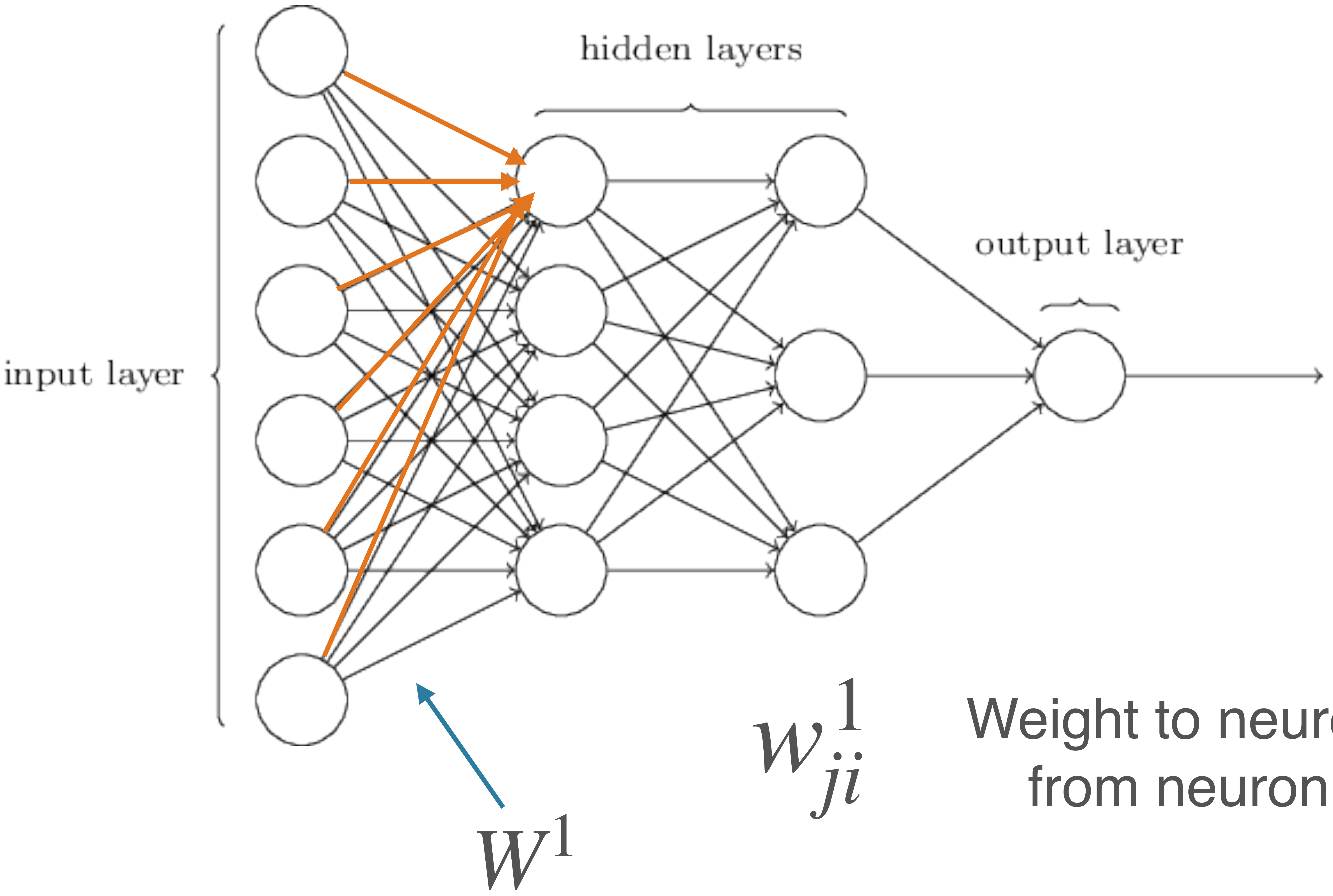

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$$W^1 = \begin{bmatrix} w_{00} & w_{10} & \cdots & w_{0n_0} \\ w_{10} & w_{11} & \cdots & w_{1n_0} \\ \vdots & \vdots & \ddots & \vdots \\ w_{n_1 0} & w_{n_1 1} & \cdots & w_{n_1 n_0} \end{bmatrix}$$

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$$b^1 = \begin{bmatrix} b_0 \\ b_1 \\ \vdots \\ b_{n_1} \end{bmatrix}$$ Shape: $(n_1, 1)$

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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  - Usually fixed by your problem / dataset
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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

