Feed-Forward Neural Networks

Ling 282/482: Deep Learning for Computational Linguistics

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Fall 2025

Note on Random Seeds

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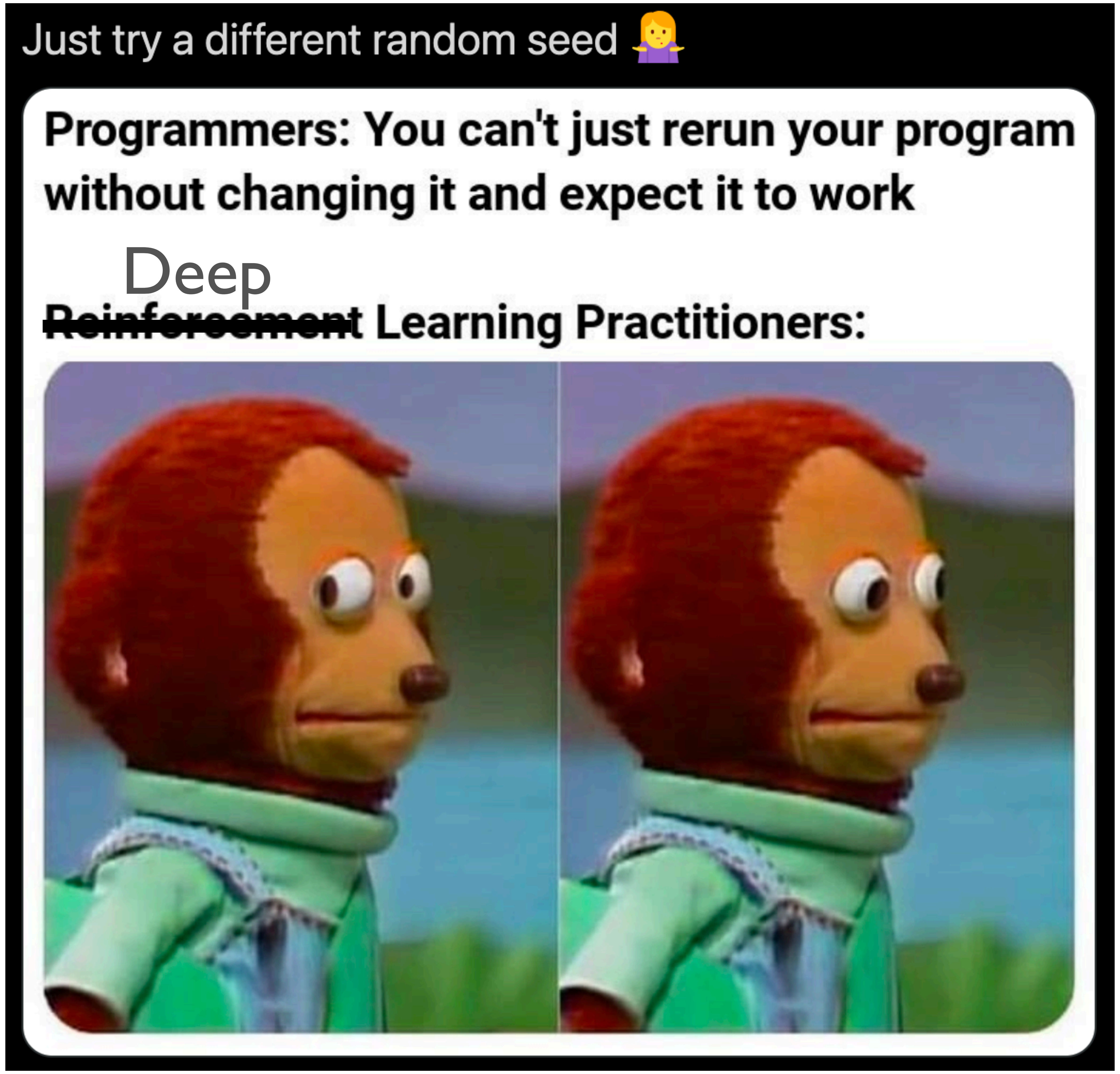
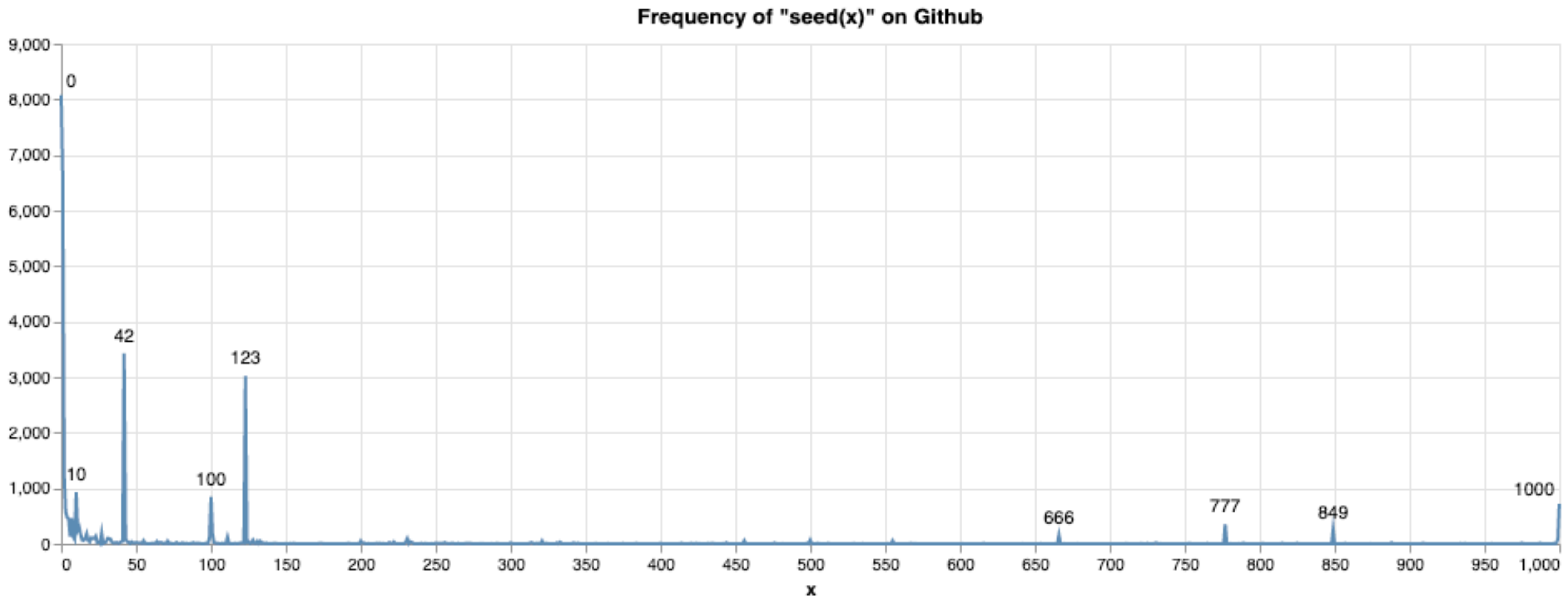
  - **Same seed —> same (non-random) behavior**
- **Sources of randomness** in DL: **shuffling the data** each epoch, **weight initialization**, negative sampling, …
- Very important for **reproducibility!**
  - In general, run on several seeds and report means / std’s

Random Seeds and Reproducibility



Random Seeds, cont

- Ideally: “randomly generate” seeds, but save/store them!
- Random seed is not a hyper-parameter! (Some discussions in these threads.)



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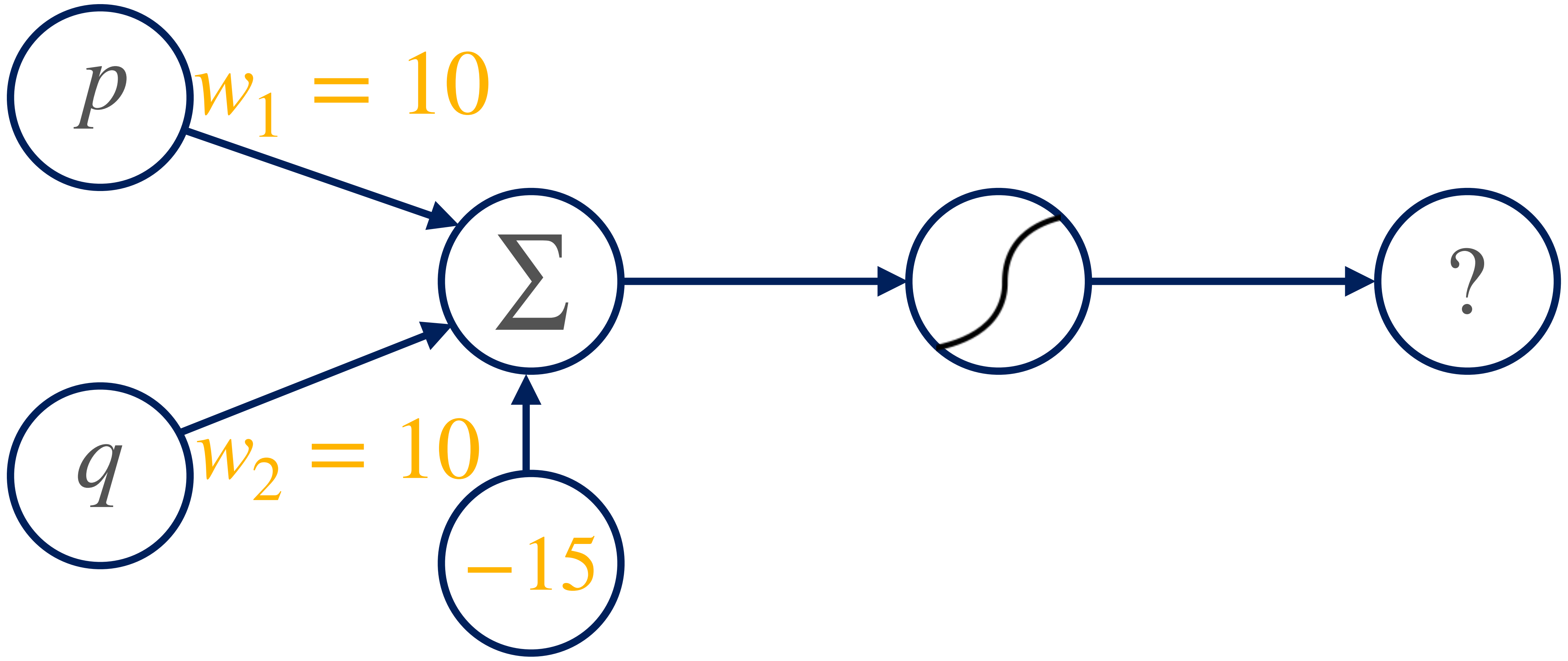
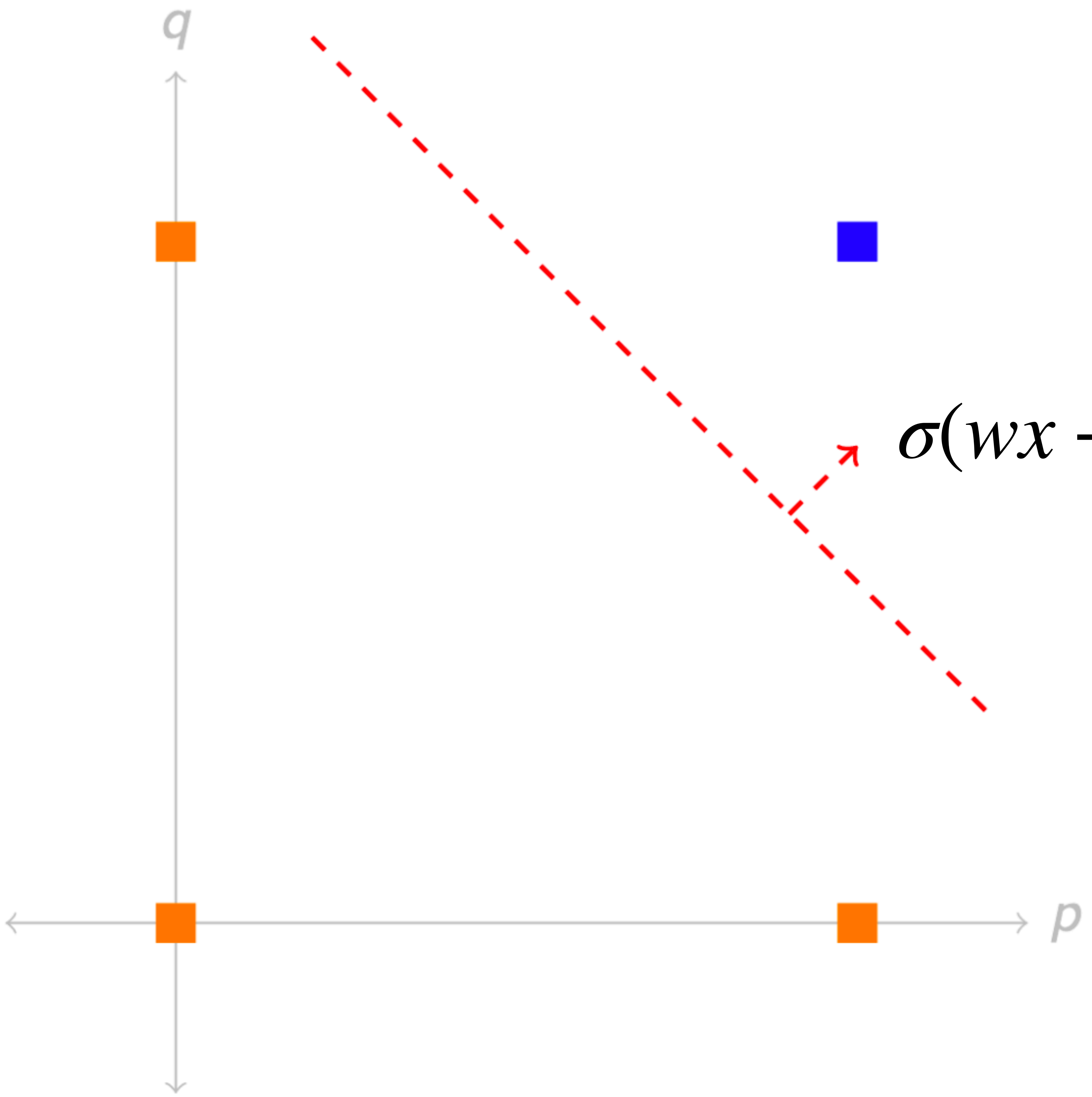
Feed-forward Neural Networks

Recall: AND Perceptron

p	q	p∧q
0	0	0
1	0	0
0	1	0
1	1	1

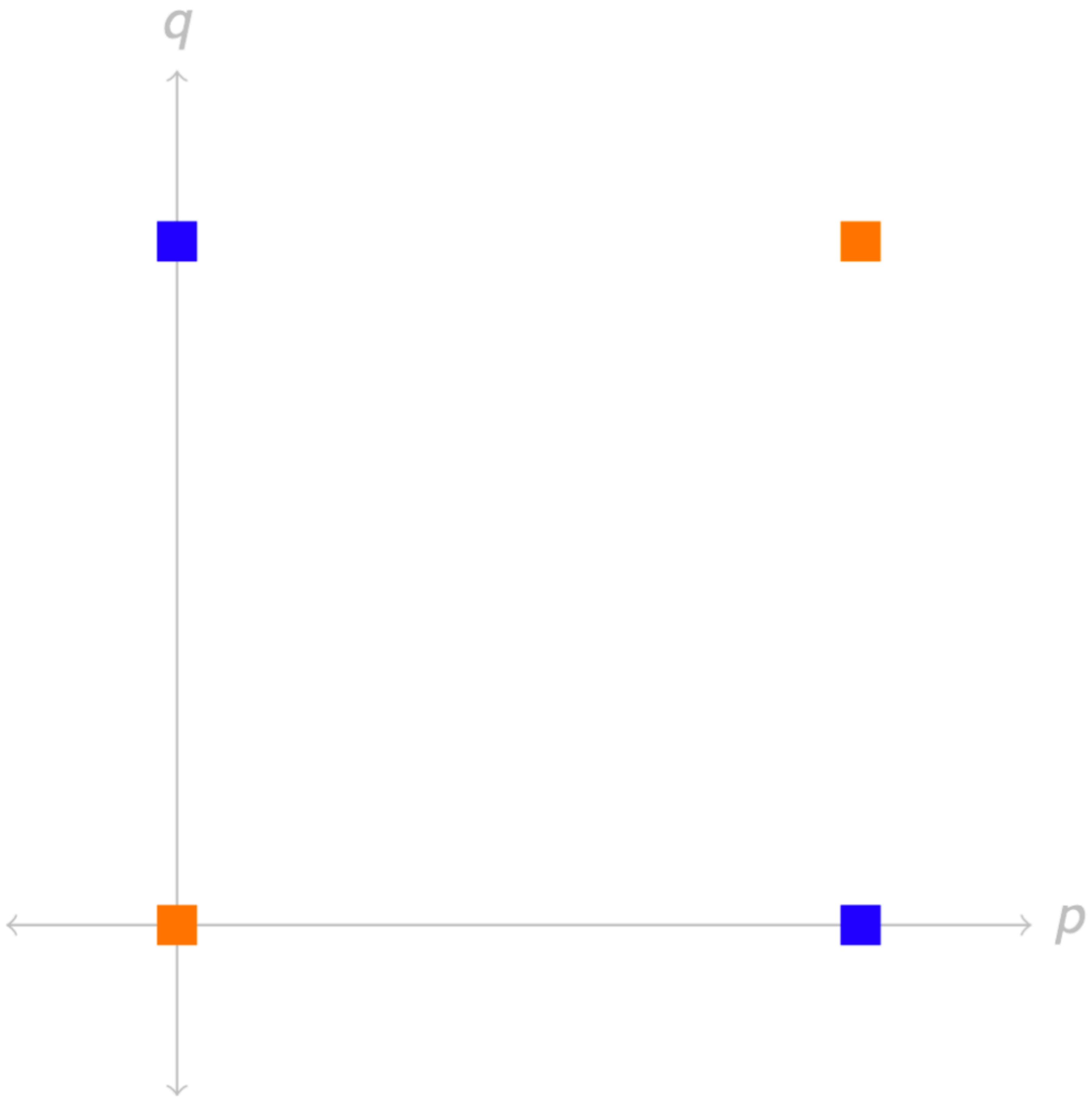


AND Linear Separation



$$\sigma(wx + b) \geq 0.5$$

The XOR problem



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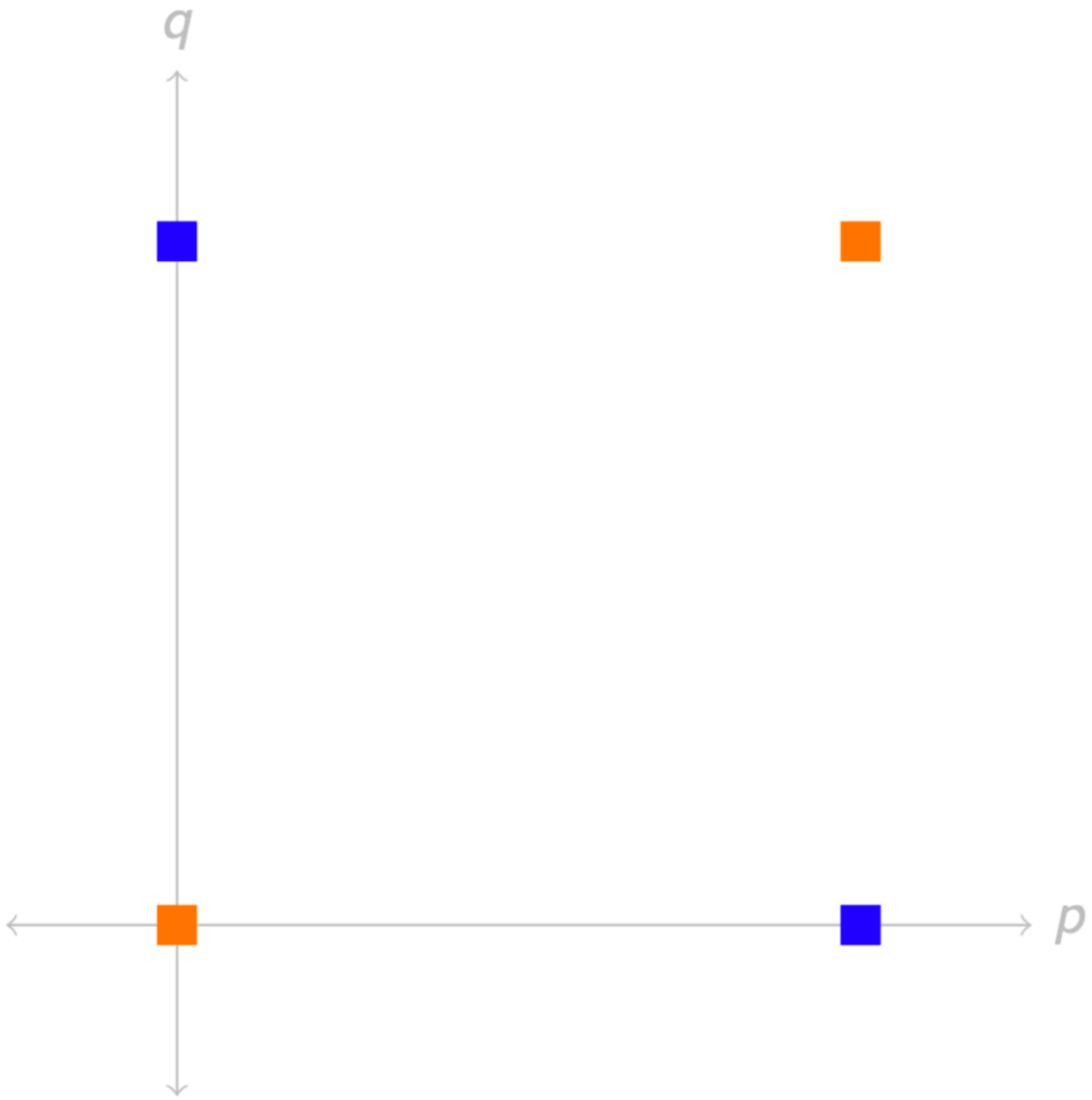
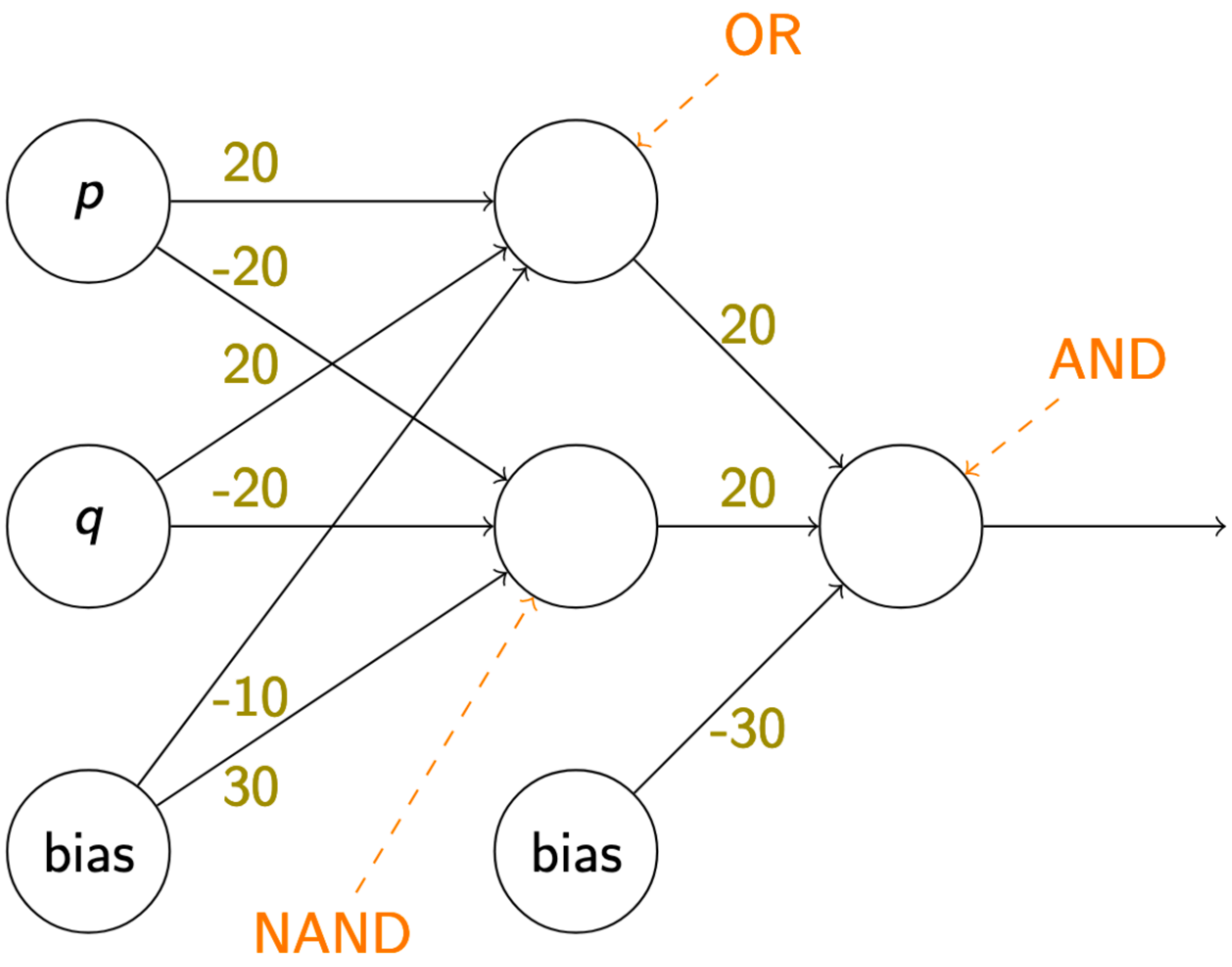


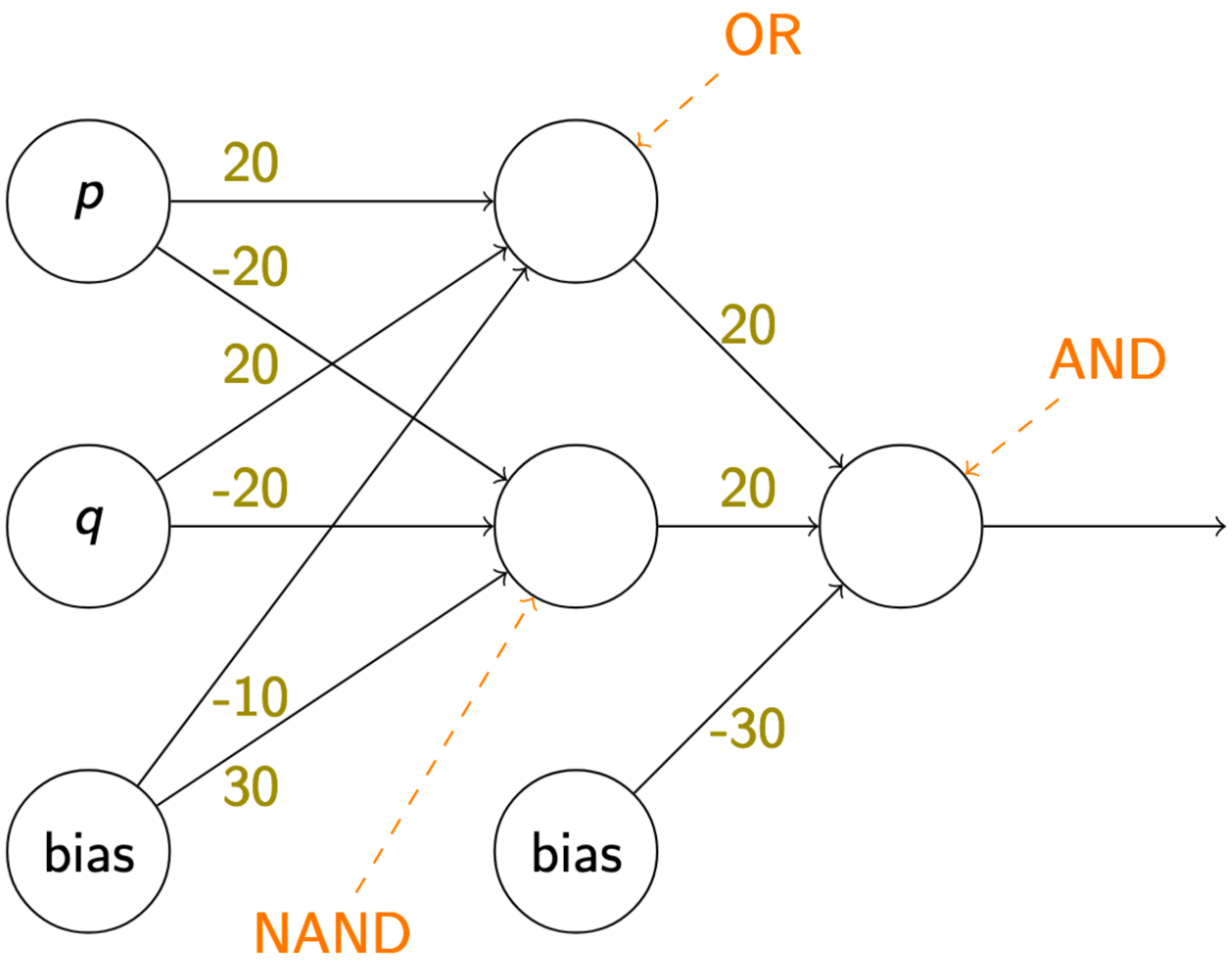
XOR is not linearly separable

Modeling XOR



Modeling XOR

- XOR is **decomposable** into other logical functions
  - (p OR q) AND (p NAND q)



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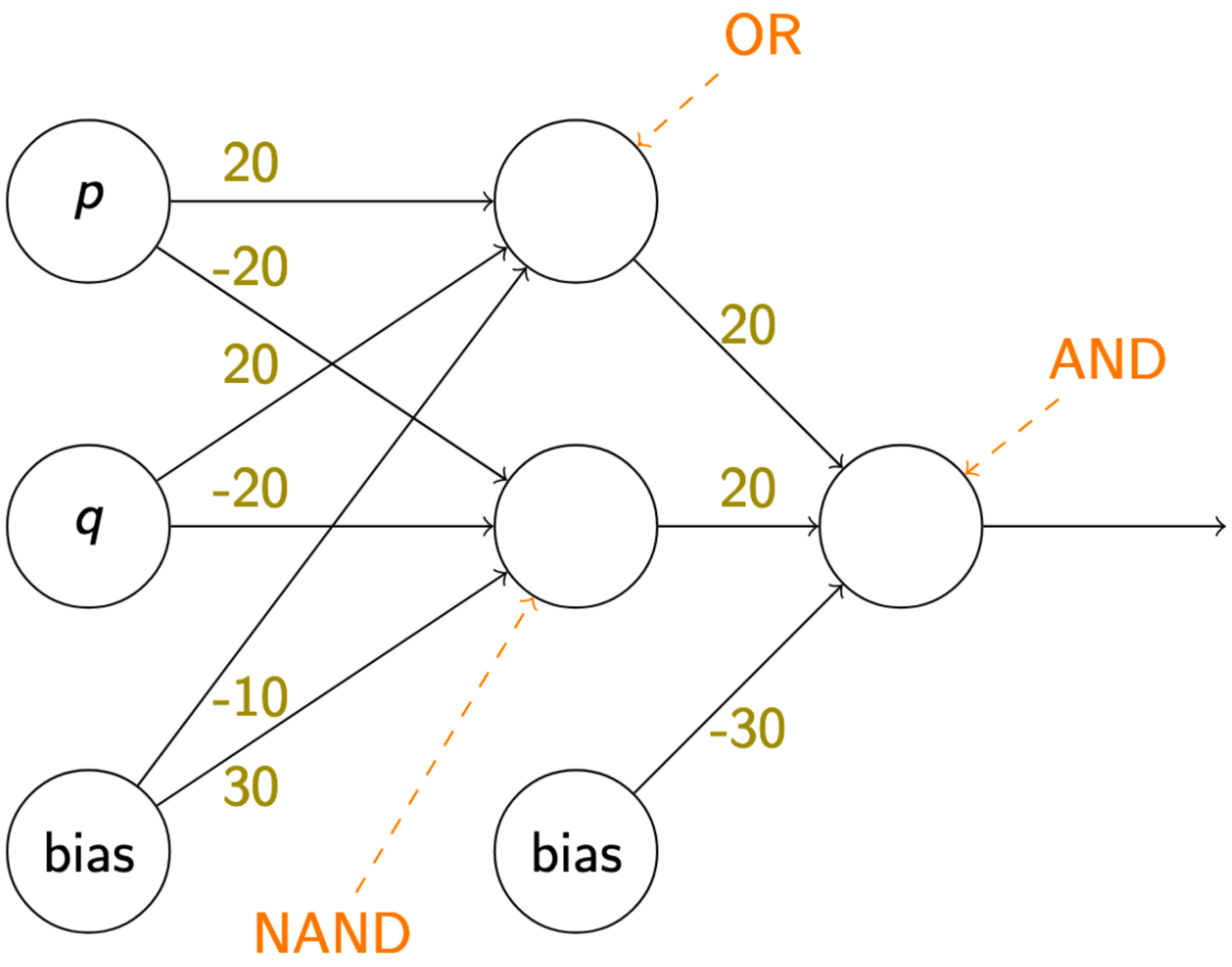

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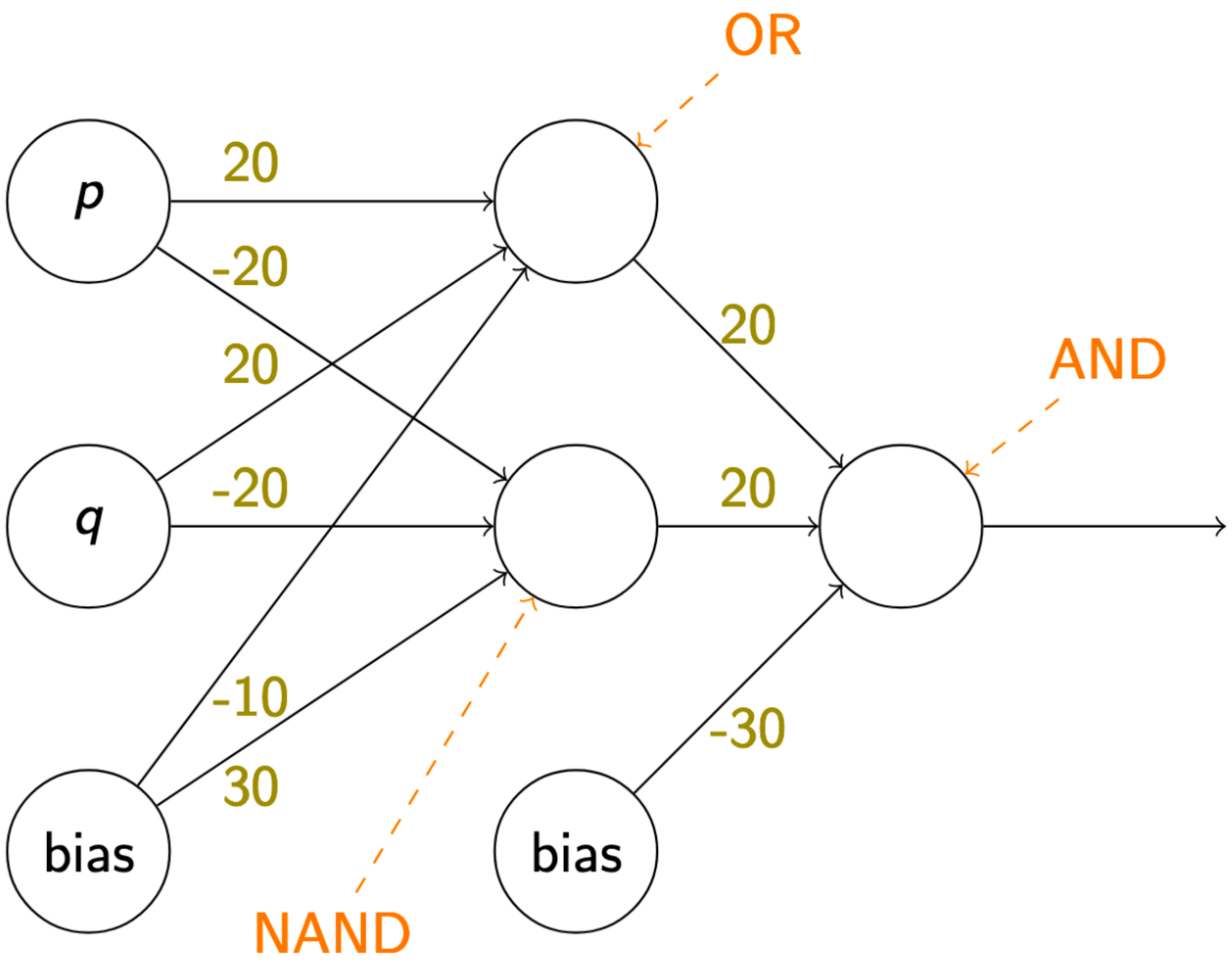

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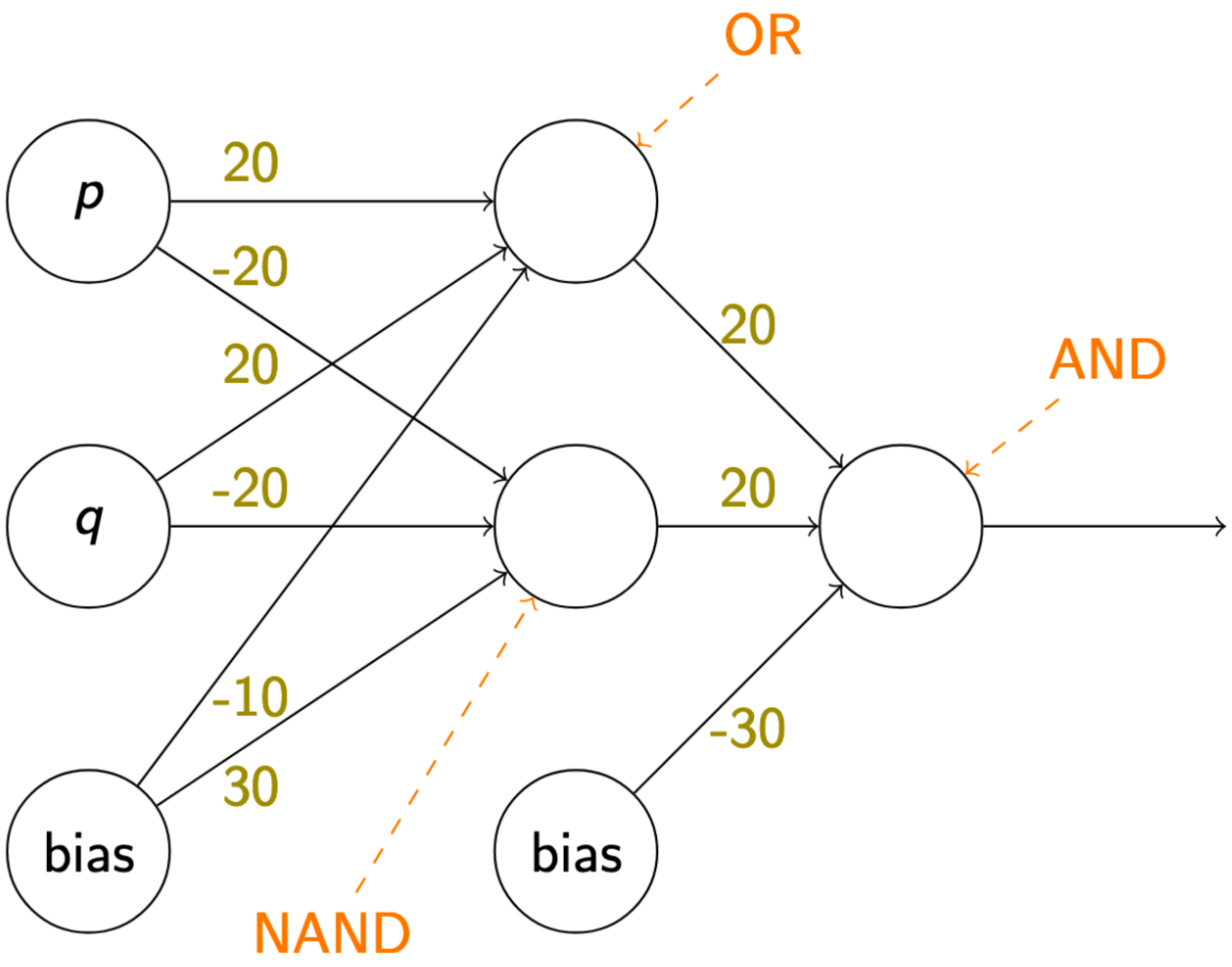
- Exercise: verify this perceptron does what we say it does