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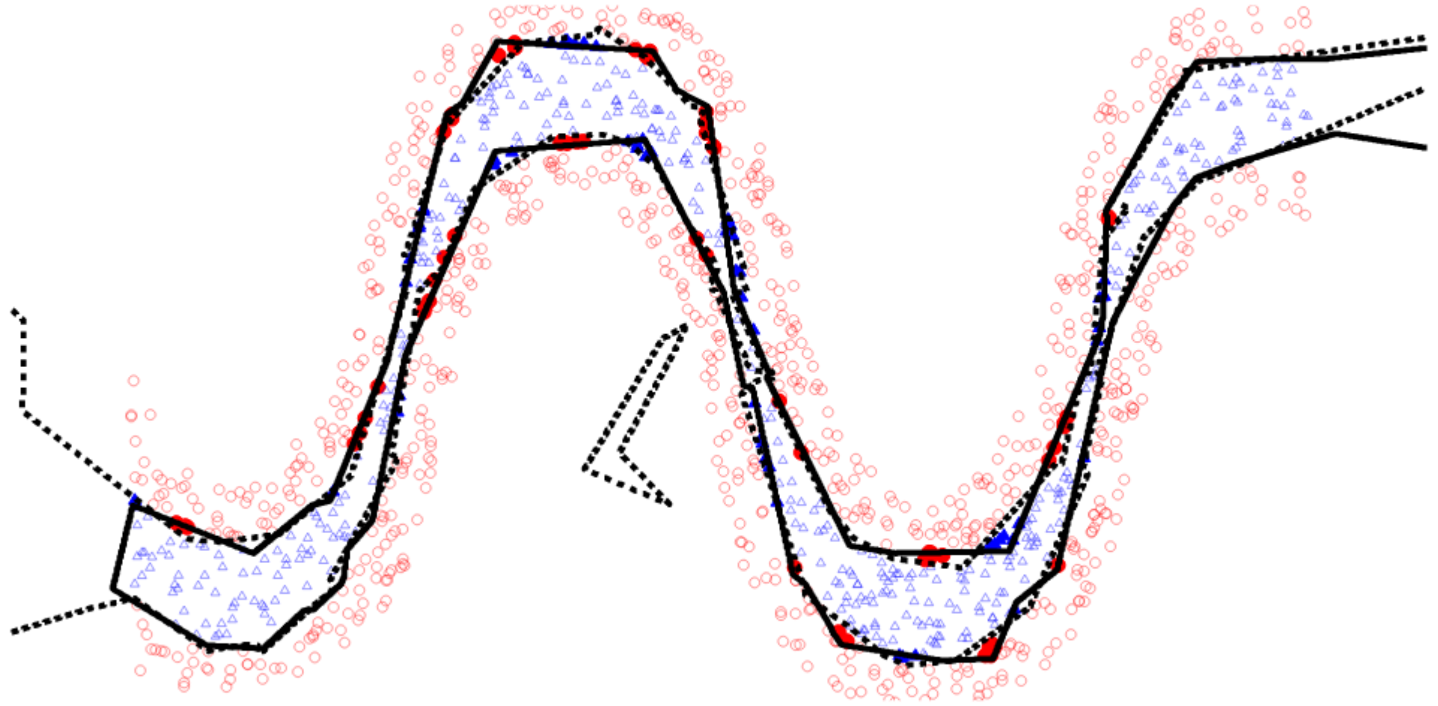
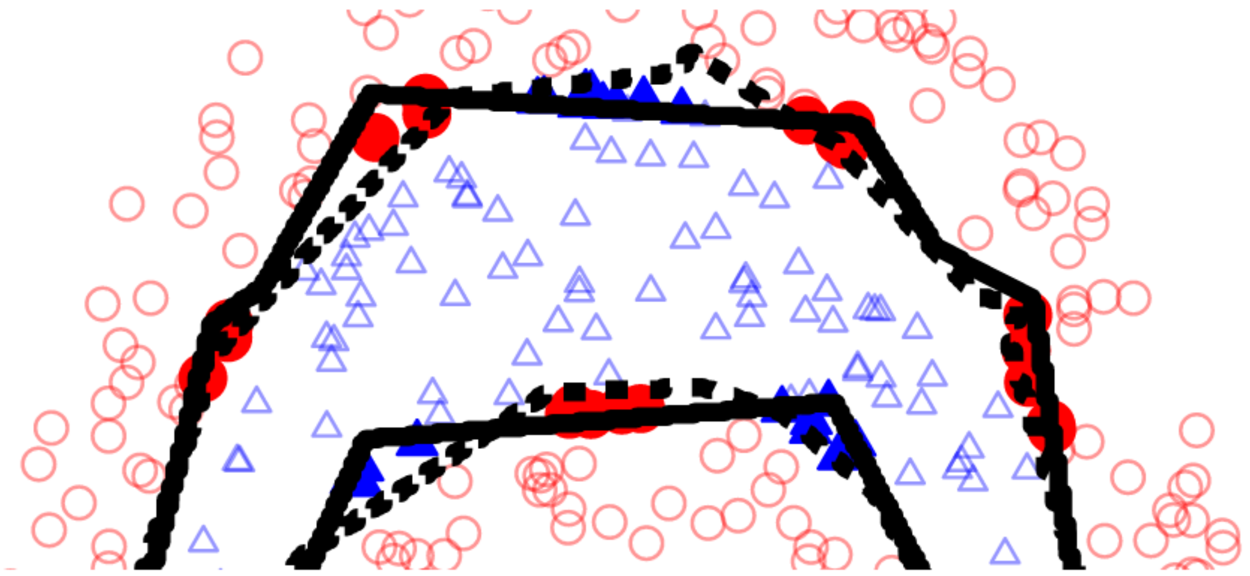
- Empirical d   discover source
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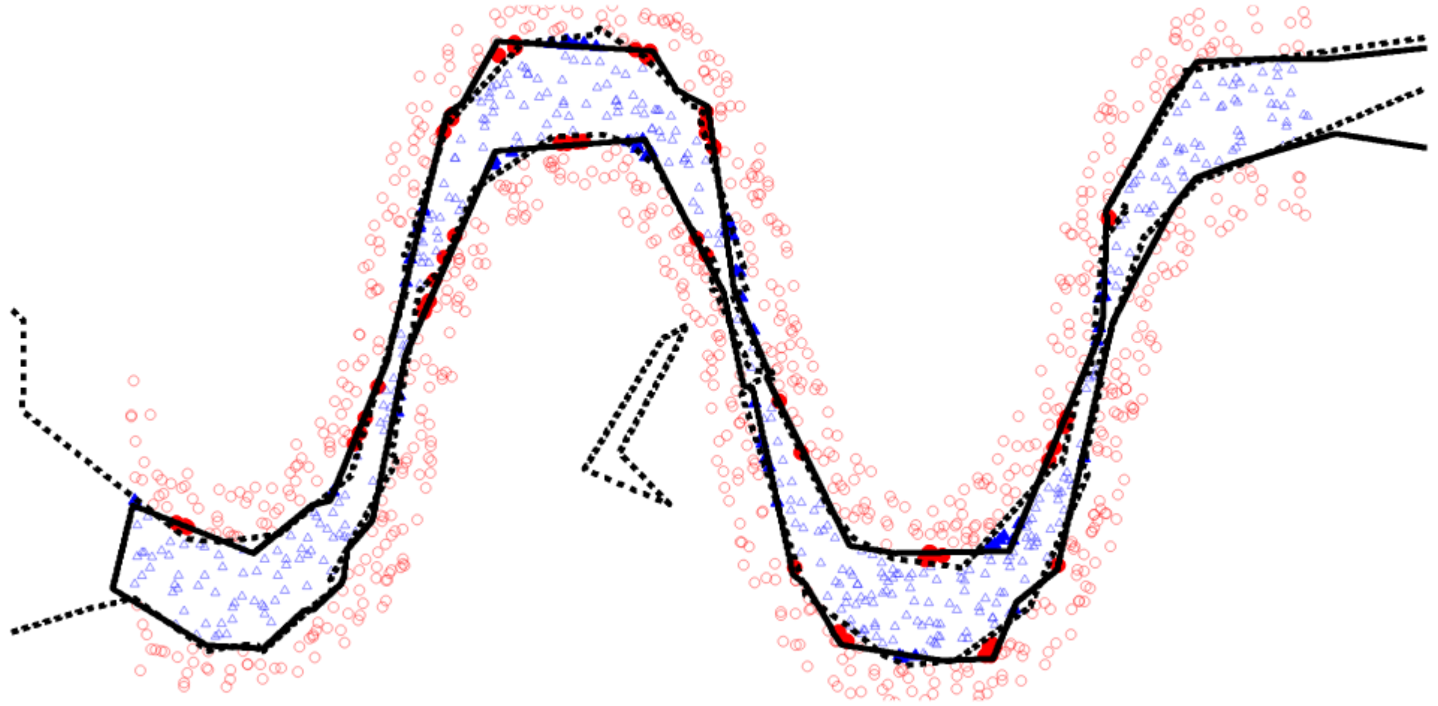

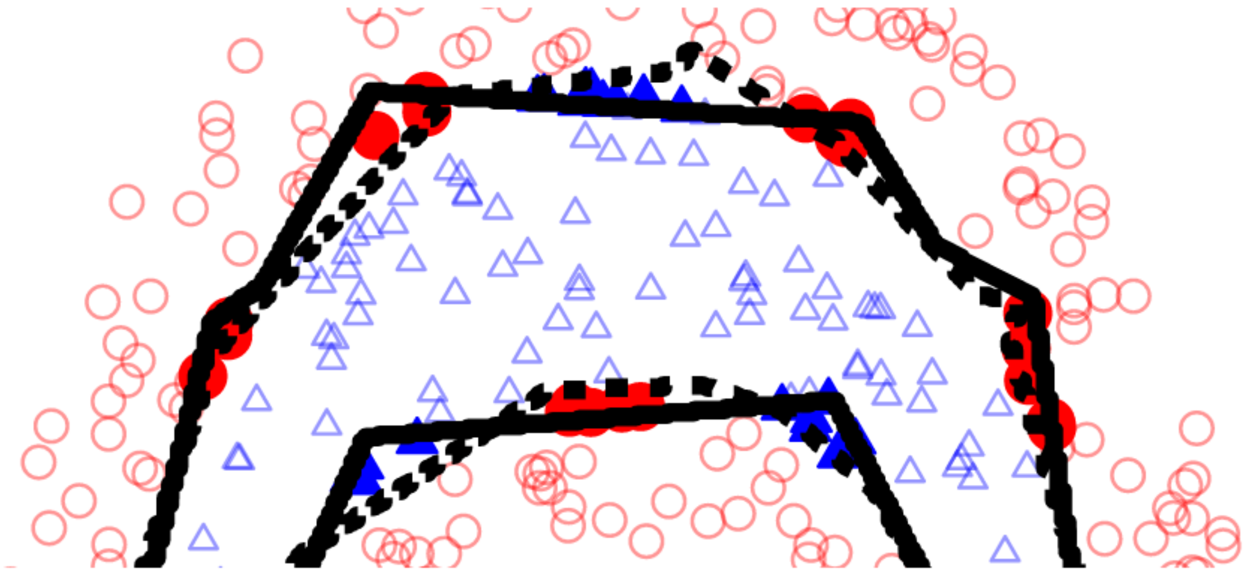

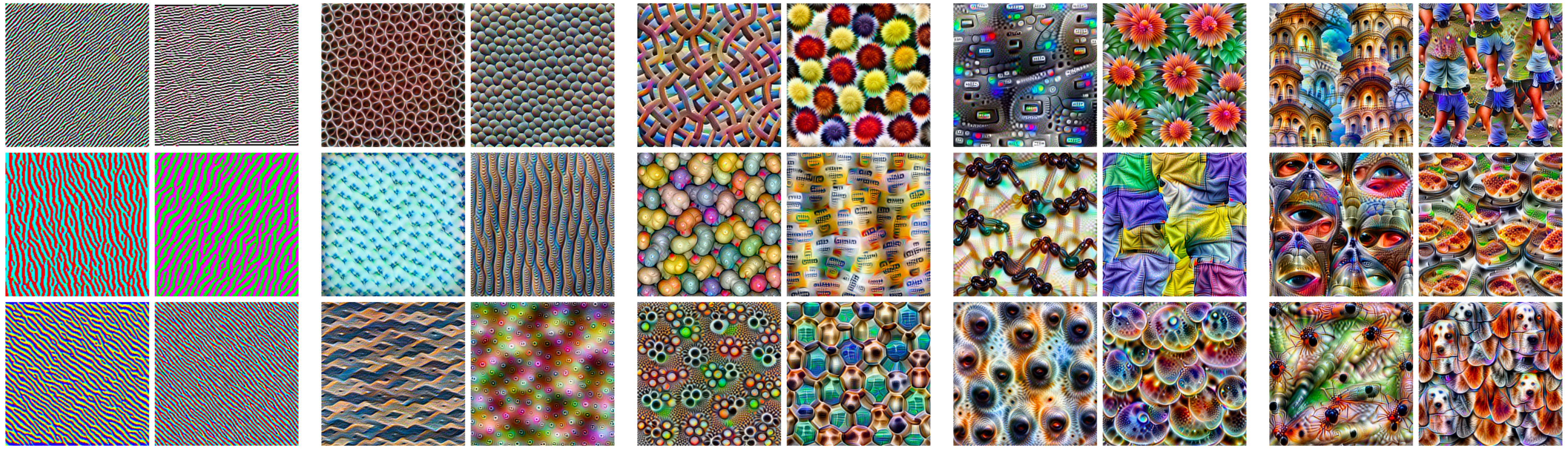

Edges (layer conv2d0) **Textures** (layer mixed3a) **Patterns** (layer mixed4a) **Parts** (layers mixed4b & mixed4c) **Objects** (layers mixed4d & mixed4e)

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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
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Non-linearity, cont.

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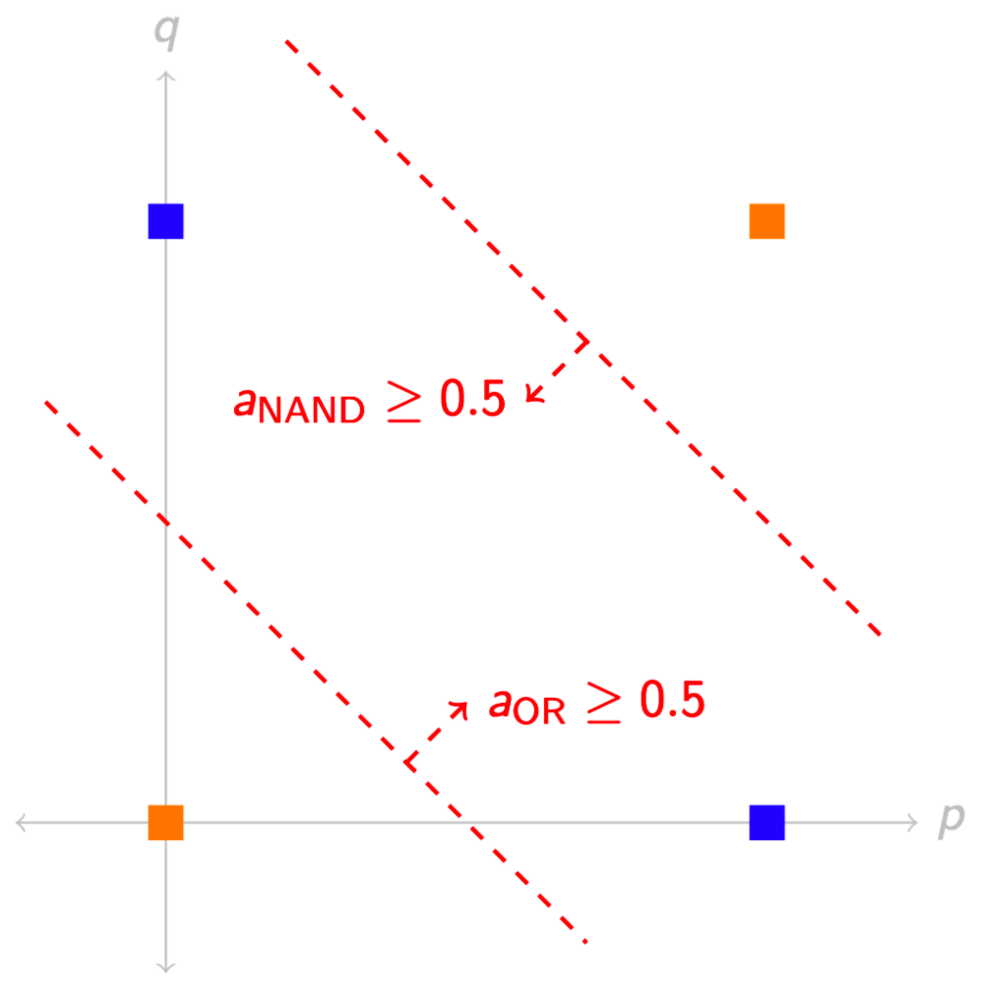
- One perspective: integrating extracted features



Non-linearity, cont.