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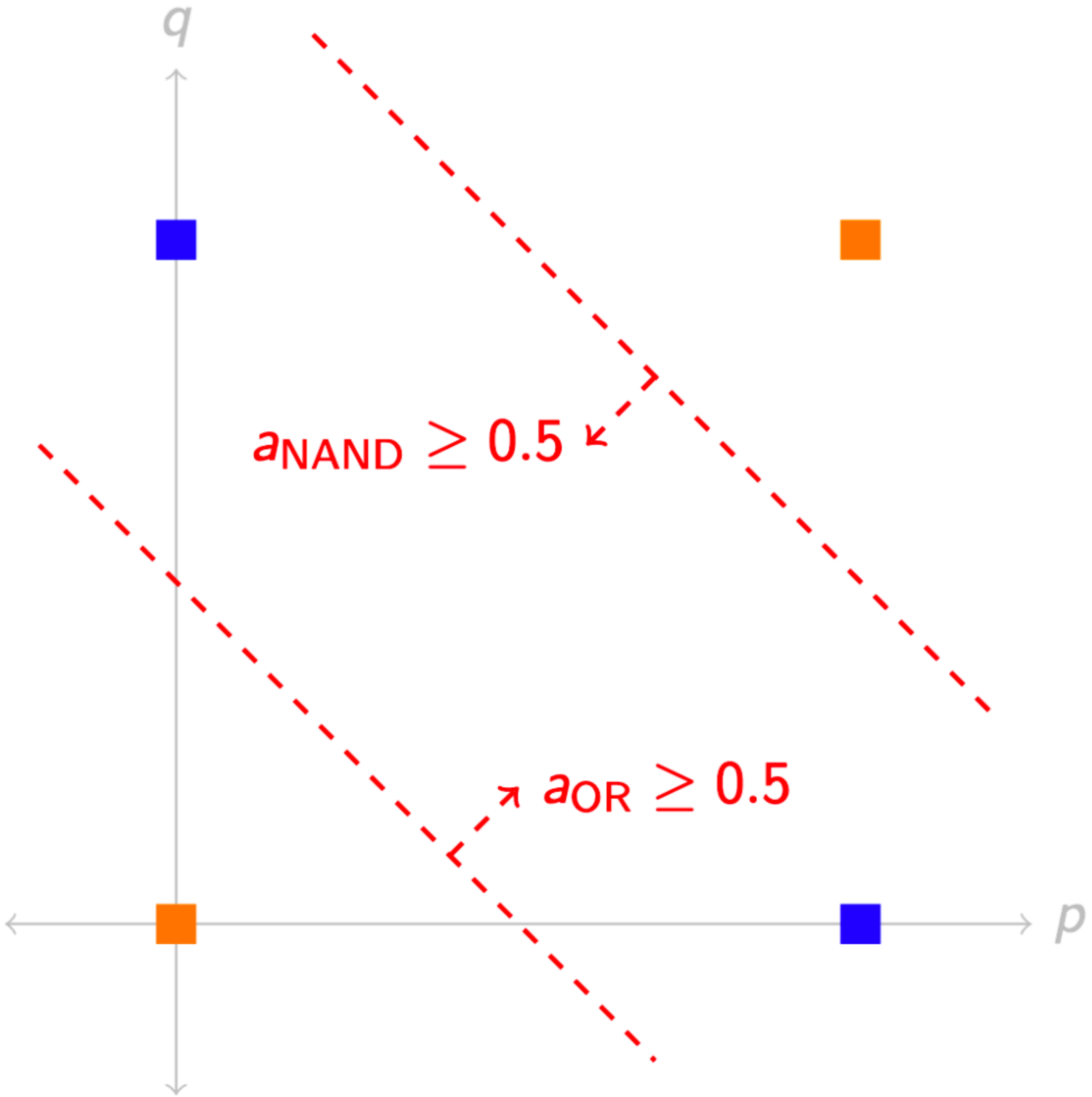

Key Ideas

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  - **Strictly more functions** can be computed with hidden layers than without
  - ***Technically** one hidden layer is all you need (see next slide)

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

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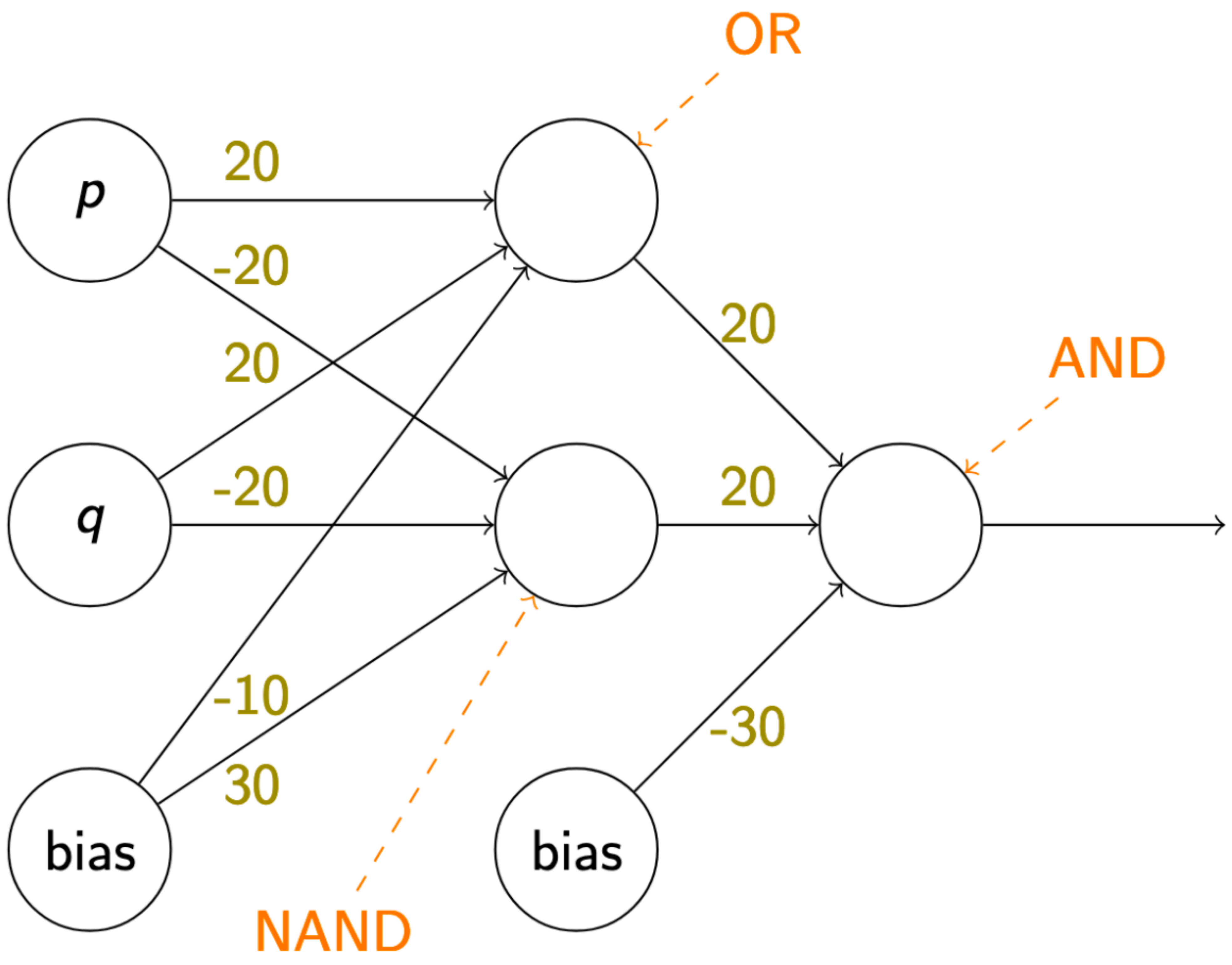
- See also GBC 6.4.1 for more references, generalizations, discussion

XOR Network



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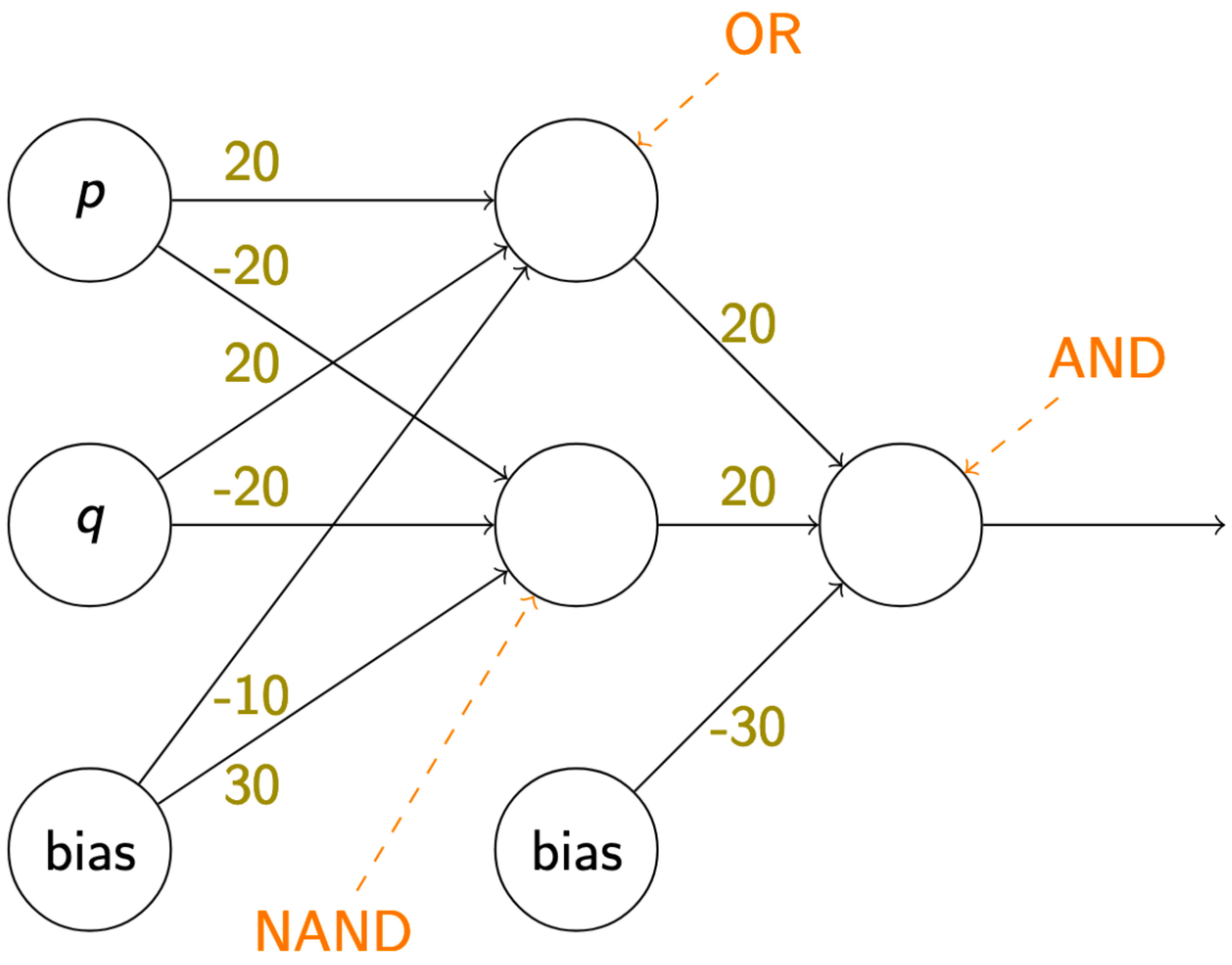

$$a_{\mathsf{or}} = \sigma\left(\begin{bmatrix} w_p^{\mathsf{or}} & w_q^{\mathsf{or}} \end{bmatrix} \begin{bmatrix} p \\ q \end{bmatrix} + b^{\mathsf{or}} \right)$$

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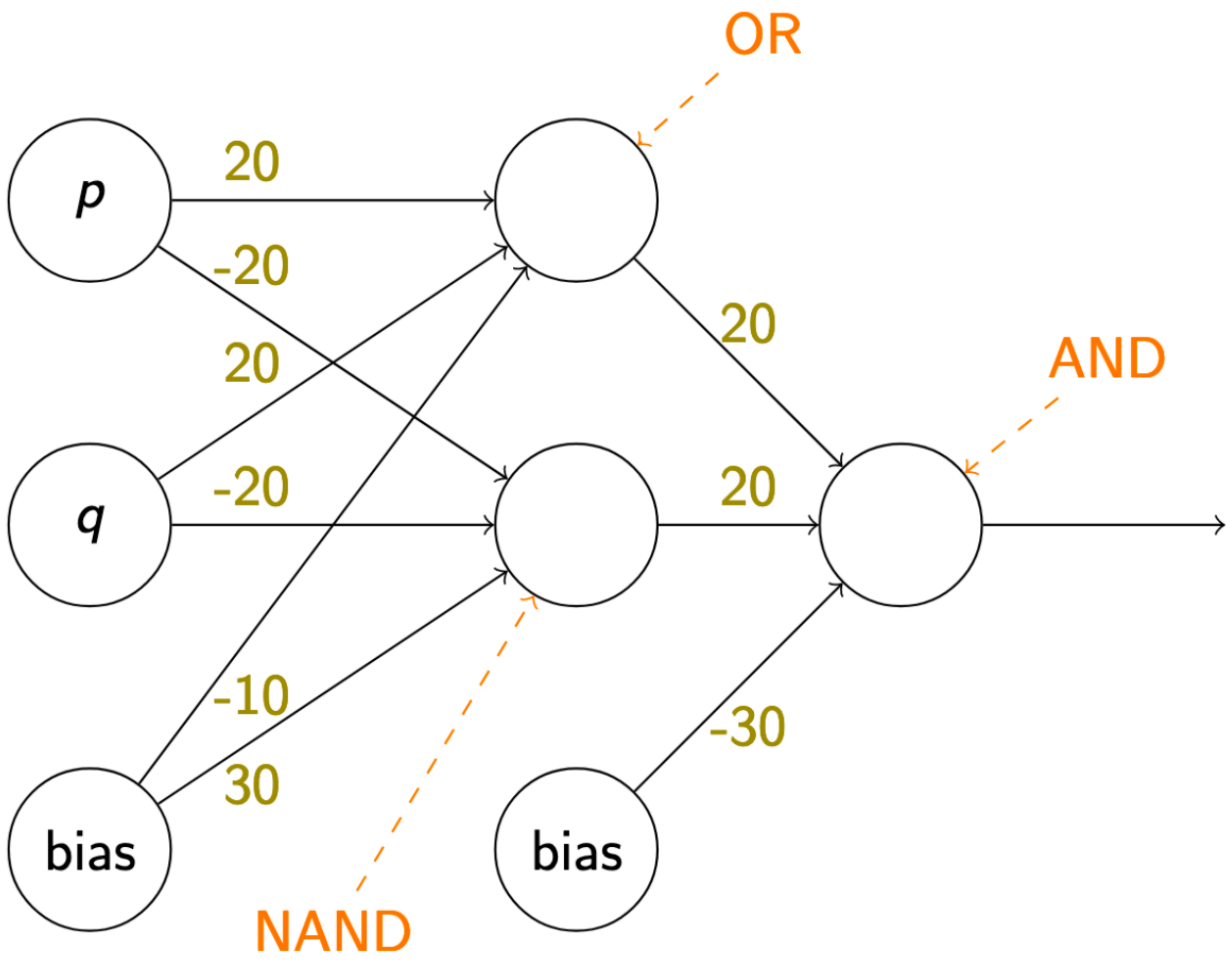

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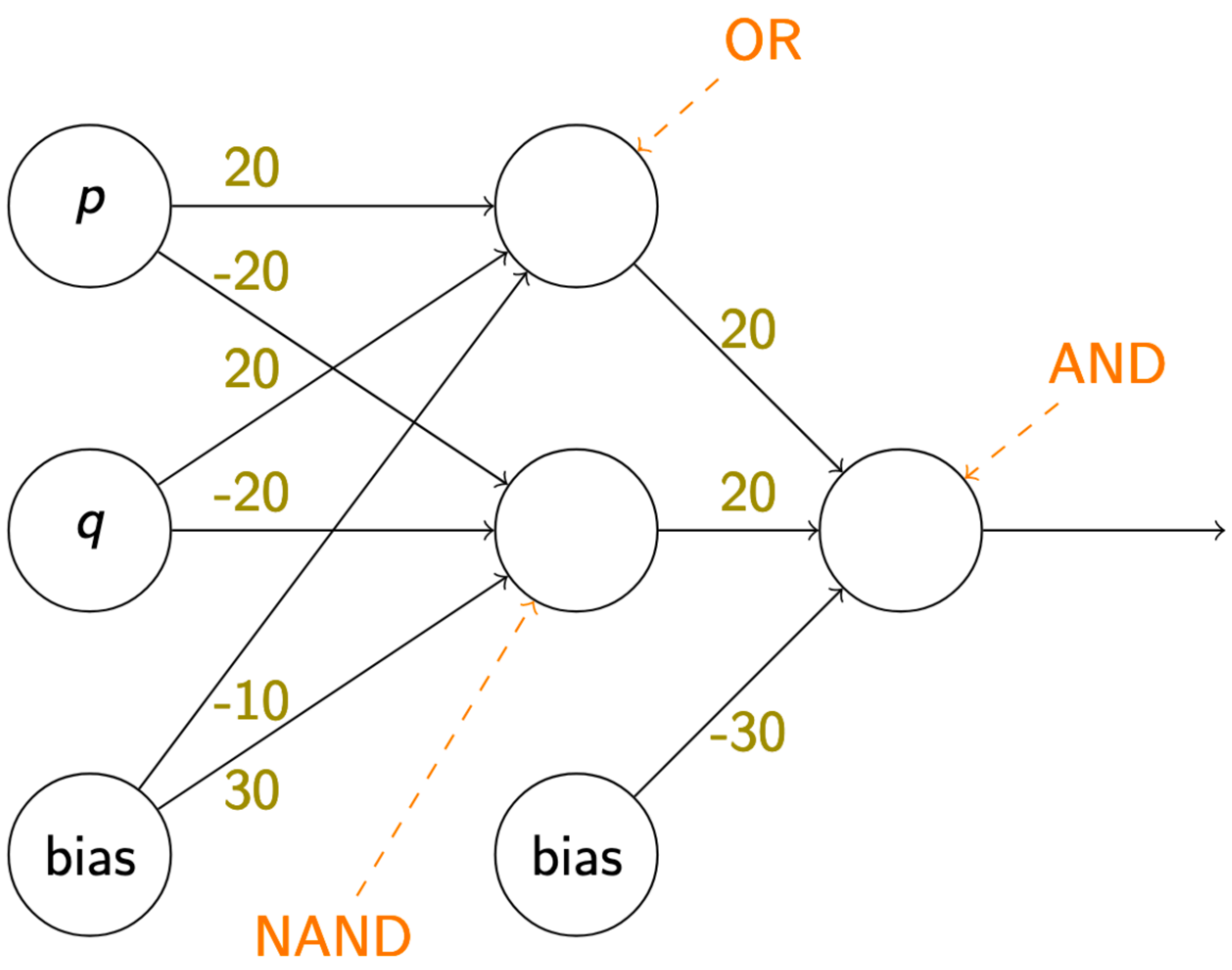