- Recall: XOR was not computable by a single neuron because the latter can only compute *linearly separable* functions
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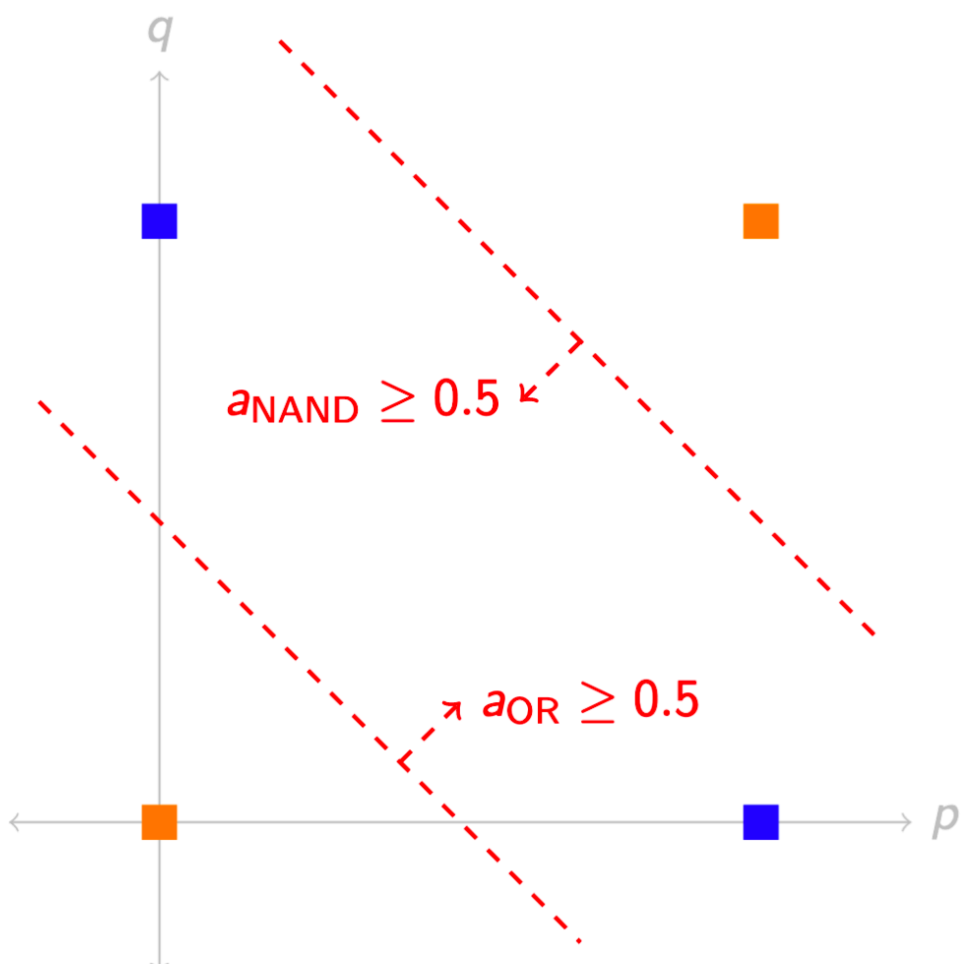
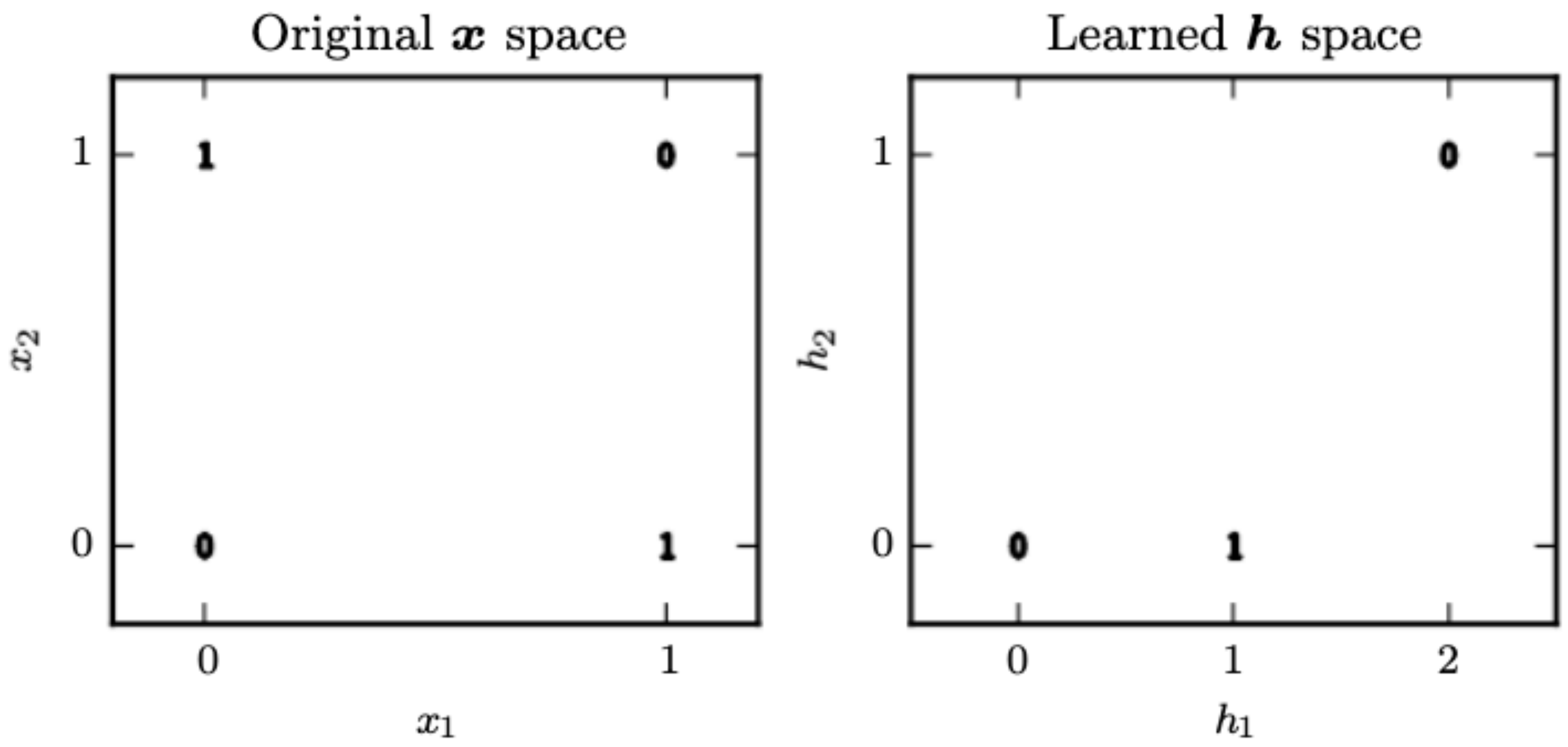
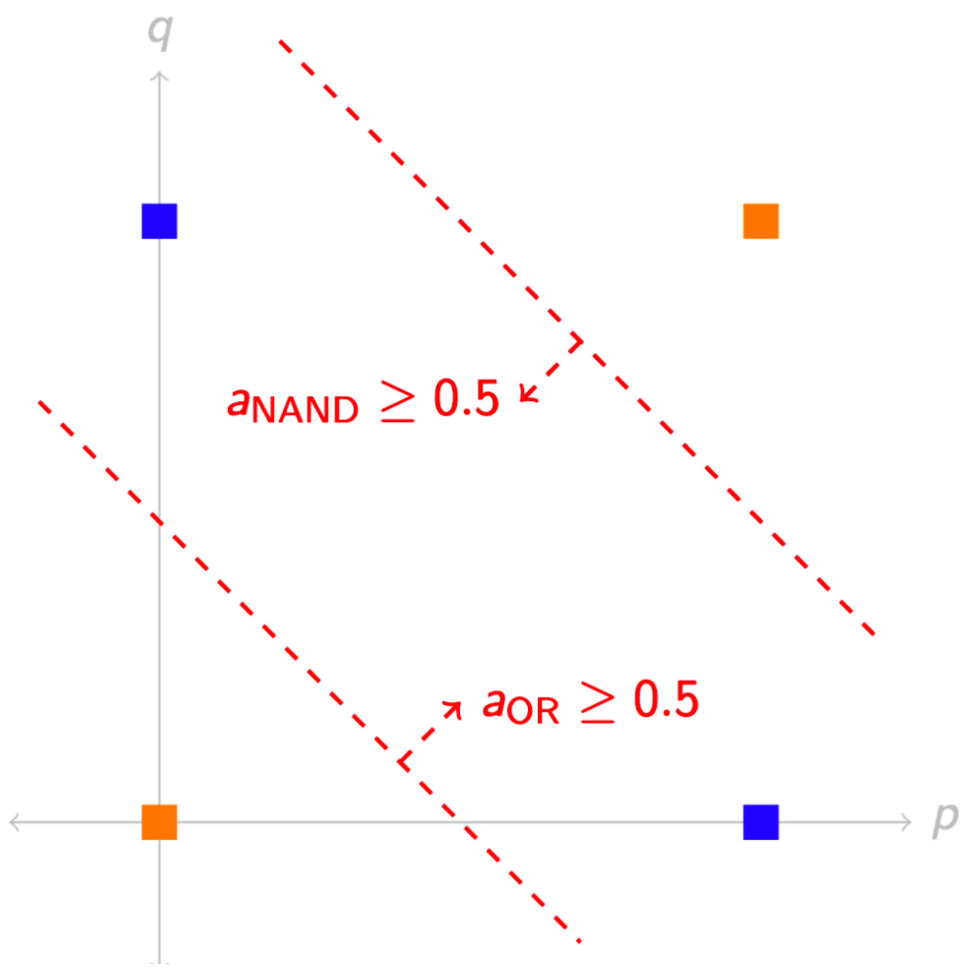
- An equivalent perspective:
  - Transforming the input space (source; p. 169)
  - This is a *non-linear* transformation
  - Space folding intuition more generally (also GBC sec 6.4.1)

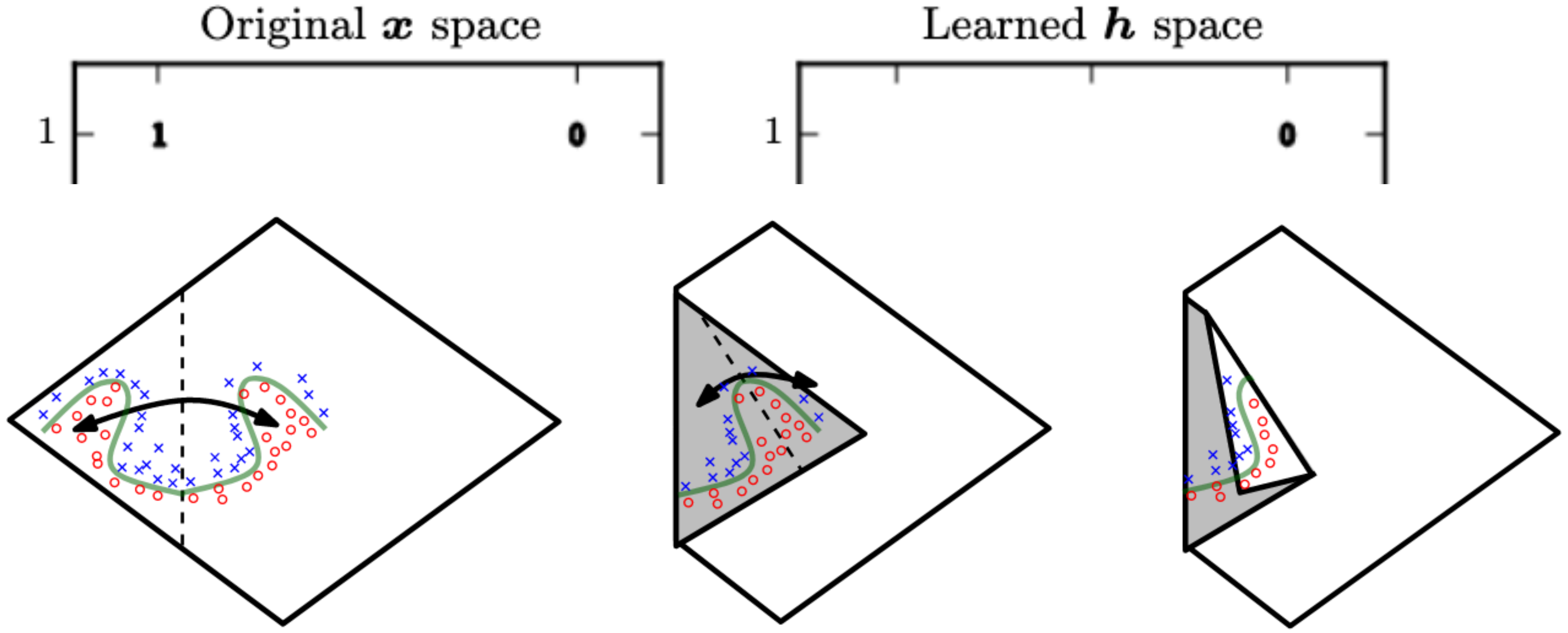




Non-linearity, cont.

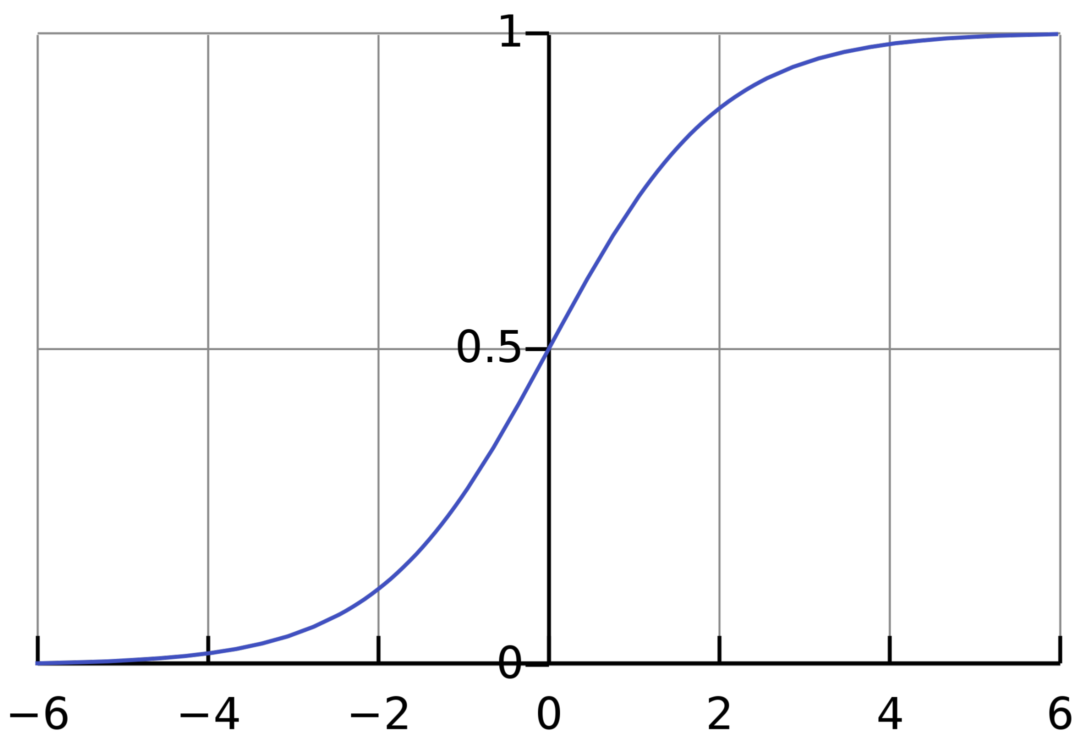
- Recall: XOR was not computable by a single neuron because the latter can only compute *linearly separable* functions
- One perspective: integrating extracted features
- An equivalent perspective:
  - Transforming the input space (source; p. 169)
  - This is a *non-linear* transformation
  - Space folding intuition more generally (also GBC sec 6.4.1)





Activation Functions: Hidden Layer

sigmoid



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

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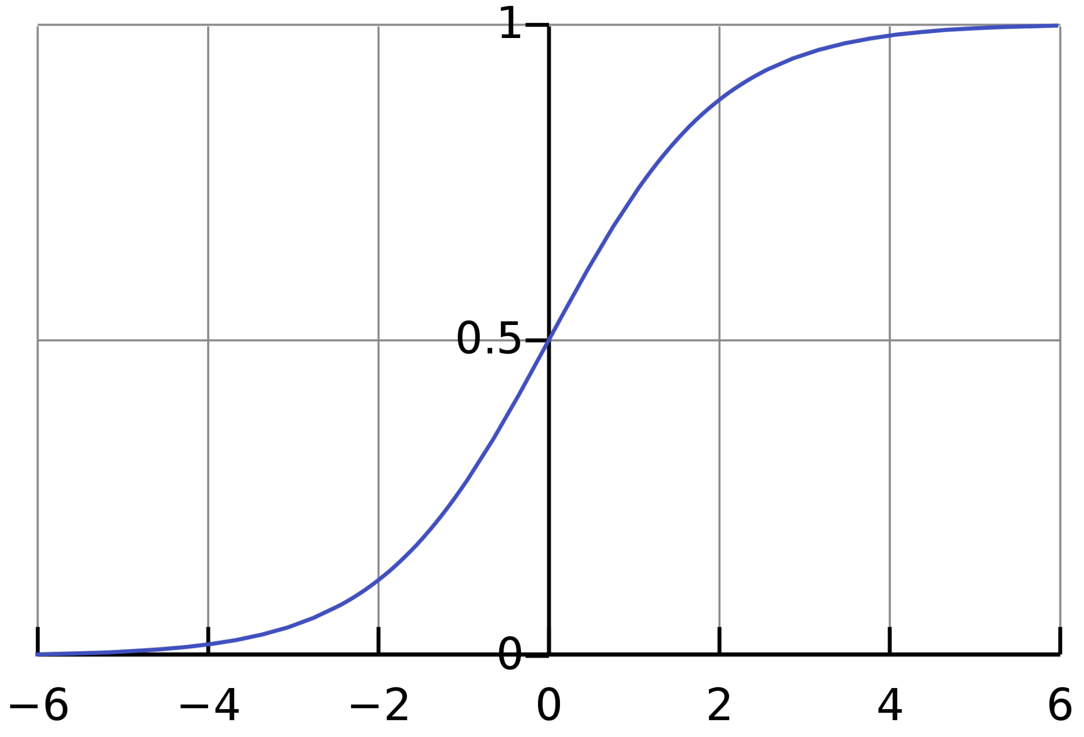