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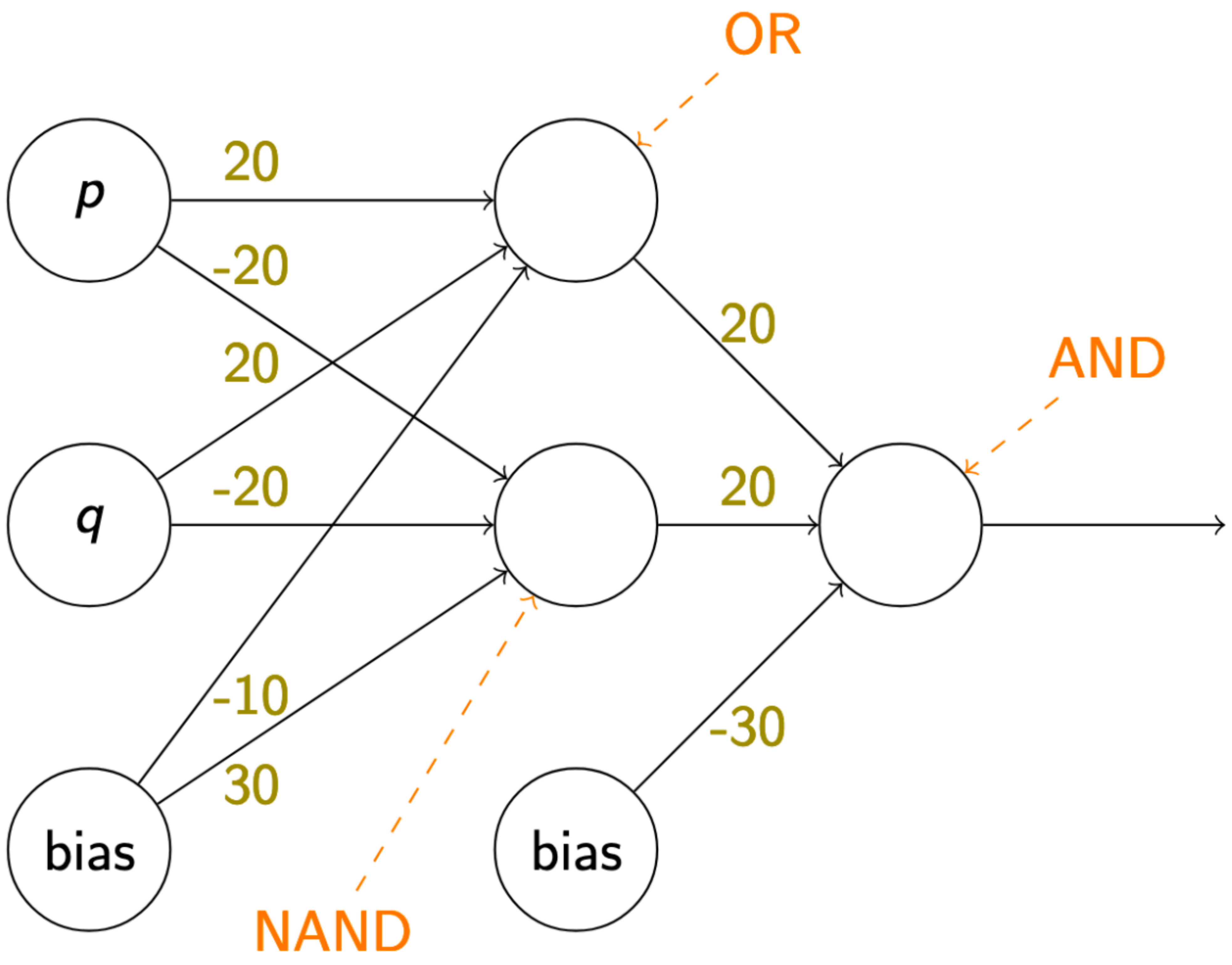

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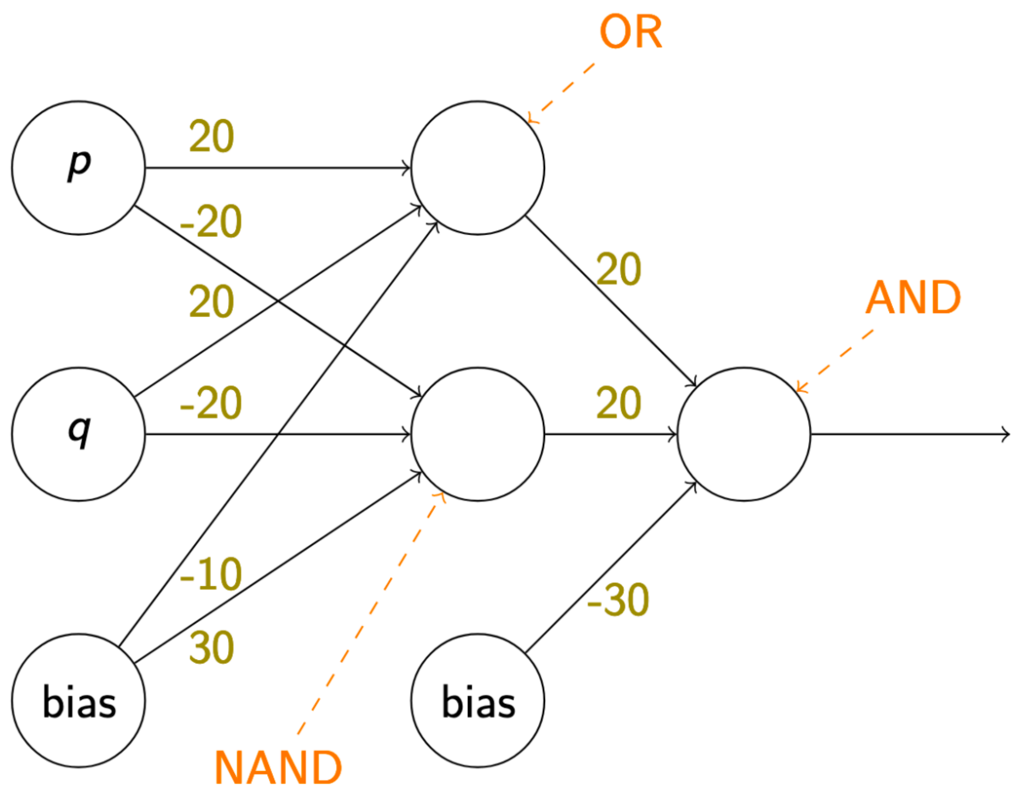

XOR Network

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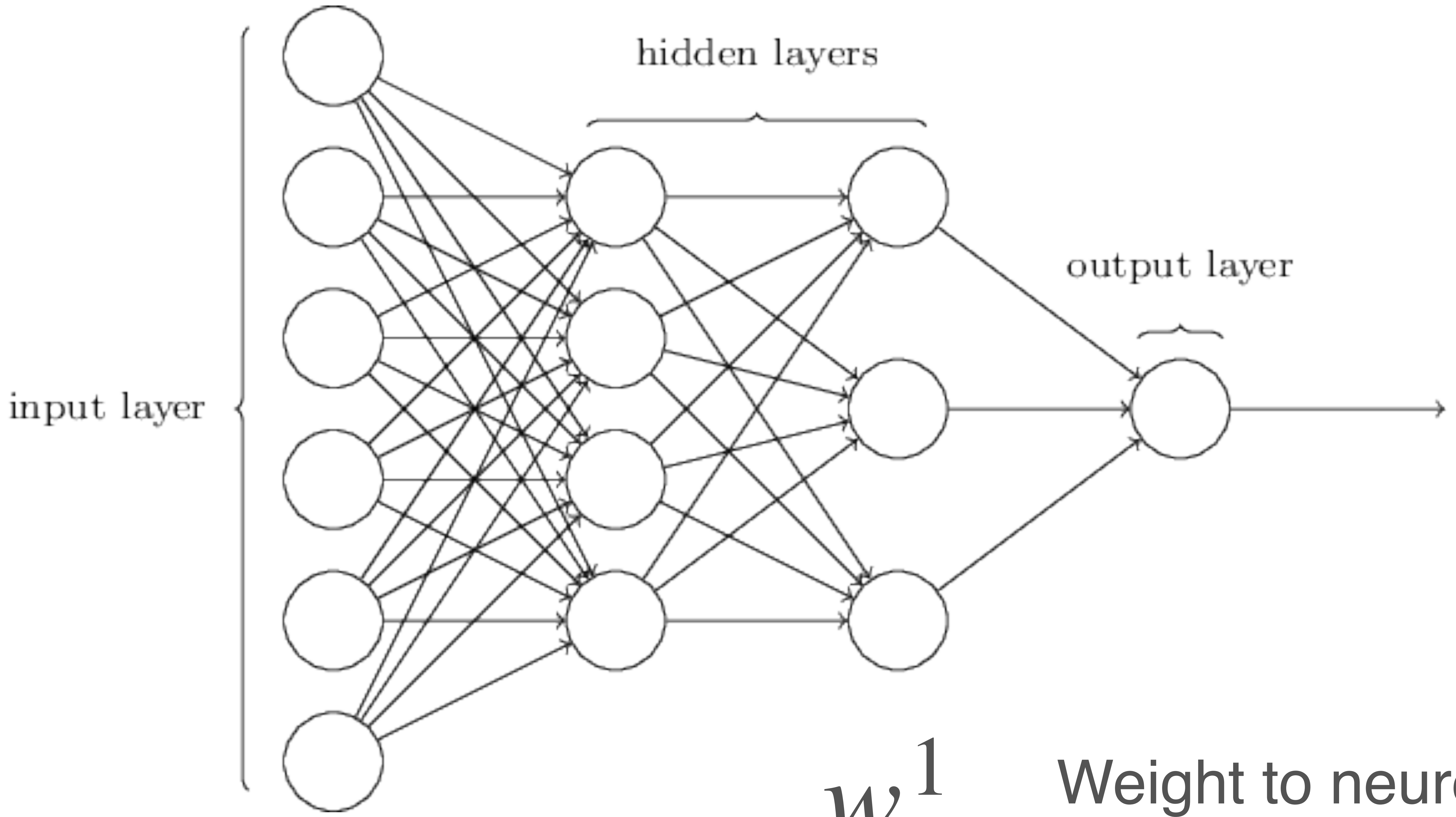
Some terminology

- Our XOR network is a **feed-forward** neural network with **one hidden layer**
  - Also called a **Multi-Layer Perceptron (MLP)**
- 2 input nodes
- 1 output node
- 1 hidden layer with 2 neurons
- Sigmoid activation function

General MLP



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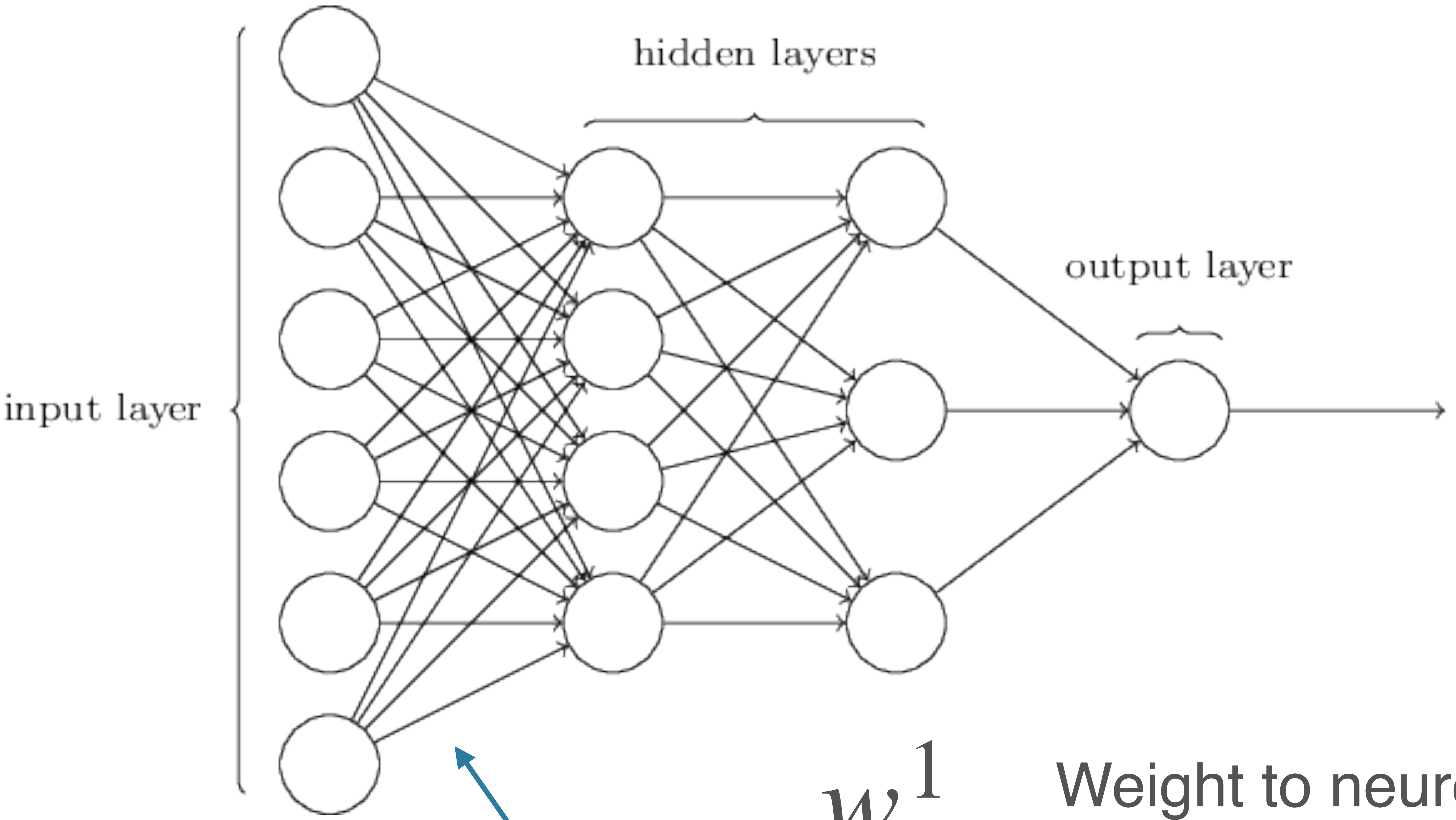
$$w_{ji}^{1}$$

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

General MLP



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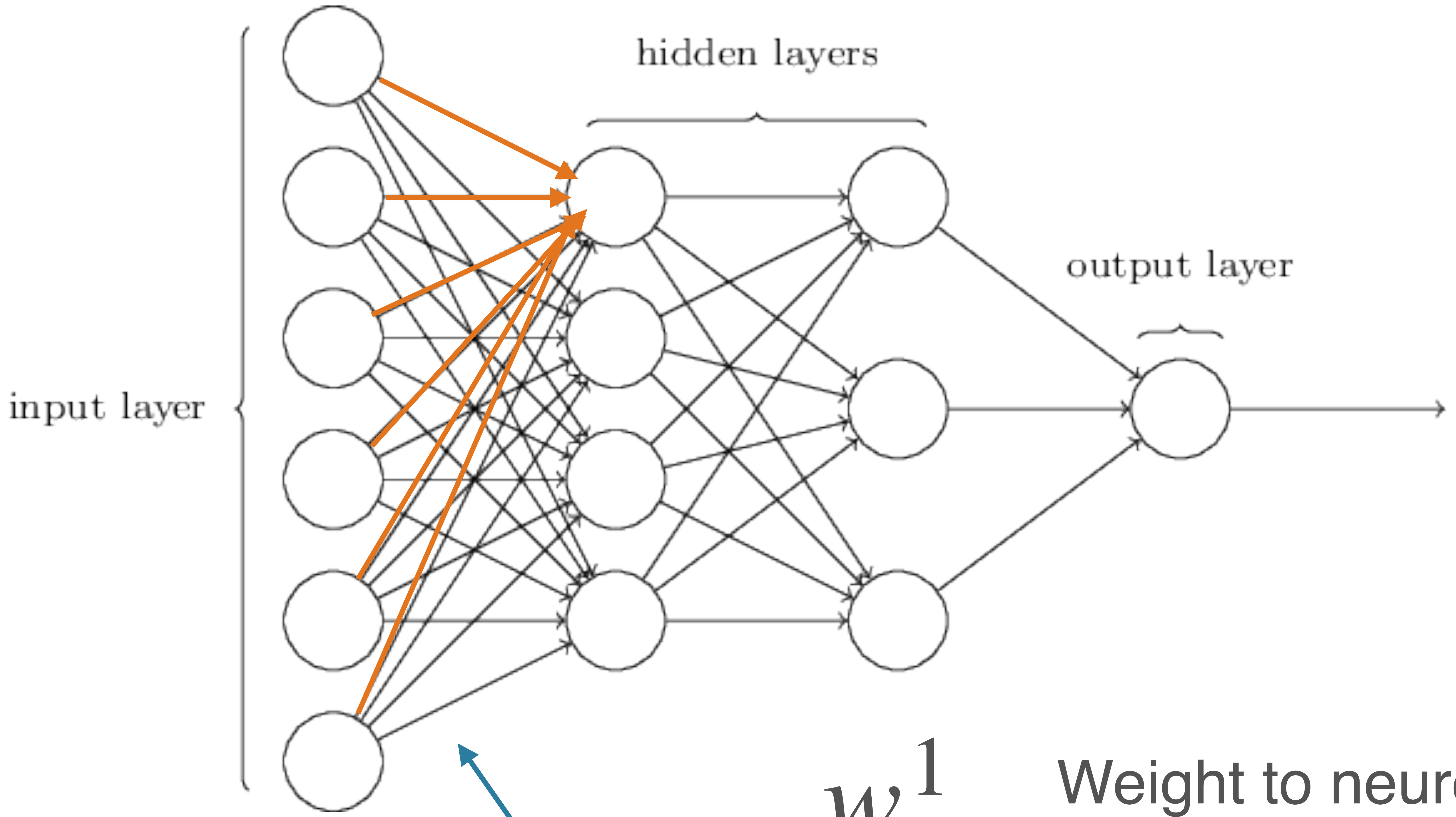

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shape: $(n_0, 1)$

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shape: (n_1, n_0)

n_0: dimension of input (layer 0)

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Parameters of an MLP

- Weights and biases
  - For **each layer** l: $n_l(n_{l-1} + 1)$
  - $n_l \cdot n_{l-1}$ weights; n_l biases
- With *k* hidden layers (considering the output as a hidden layer):
  - $\sum_{i=1}^{k} n_i(n_{i-1} + 1)$ trainable parameters

Hyper-parameters of an MLP

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- **Input & output size**
  - Usually **fixed by your problem / dataset**
  - Input: image size, vocab size; number of “raw” features in general
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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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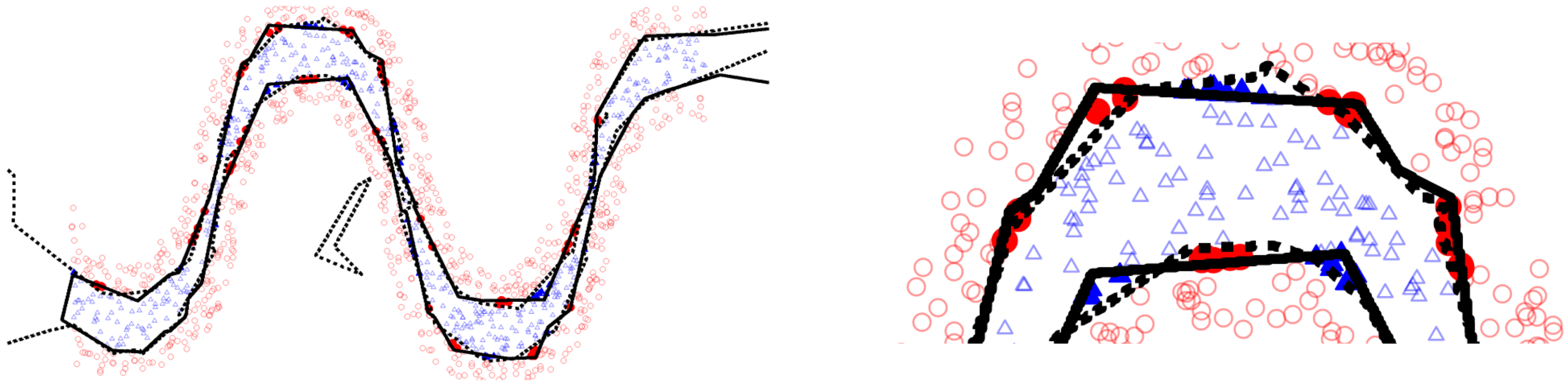