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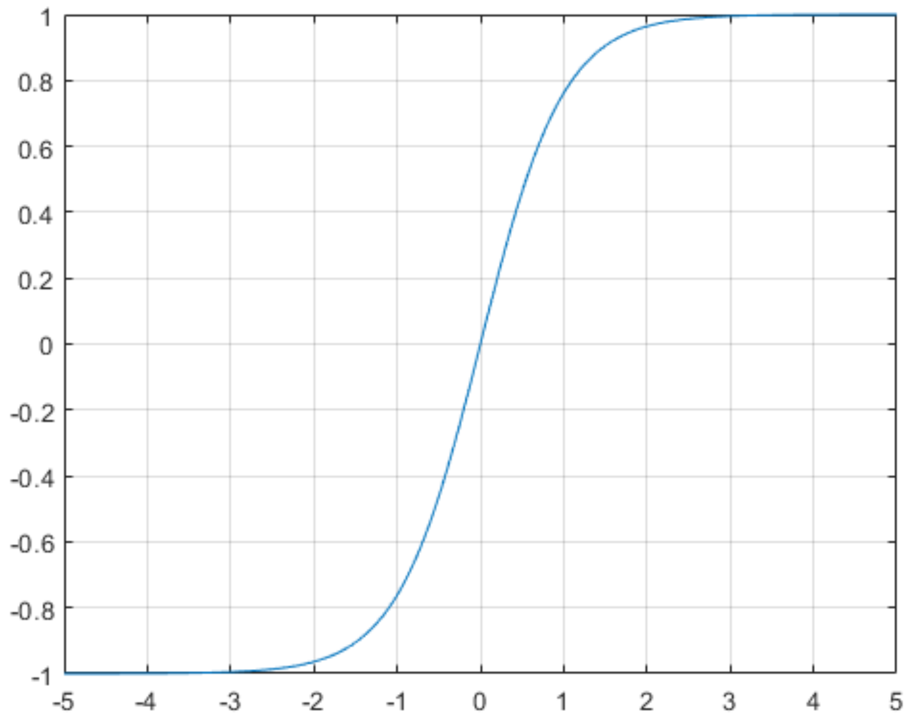
tanh



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

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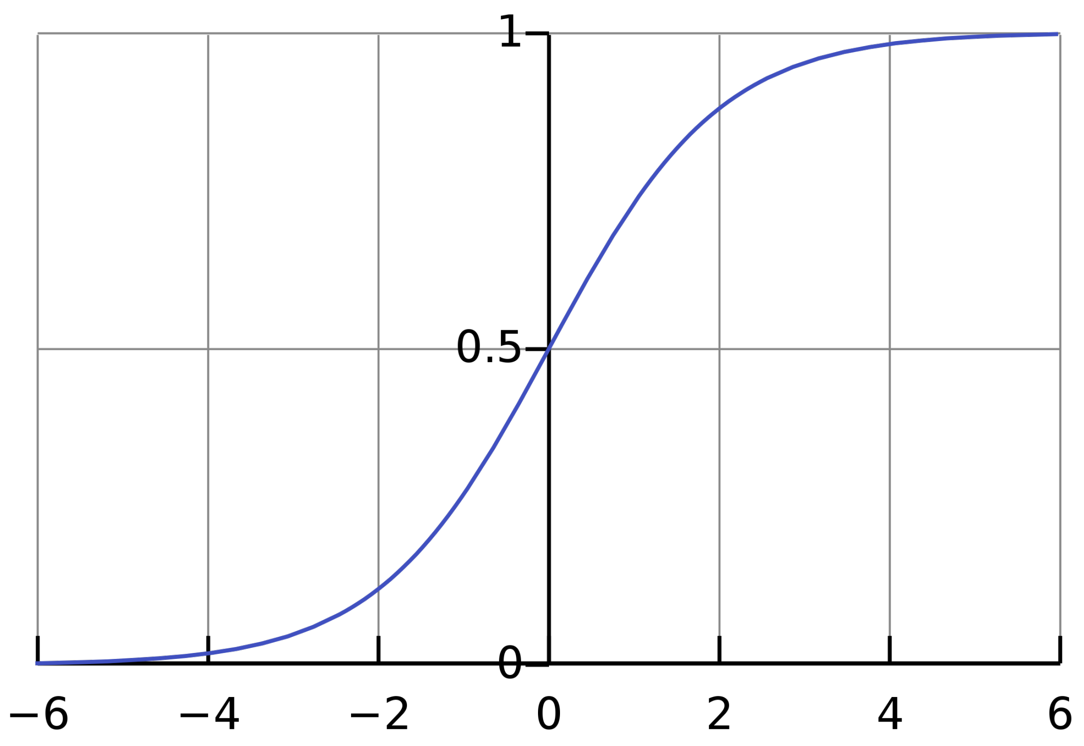

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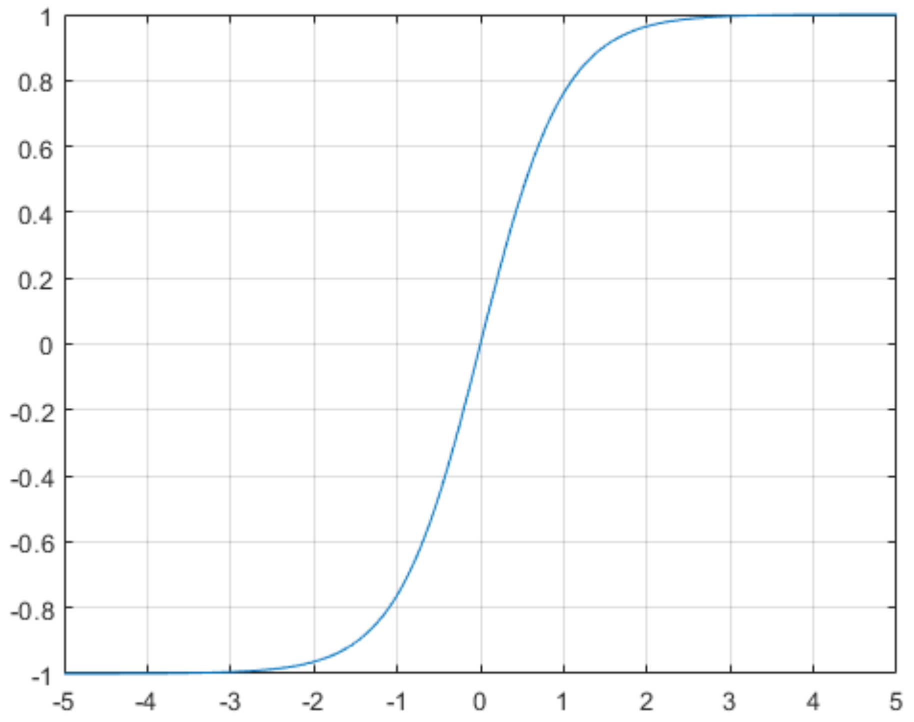