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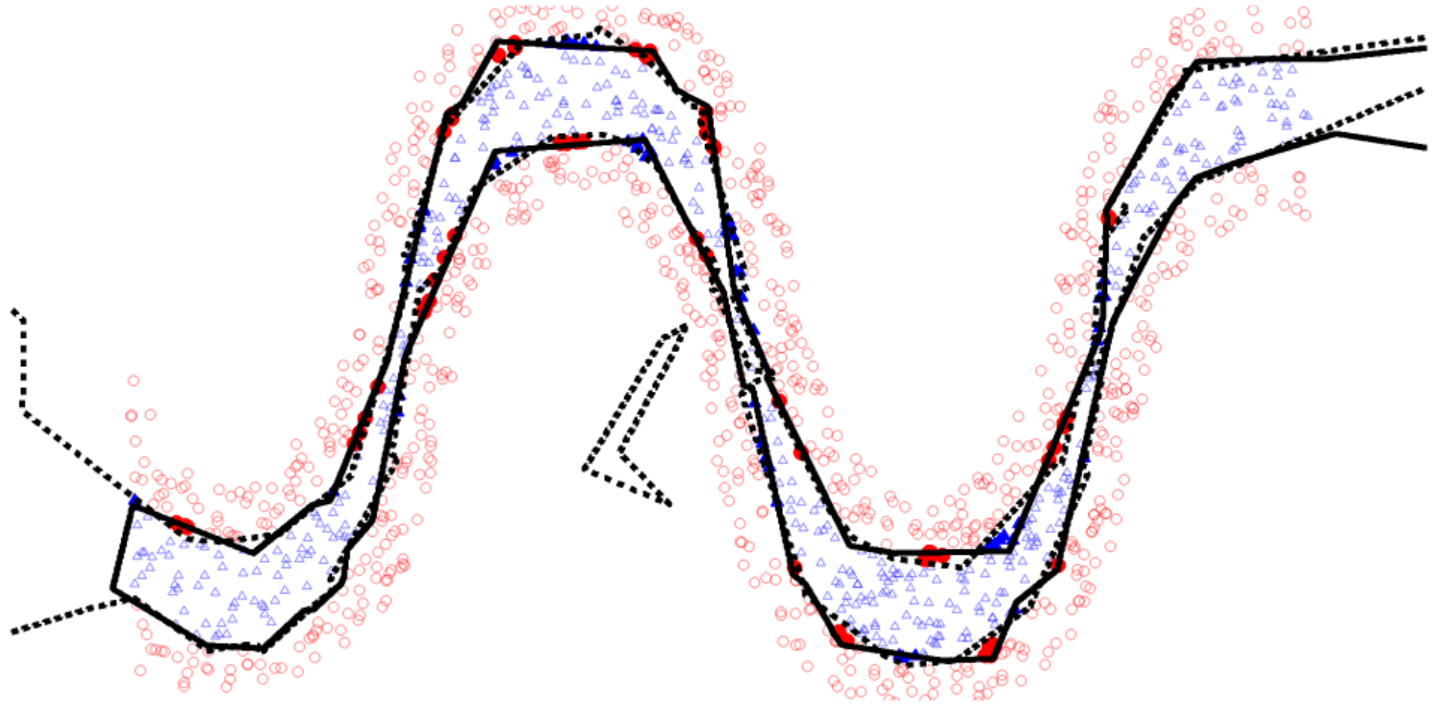

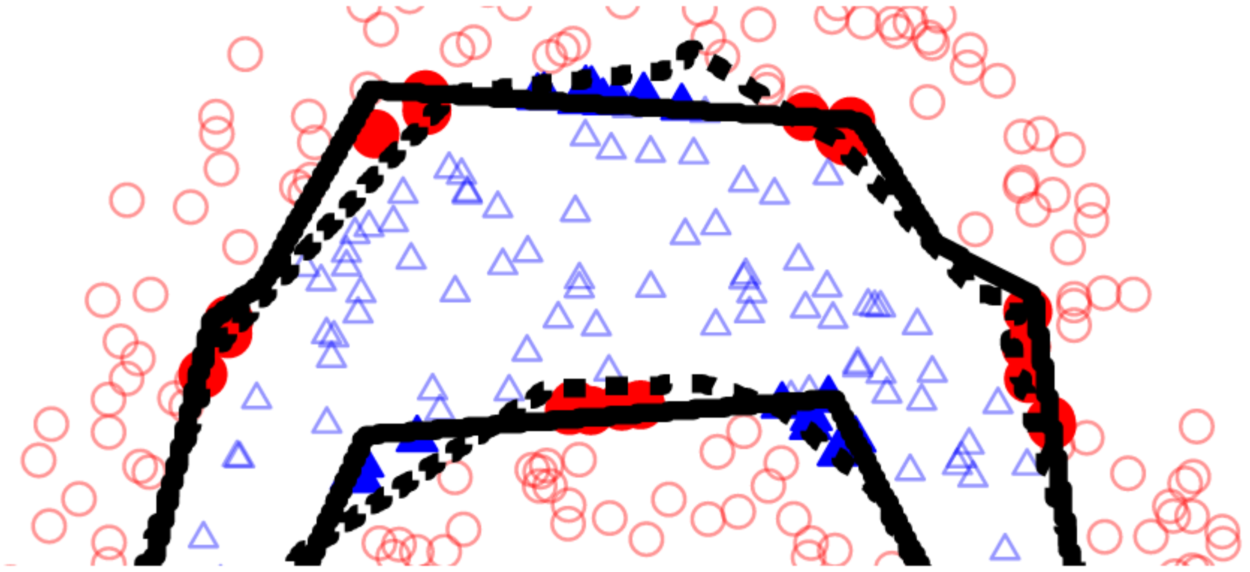

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  - In principle
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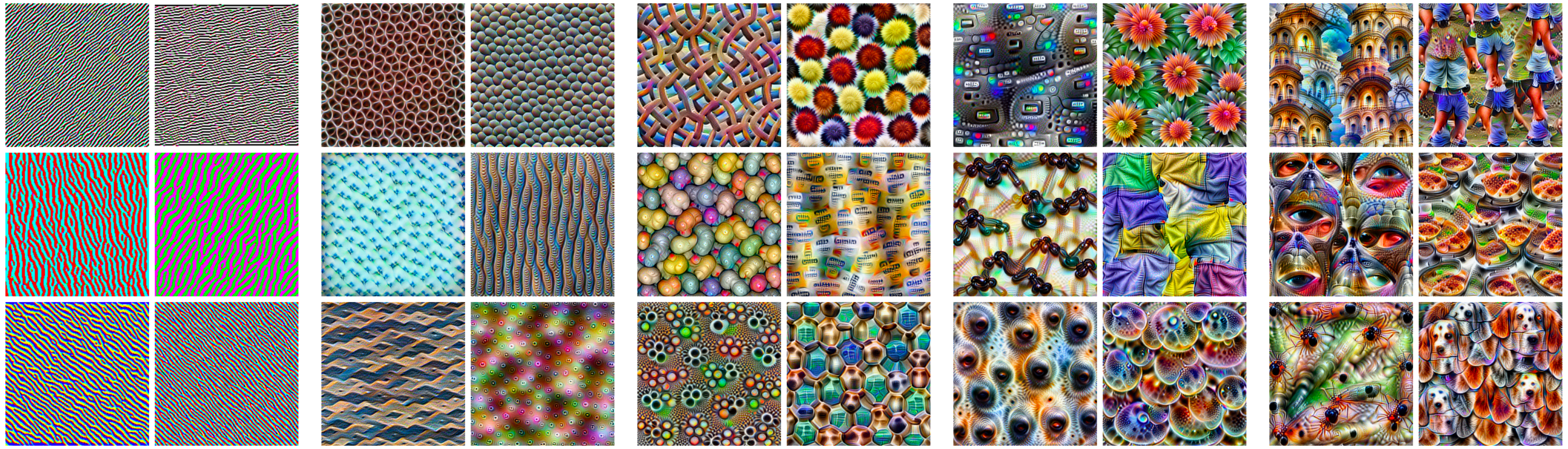

Edges (layer conv2d0) **Textures** (layer mixed3a) **Patterns** (layer mixed4a) **Parts** (layers mixed4b & mixed4c) **Objects** (layers mixed4d & mixed4e)

source

Activation Functions

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

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

Non-linearity, cont.

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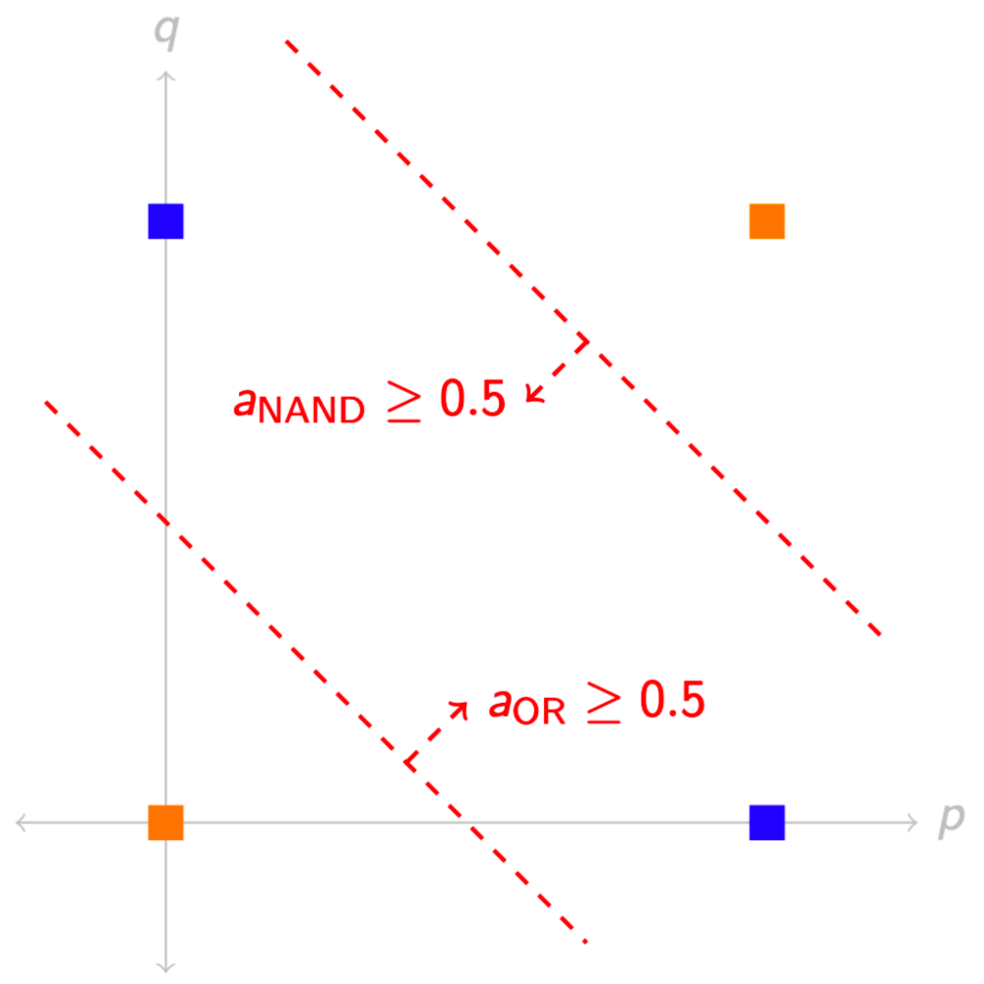

Non-linearity, cont.

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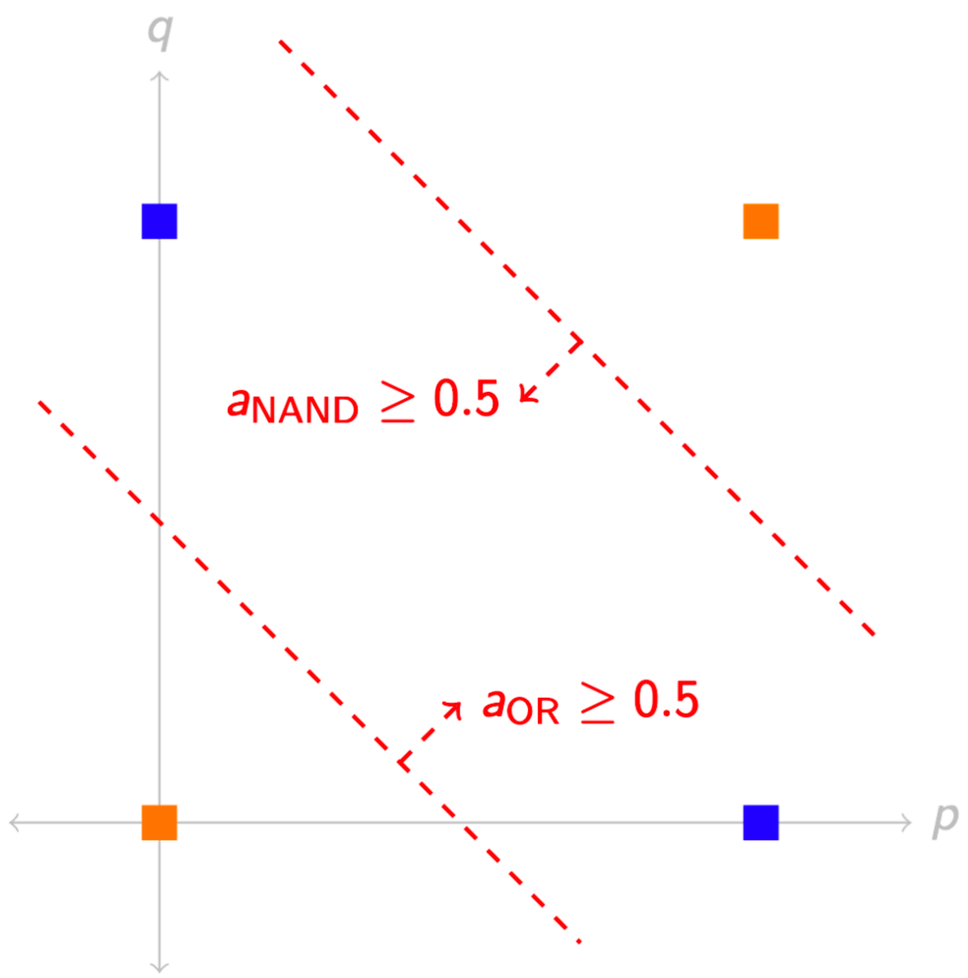
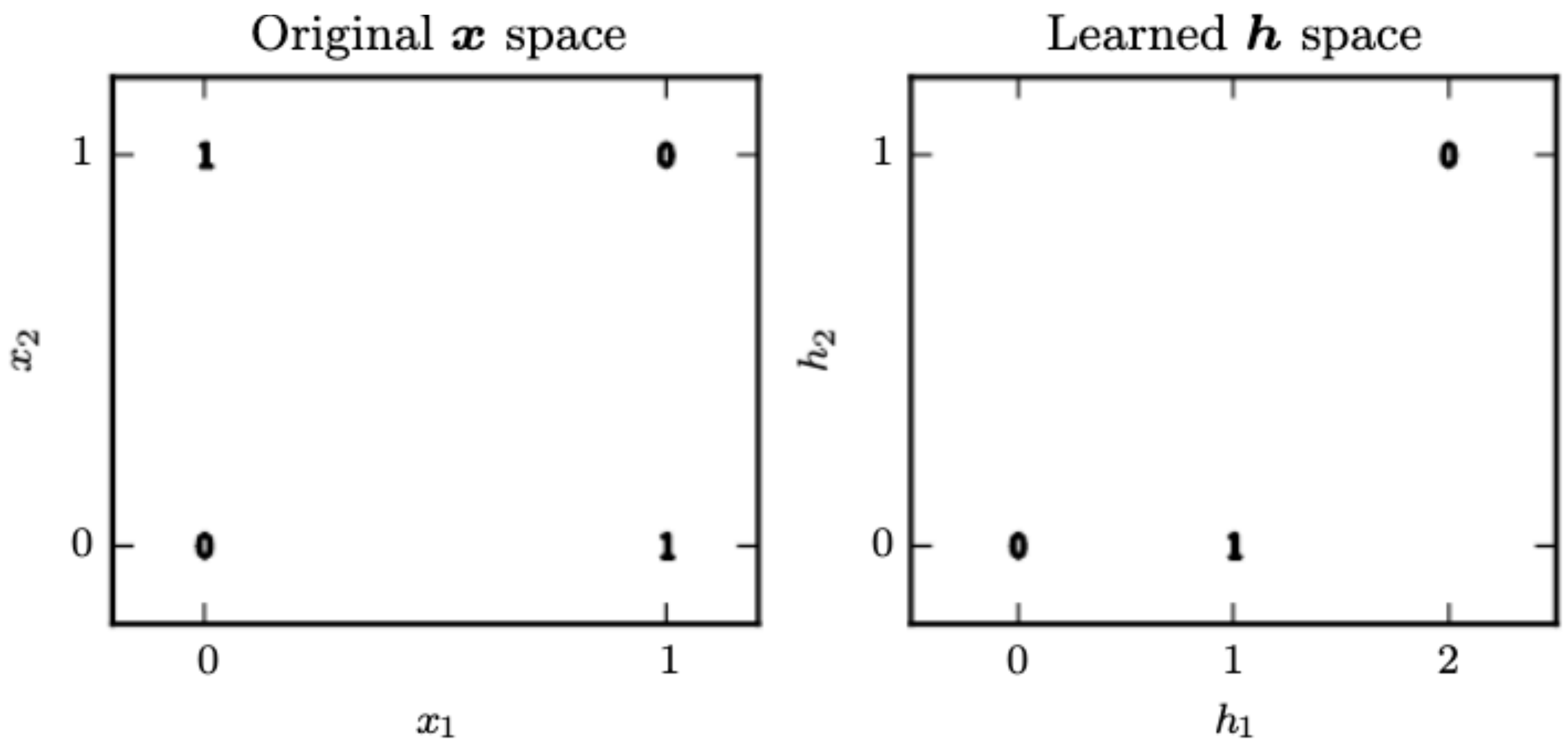
  - This is a *non-linear* transformation
  - Space folding intuition more generally (also GBC sec 6.4.1)





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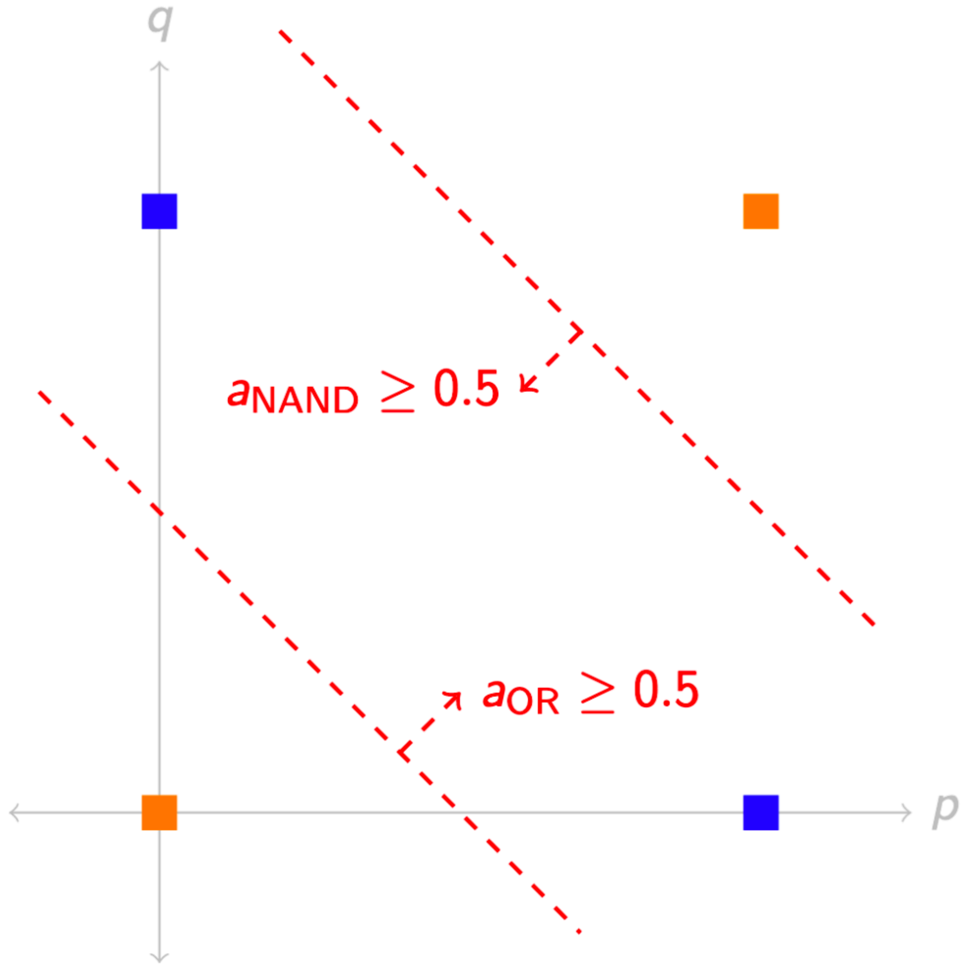
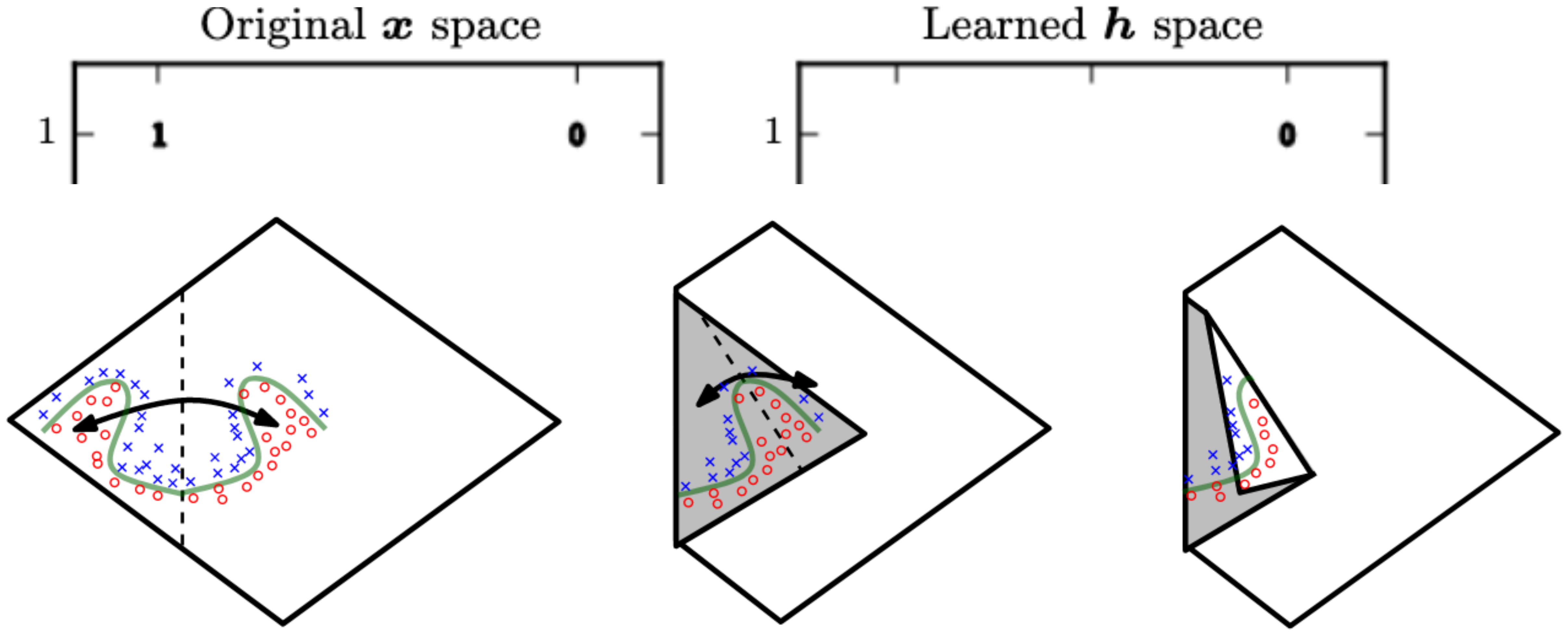
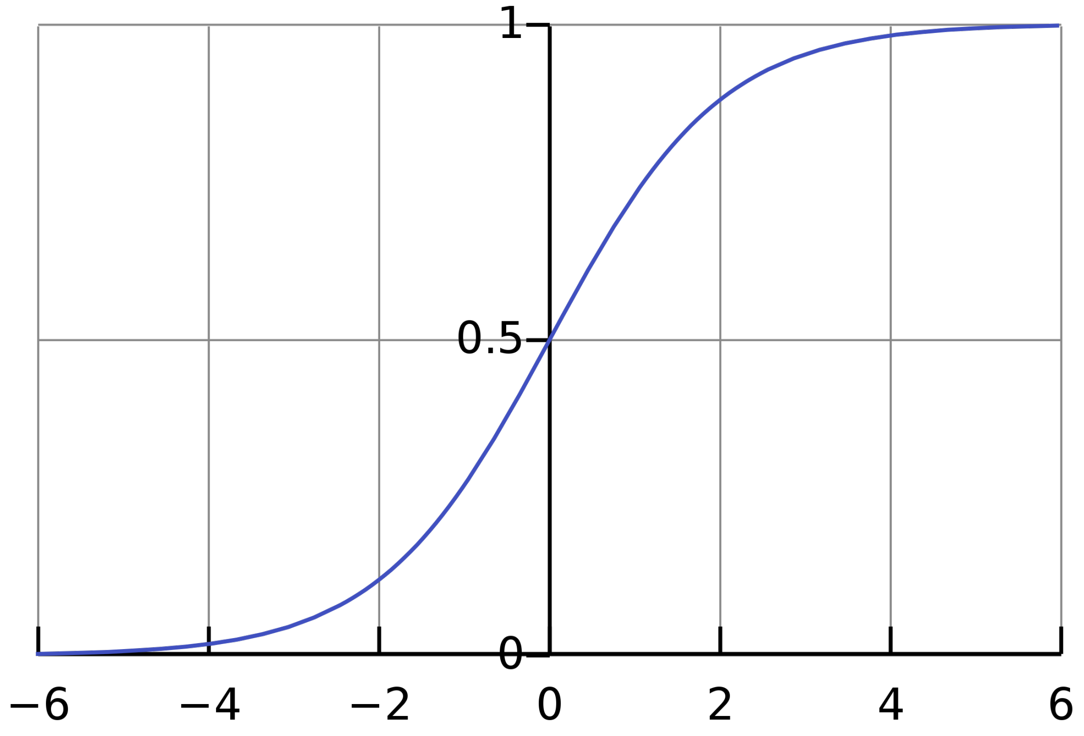




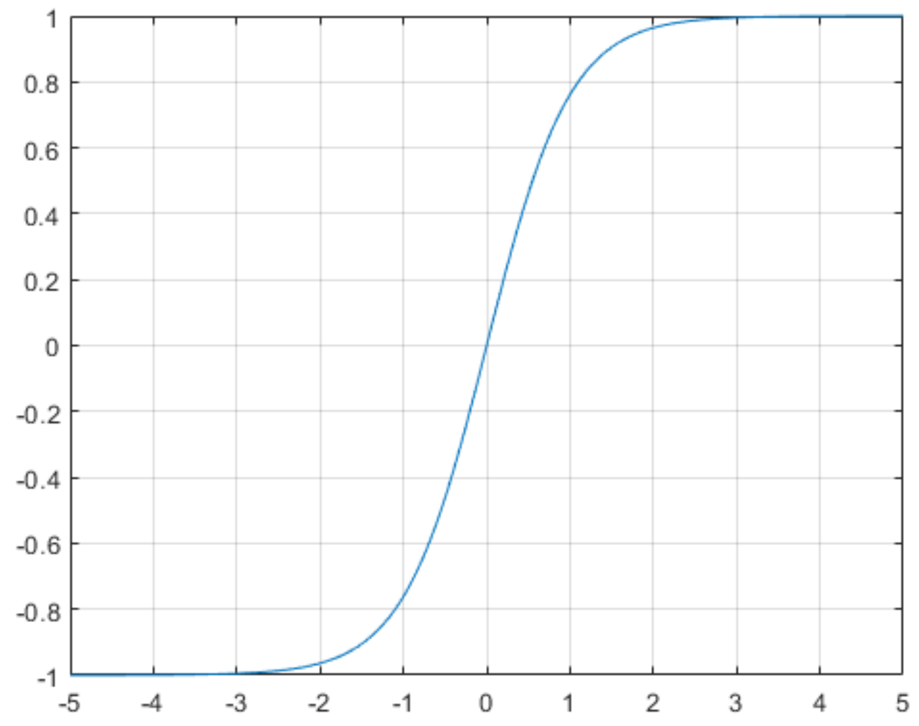
Activation Functions: Hidden Layer

sigmoid



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

tanh



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

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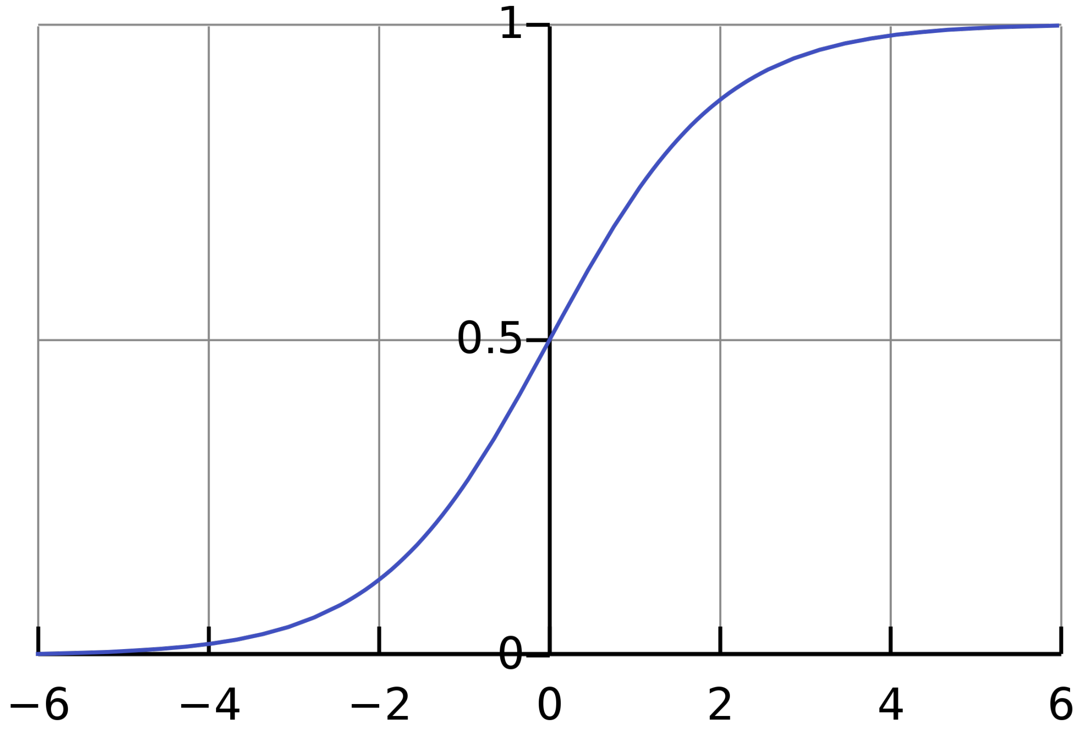

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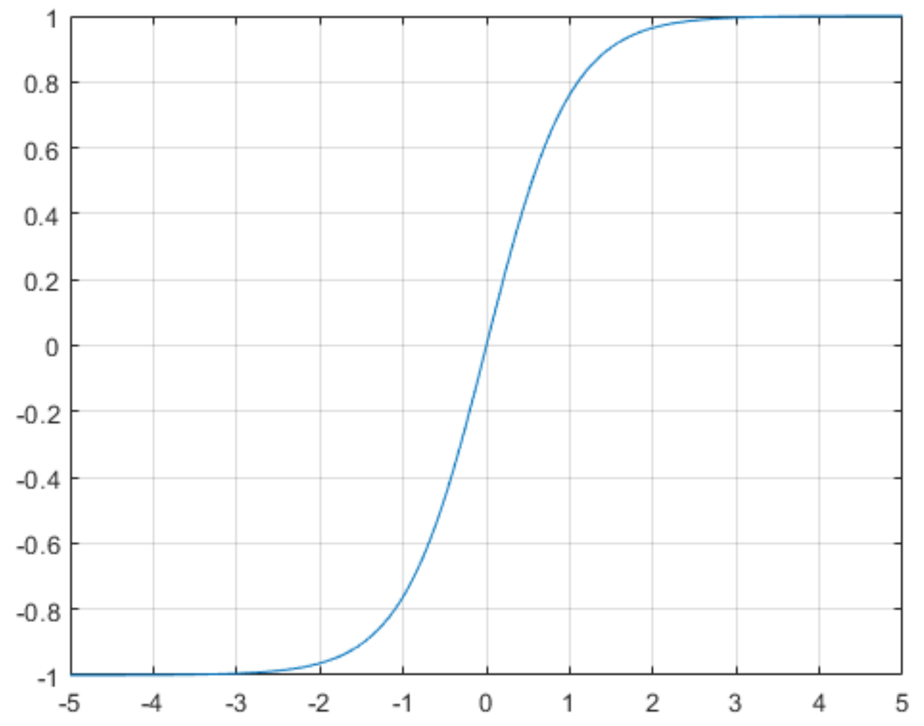

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Problem with these two: derivative "saturates" (nearly 0) everywhere except near origin

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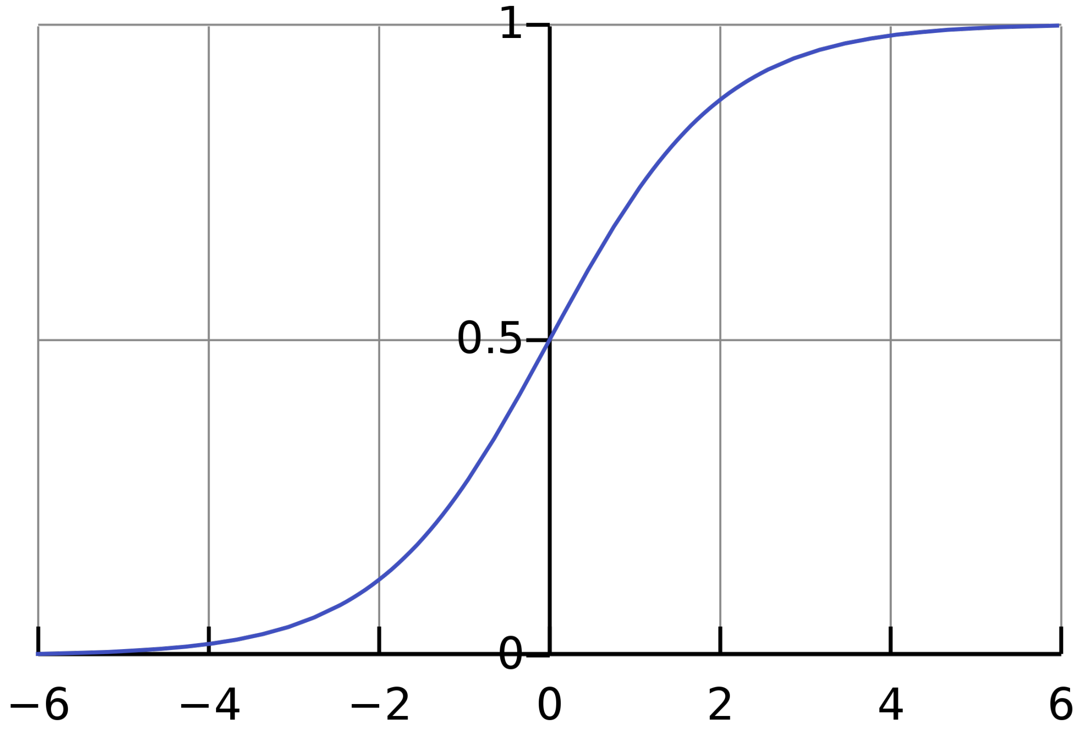

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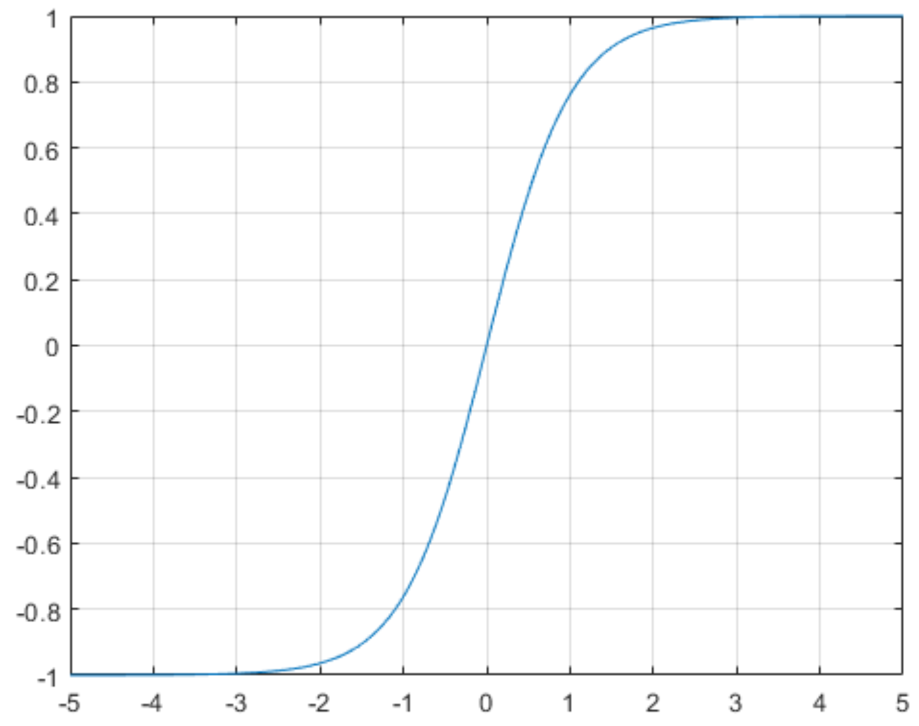

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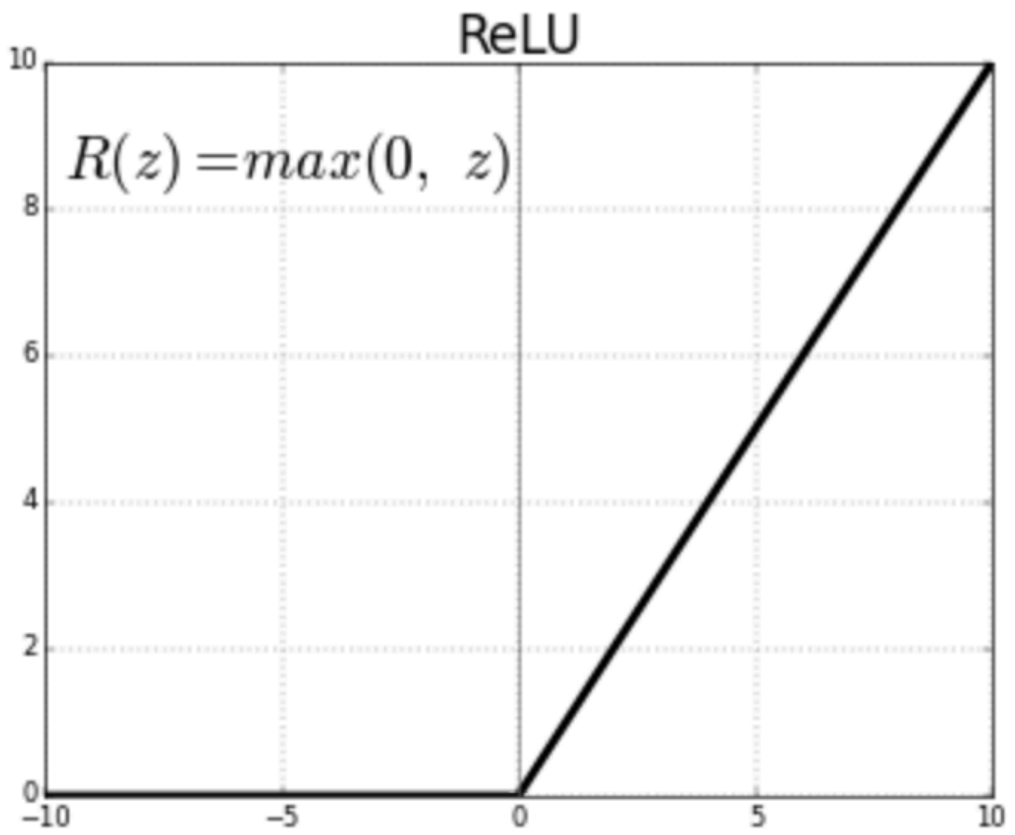