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Problem: derivative “saturates” (nearly 0) everywhere except near origin

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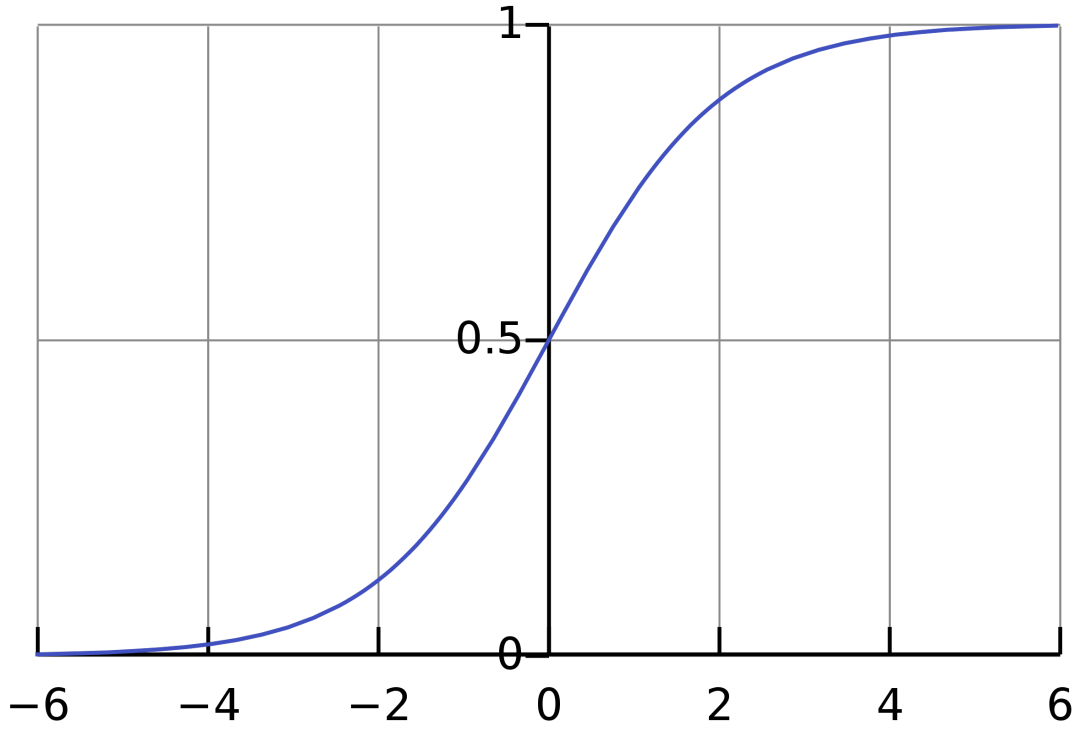

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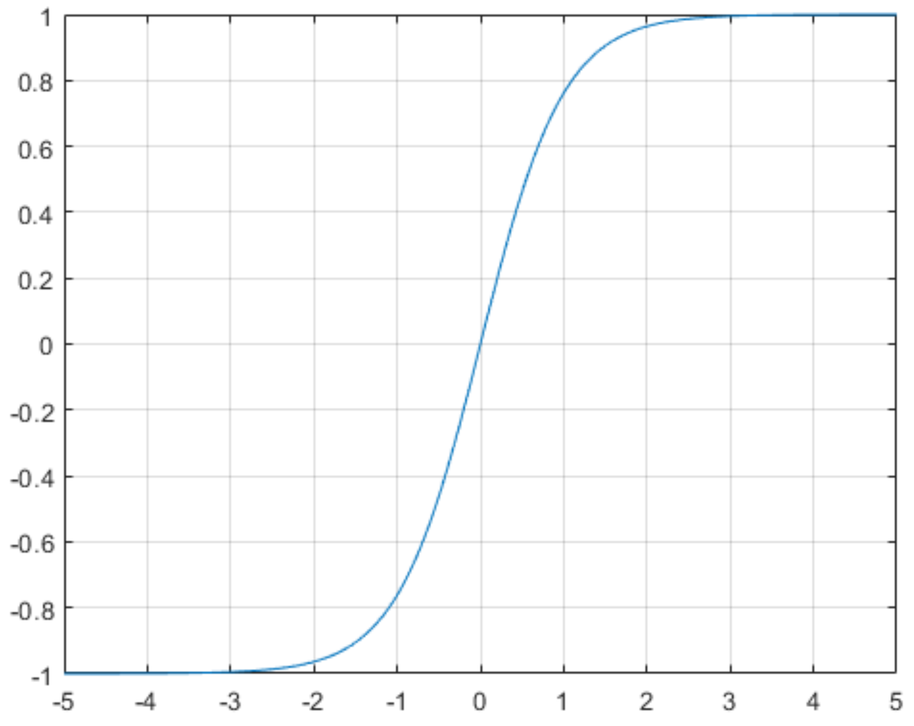

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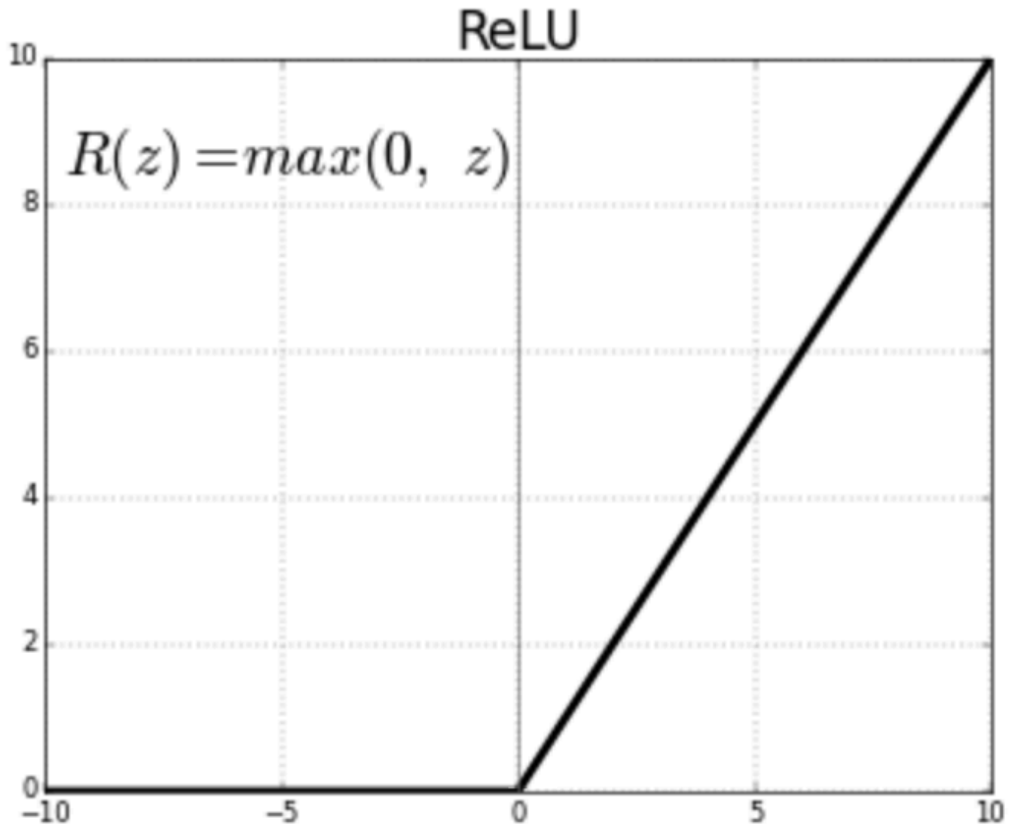