Problem with these two: derivative "saturates" (nearly 0) everywhere except near origin

ReLU does not saturate. Good "default"

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

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

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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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$$W^1 = \begin{bmatrix} w_{00} & w_{10} & \cdots & w_{0n_0} \\ w_{10} & w_{11} & \cdots & w_{1n_0} \\ \vdots & \vdots & \ddots & \vdots \\ w_{n_10} & w_{n_11} & \cdots & w_{n_1n_0} \end{bmatrix}$$

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Shape: (n_1, n_0)
n_0: dimension of input (layer 0)
n_1: output dimension of layer 1

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

Shape: $(n_0, 1)$

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

Shape: $(n_1, 1)$

Mini-batch Gradient Descent

```
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 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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Shape: (n_0, k)

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Shape: (n_1, n_0)
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Shape: $(n_1, 1)$
Added to each col. of $W^1 X$

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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  - Images: (batch_size, width, height, 3)
  - Sequences: (batch_size, seq_len, representation_size)
- Two comments:
  - In your code, **annotate every tensor** with a comment showing **intended shape**
  - When debugging, look at shapes early on!!

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

Neural Probabilistic Language Model

Language Modeling

- A language model parametrized by θ computes: $P_\theta(w_1, \ldots, w_n)$
- Typically (though we'll see variations): $P_\theta(w_1, \ldots, w_n) = \prod_i P_\theta(w_i \mid w_1, \ldots, w_{i-1})$
- E.g. of labeled data: "Today is the seventh day of 282." —>
  - (<s>, Today)
  - (<s> Today, is)
  - (<s> Today is, the)
  - (<s> Today is the, seventh)

N-gram LMs

- Dominant approach for a long time uses **n-grams**:

$$P_\theta(w_i \mid w_1, \ldots, w_{i-1}) \approx P_\theta(w_i \mid w_{i-1}, w_{i-2}, \ldots, w_{i-n})$$

- Estimate the probabilities by **counting** in a corpus
  - Fancy variants (back-off, smoothing, etc)
- Some problems:
  - **Huge number of parameters**: $\approx |V|^n$
  - Doesn't generalize to unseen n-grams

Neural LM

- Core idea behind the Neural Probabilistic LM
  - Make **n-gram assumption**
  - But: learn **word embeddings**
  - “n-gram of word vectors”
  - Probabilities represented by a neural network, not counts

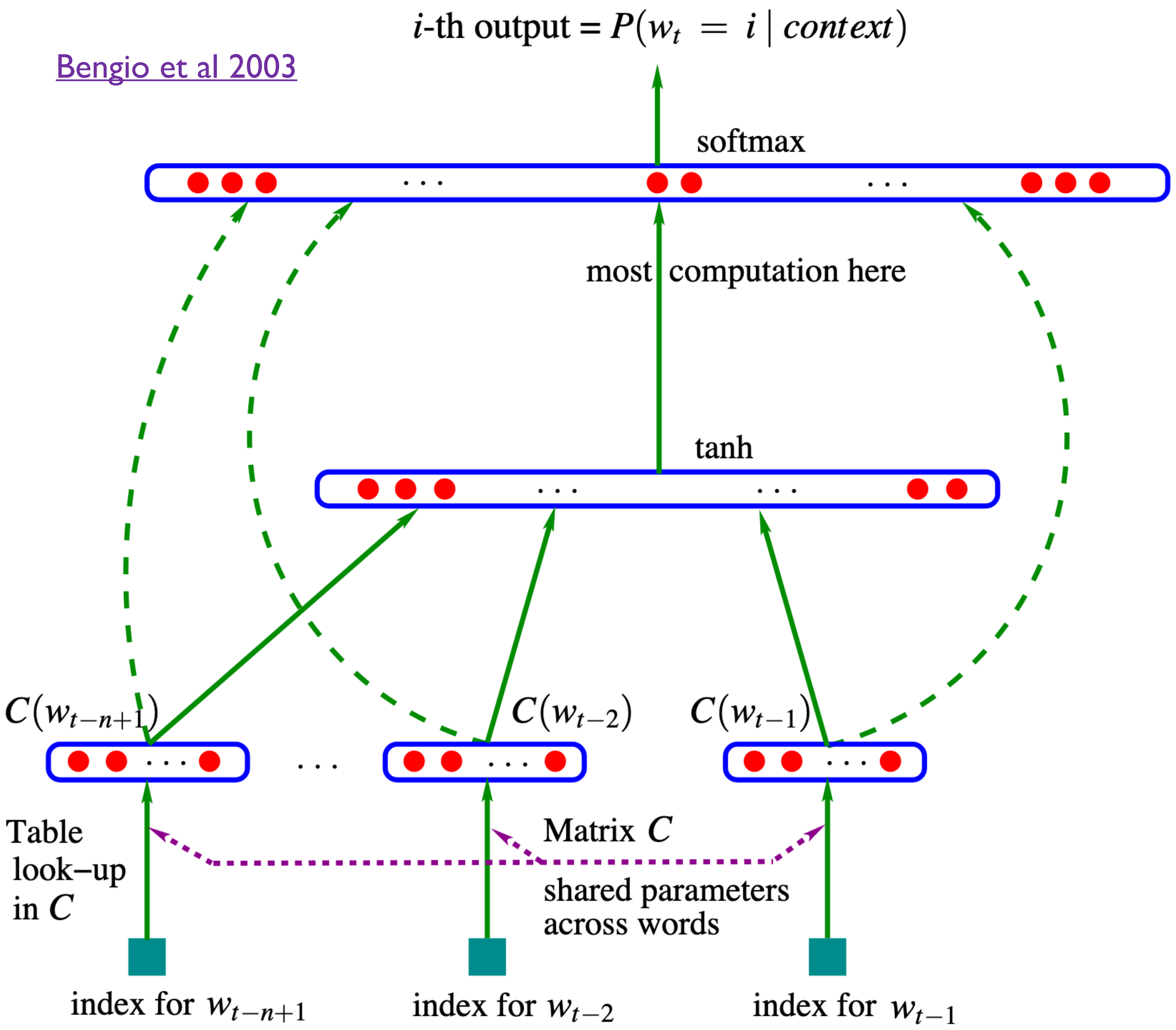
Pros of Neural LM

- Number of parameters:
  - Significantly lower, thanks to **“low”-dimensional embeddings**
- Generalization: embeddings enable **generalizing to similar words**