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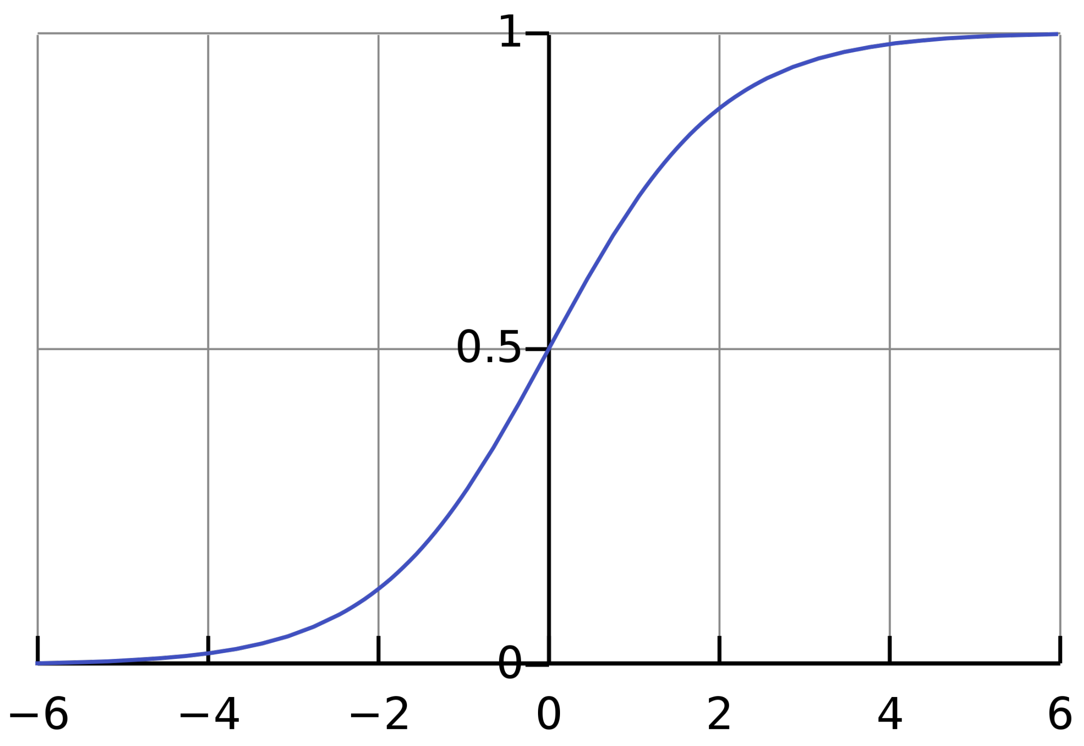

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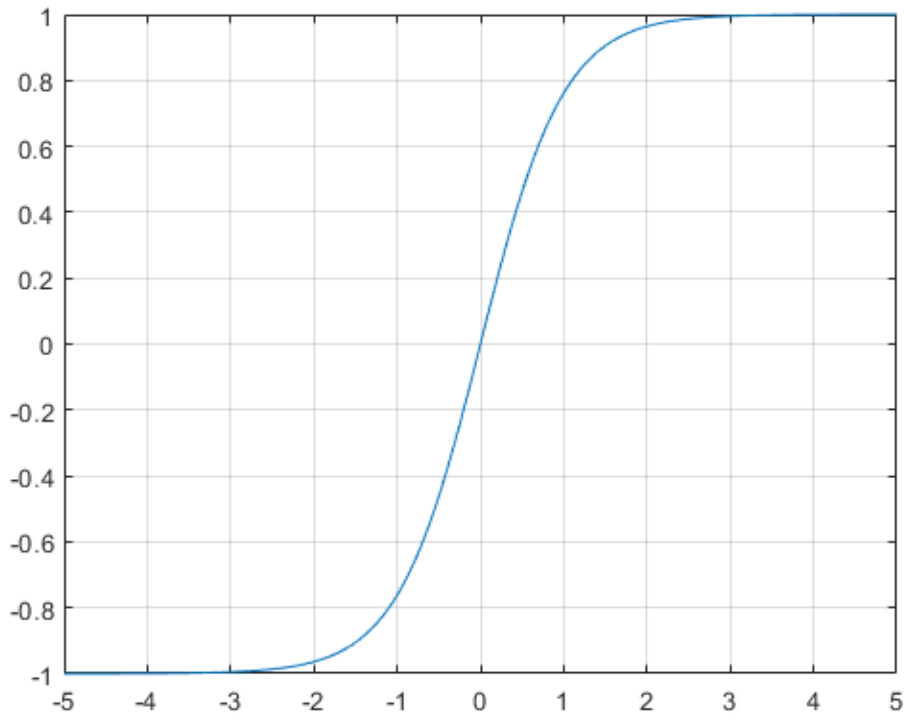

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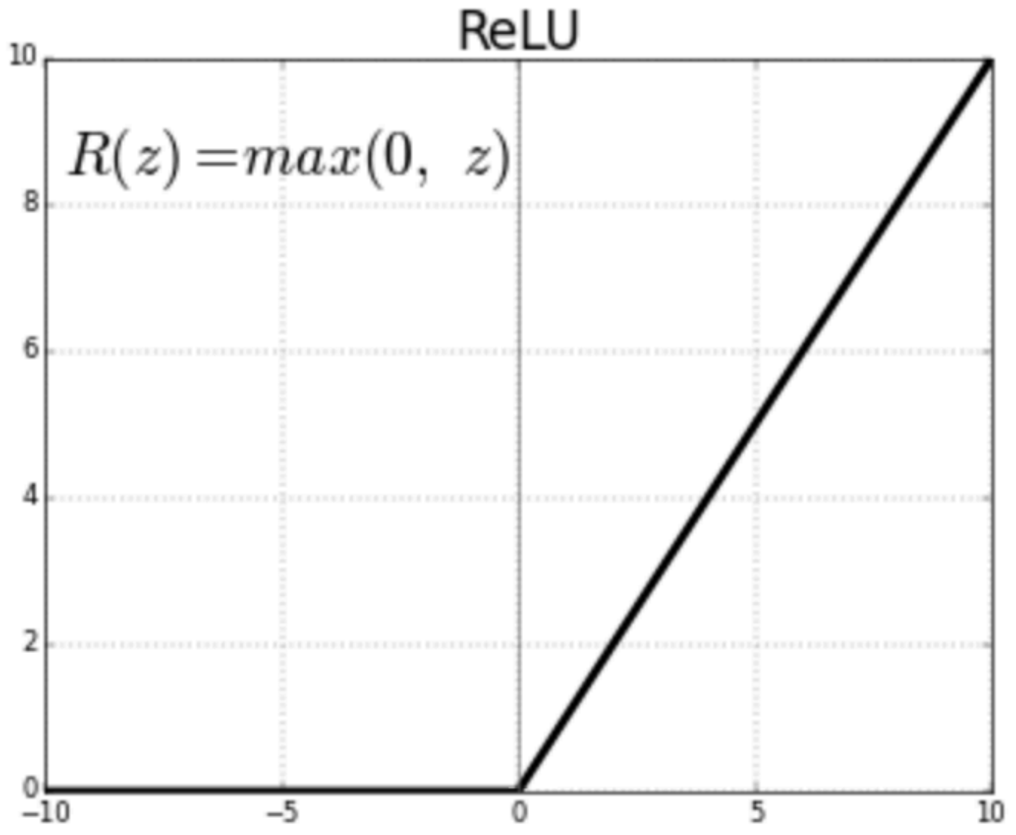

- Use ReLU by default
- Generalizations:
  - Leaky
  - ELU
  - Softplus
  - …

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

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

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

Computing with a Single Input

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$$x = \begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_{n_0} \end{bmatrix}$$ Shape: $(n_0, 1)$

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Shape: (n_1, n_0)

n_0: dimension of input (layer 0)

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$$b^1 = \begin{bmatrix} b_0 \\ b_1 \\ \vdots \\ b_{n_1} \end{bmatrix}$$ Shape: $(n_1, 1)$

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

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

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k: batch_size

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Added to each col. of W^1X

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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- Two comments:
  - In your code, **annotate every tensor** with a comment saying intended shape
  - When debugging, look at shapes early on!!

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  - (The result of this multiplication is the same, just transposed)

Next Time

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