```
                    The cat is walking in the bedroom
to                  A dog was running in a room
and likewise to     The cat is running in a room
                    A dog is walking in a bedroom
                    The dog was walking in the room
```

Neural LM Architecture

Bengio et al 2003



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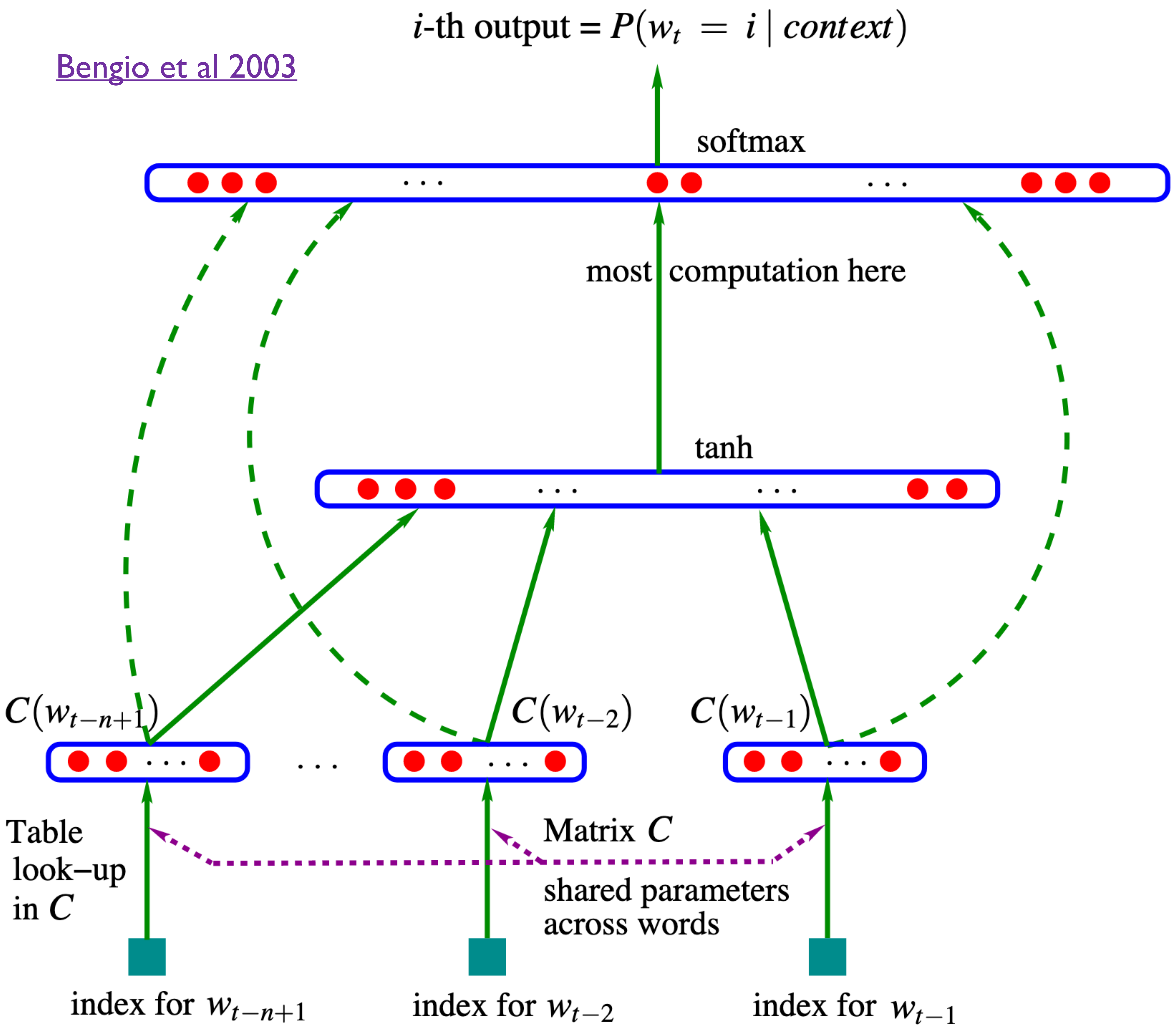

w_t: one-hot vector

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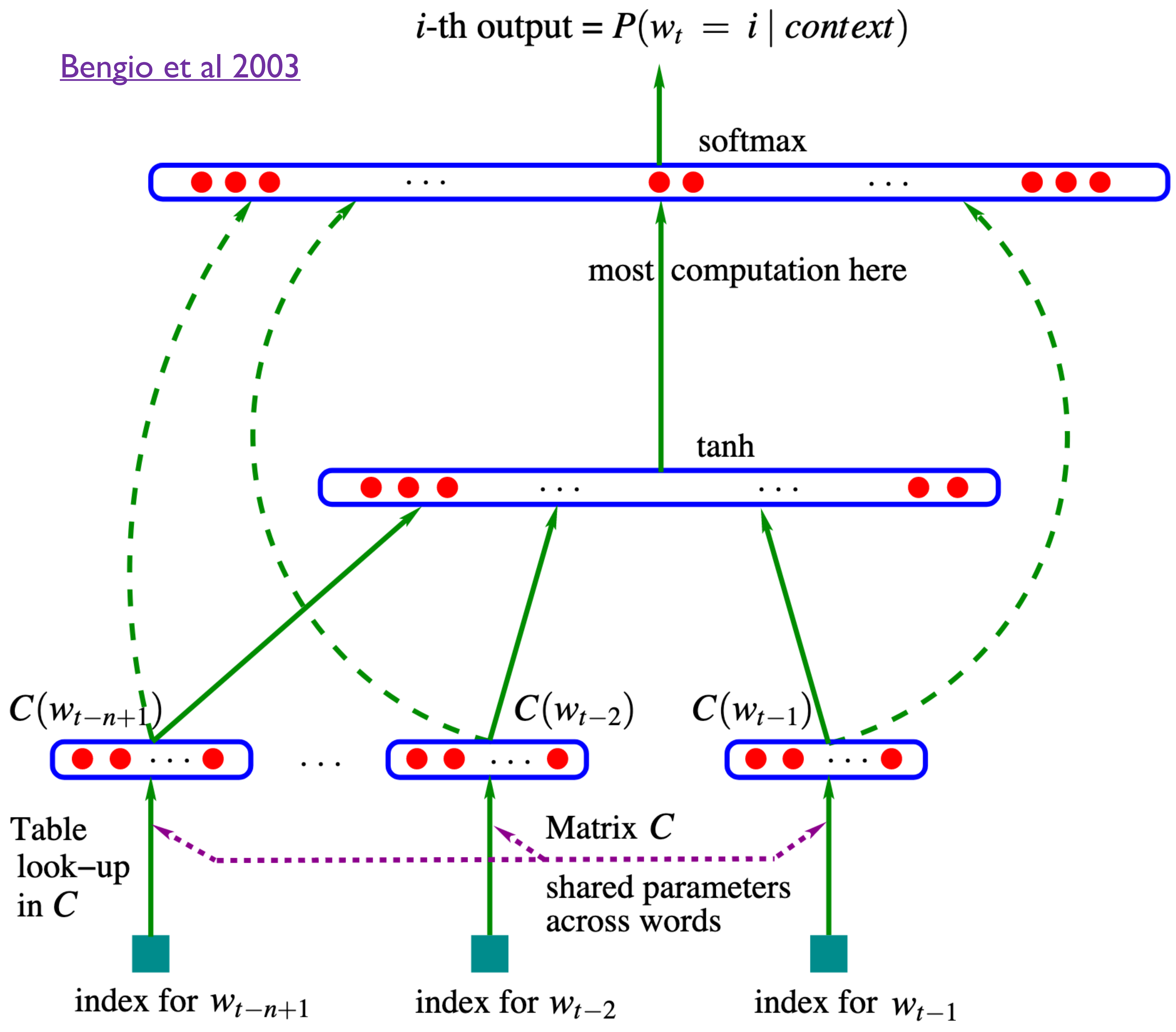

embeddings = concat$(Cw_{t-1}, Cw_{t-2}, \ldots, Cw_{t-(n+1)})$

w_t: one-hot vector

Neural LM Architecture

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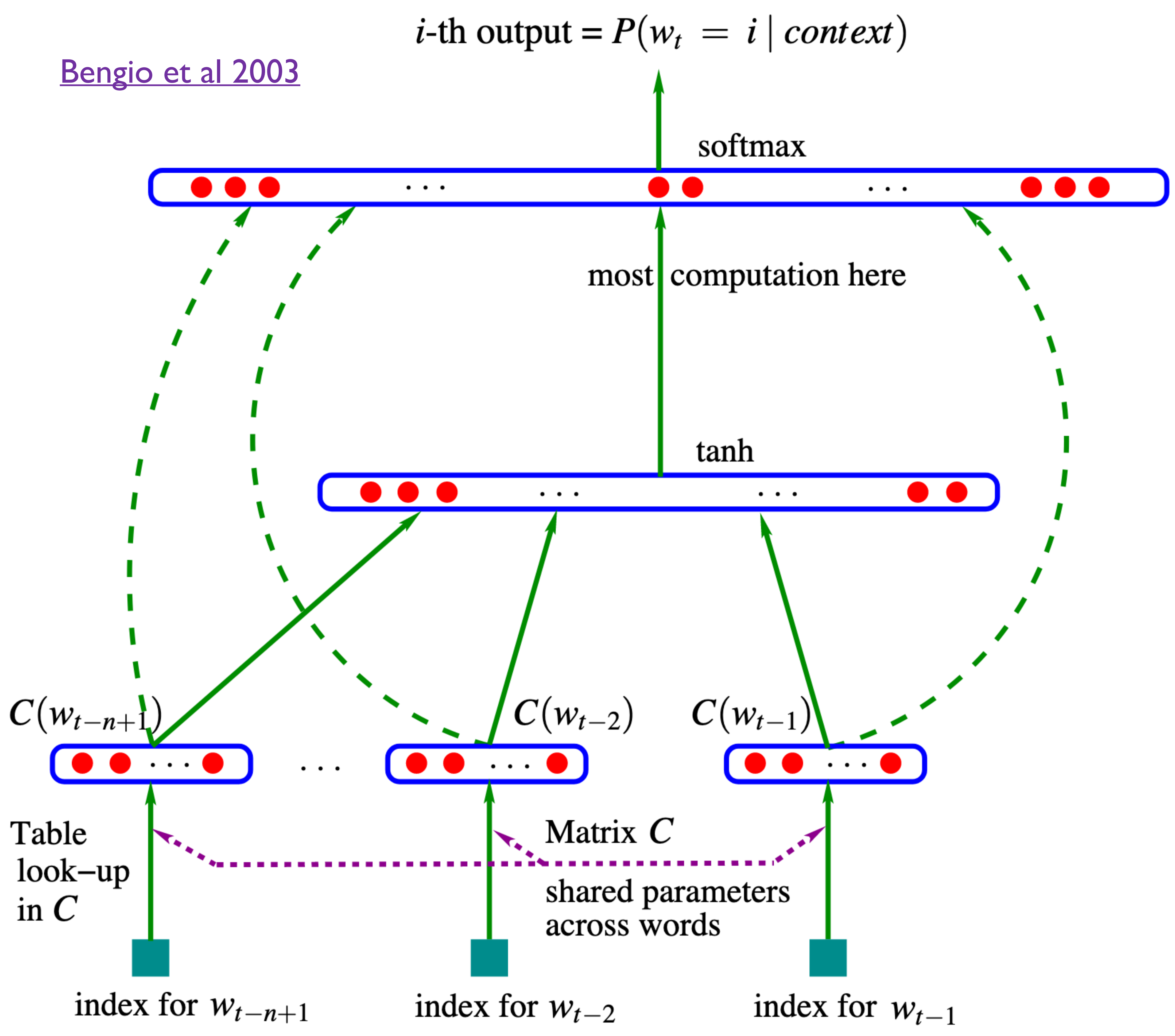
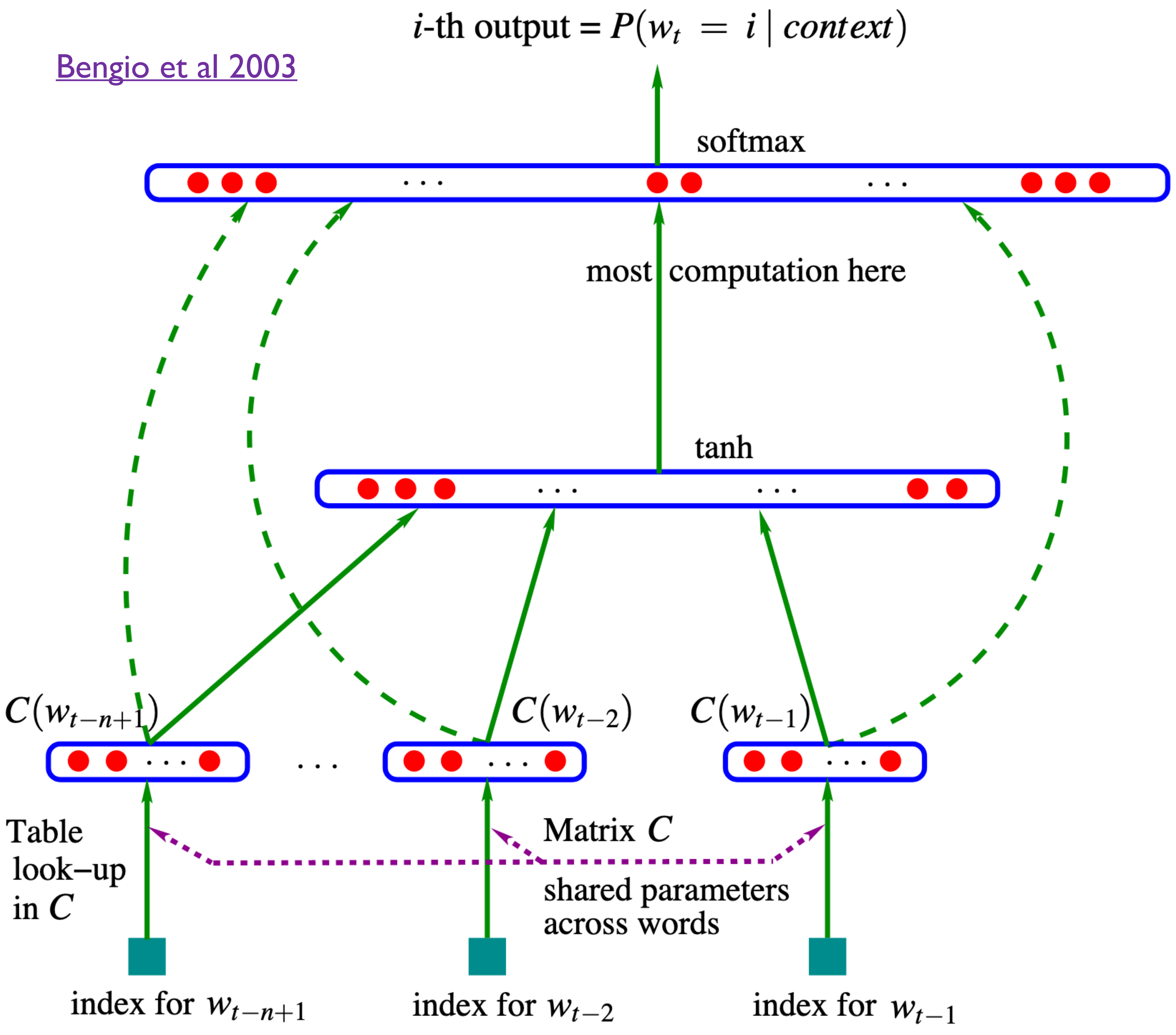


$$\text{hidden} = \tanh(W^1 \cdot \text{embeddings} + b^1)$$

$$\text{embeddings} = \text{concat}(Cw_{t-1}, Cw_{t-2}, \ldots, Cw_{t-(n+1)})$$

w_t: one-hot vector

Neural LM Architecture



$$\text{probabilities} = \text{softmax}(W^2 \cdot \text{hidden} + b^2)$$

$$\text{hidden} = \tanh(W^1 \cdot \text{embeddings} + b^1)$$

$$\text{embeddings} = \text{concat}(Cw_{t-1}, Cw_{t-2}, \ldots, Cw_{t-(n+1)})$$

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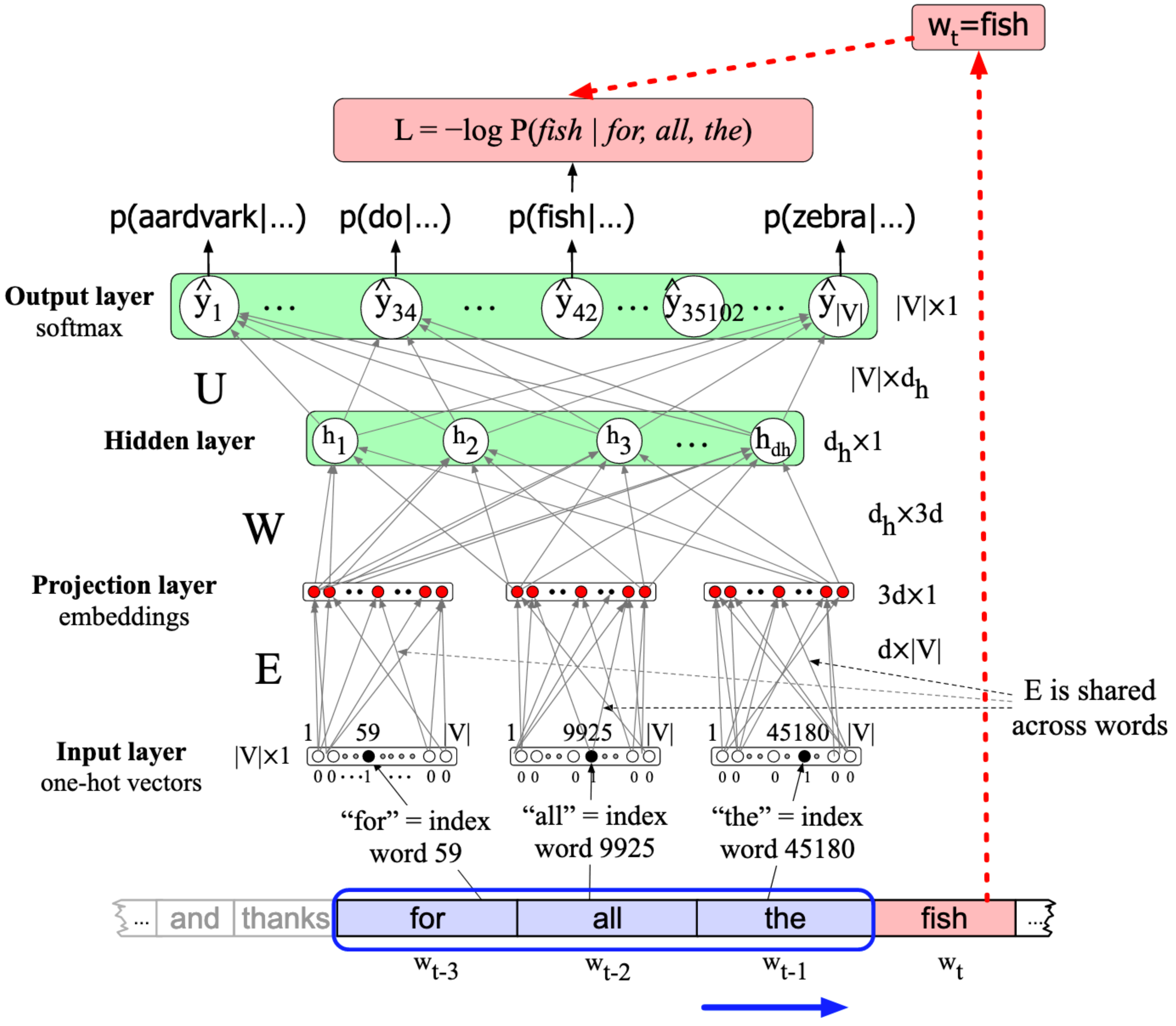
More Detailed Diagram of Architecture



JM sec 7.5

Output and Loss for Classification

$$\text{logits} = W \cdot \text{hidden} + b$$

$$\hat{y} = \text{probs} = \text{softmax}(\text{logits})$$

$$\ell_{CE}(\hat{y}, y) = -\sum_{i=0}^{|\text{classes}|} y_i \log \hat{y}_i$$

One hot for true class label

Evaluation of LMs

- **Extrinsic**: use in other NLP systems
- **Intrinsic**: intuitively, want probability of a test corpus
  - **Perplexity**: inverse probability, weighted by size of corpus
  - **Lower** is better!
  - **Only comparable w/ same vocab**

Perplexity

$$PP(W) = P(w_1 w_2 \cdots w_N)^{-1/N}$$

$$= \sqrt[N]{\frac{1}{P(w_1 w_2 \cdots w_N)}}$$

$$= \sqrt[N]{\frac{1}{\prod_{i=0}^{N} P(w_i \mid w_1, \ldots, w_{i-1})}}$$

$$= 2^{-\frac{1}{N}\sum_{i=0}^{N} \log P(w_i | w_1, \ldots, w_{i-1})}$$

More Complete Picture of This Model

Revisiting Simple Neural Probabilistic Language Models

Simeng Sun and **Mohit Iyyer**
College of Information and Computer Sciences
University of Massachusetts Amherst
`{simengsun, miyyer}@cs.umass.edu`

Abstract

Recent progress in language modeling has been driven not only by advances in neural architectures, but also through hardware and optimization improvements. In this paper, we revisit the neural probabilistic language model (NPLM) of Bengio et al. (2003), which simply concatenates word embeddings within a fixed window and passes the result through a feed-forward network to predict the next word. When scaled up to modern hardware, this model (despite its many limitations) performs

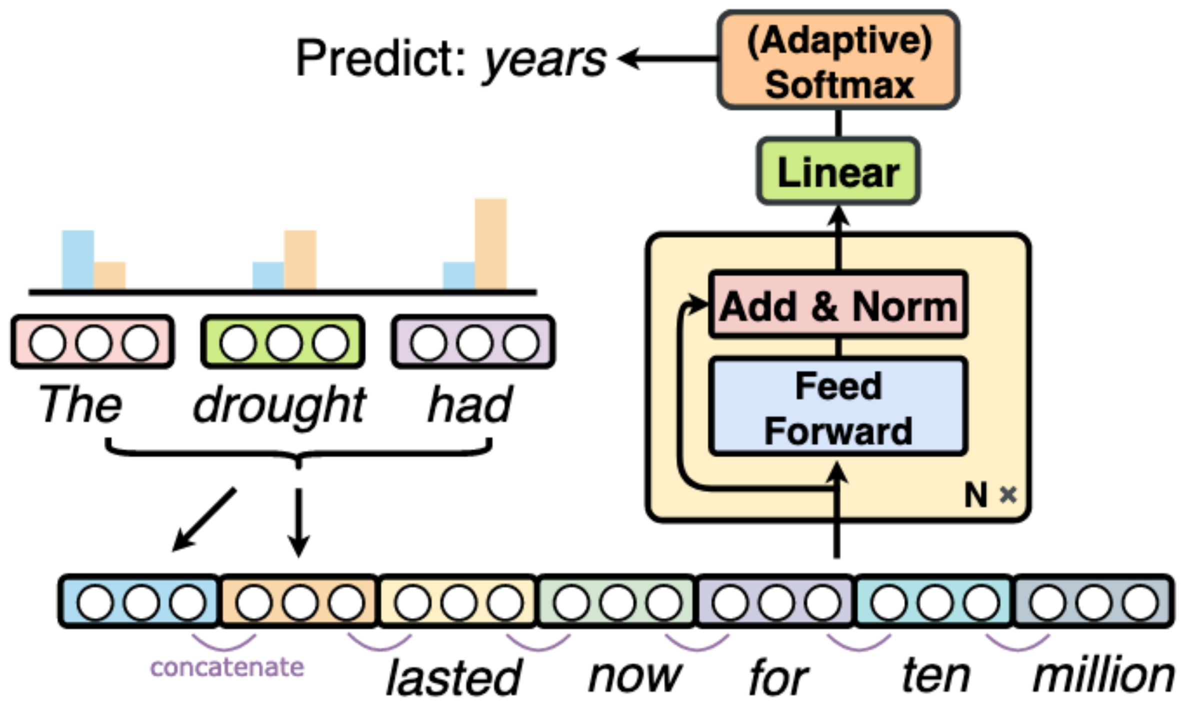
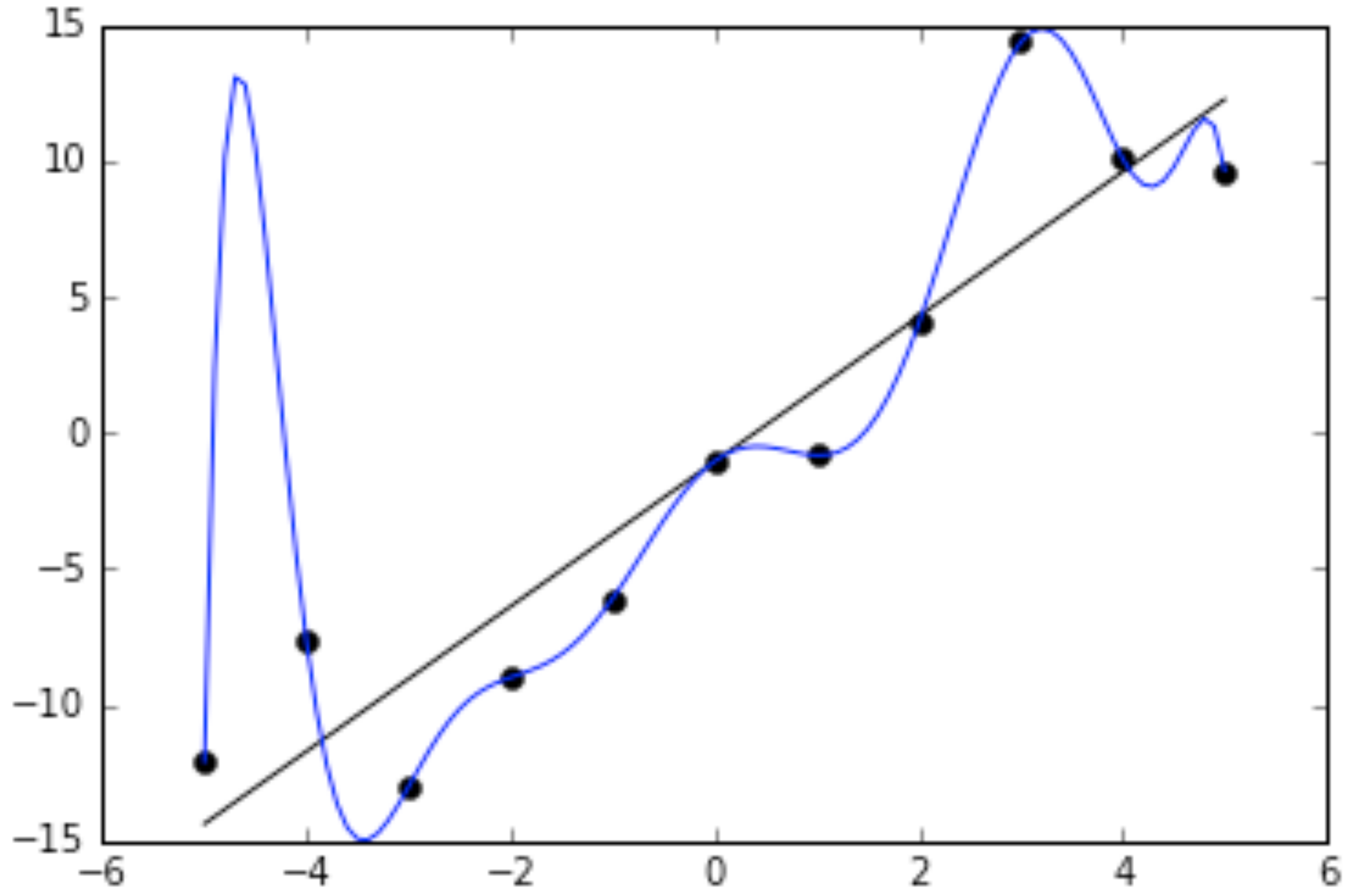


Figure 1: A modernized version of the neural probabilistic language model of Bengio et al. (2003), which

Additional Training Notes: Regularization and Hyper-Parameters

Overfitting

- Over-fitting: model too closely mimics the training data
  - Therefore, **cannot *generalize* well**
- Common when models are "**over-parameterized**"
  - E.g. fitting a high-degree polynomial
  - Neural models are typically over-parameterized
- Key questions:
  - How to detect overfitting?
  - How to prevent it?

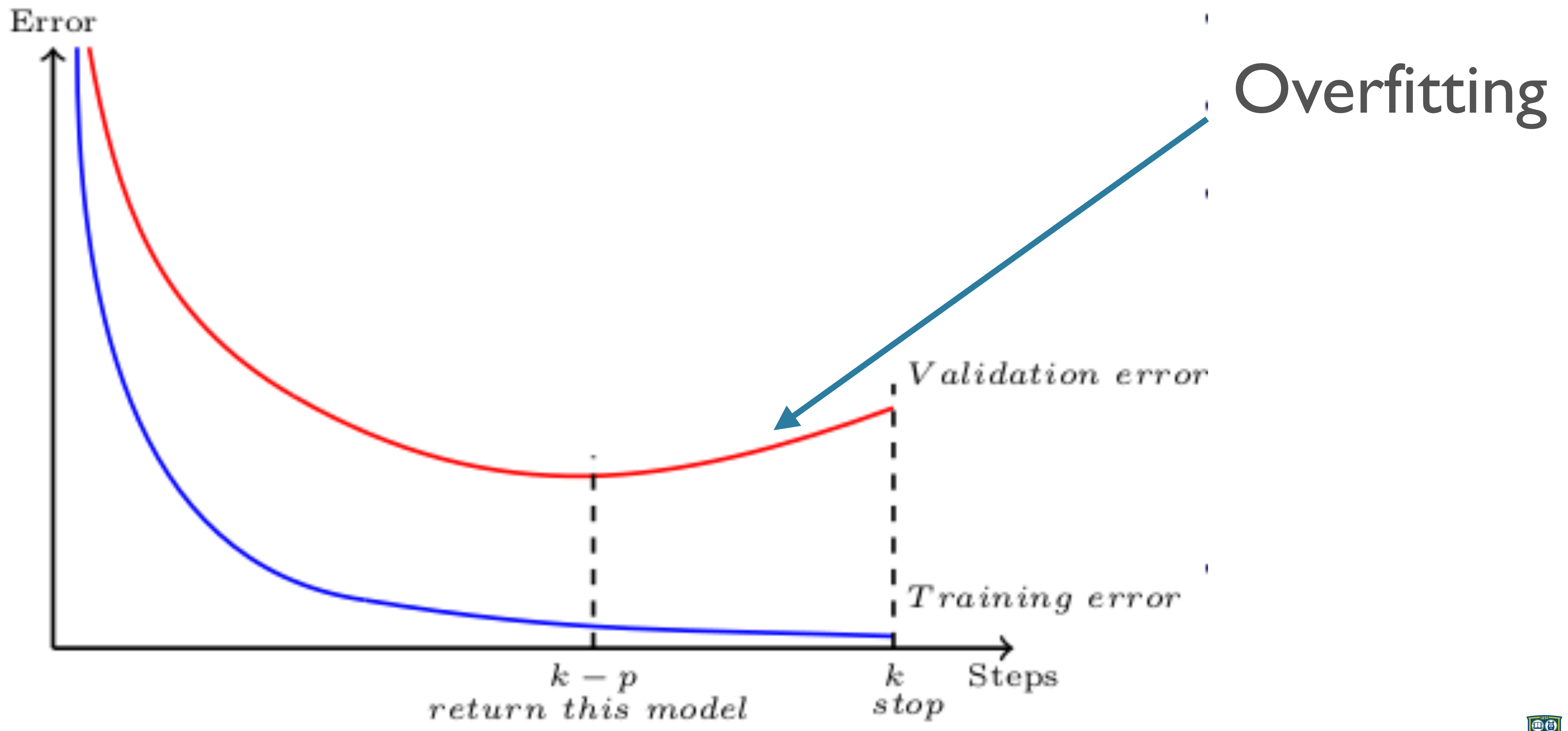


Train, Dev, Test Set Splits

- Split total data into three chunks: train, dev (aka valid), test
  - Common: 70/15/15, 80/10/10%
- **Train**: used for individual model training, as we've seen so far
- **Dev/valid**:
  - Evaluation during training
  - Hyper-parameter tuning
  - Model selection
- **Test**:
  - Final evaluation; **DO NOT TOUCH** otherwise

Early stopping

- Naive idea: pick # of epochs, hope for no overfitting
- Better: pick **max # of epochs**, and "**patience**"
  - Halt when **validation error does not improve** over patience-many epochs



source

Regularization

- NNs are often *overparameterized*, so regularization helps
- L1/L2: $\mathscr{L}'(\theta, y) = \mathscr{L}(\theta, y) + \lambda ||\theta||^2$
  - (penalty for **higher magnitude** parameters)
- Dropout:
  - During training, randomly **turn off X% of neurons** in each layer
  - (Don't do this during testing/predicting)
- Batch Normalization / Layer Norm
- Batch size choice can also be regulating

Input: Values of x over a mini-batch: $\mathcal{B} = \{x_{1...m}\}$;
Parameters to be learned: γ, β

Output: $\{y_i = \mathrm{BN}_{\gamma,\beta}(x_i)\}$

$$\mu_\mathcal{B} \leftarrow \frac{1}{m}\sum_{i=1}^{m} x_i \qquad \text{// mini-batch mean}$$

$$\sigma_\mathcal{B}^2 \leftarrow \frac{1}{m}\sum_{i=1}^{m} (x_i - \mu_\mathcal{B})^2 \qquad \text{// mini-batch variance}$$

$$\widehat{x}_i \leftarrow \frac{x_i - \mu_\mathcal{B}}{\sqrt{\sigma_\mathcal{B}^2 + \epsilon}} \qquad \text{// normalize}$$

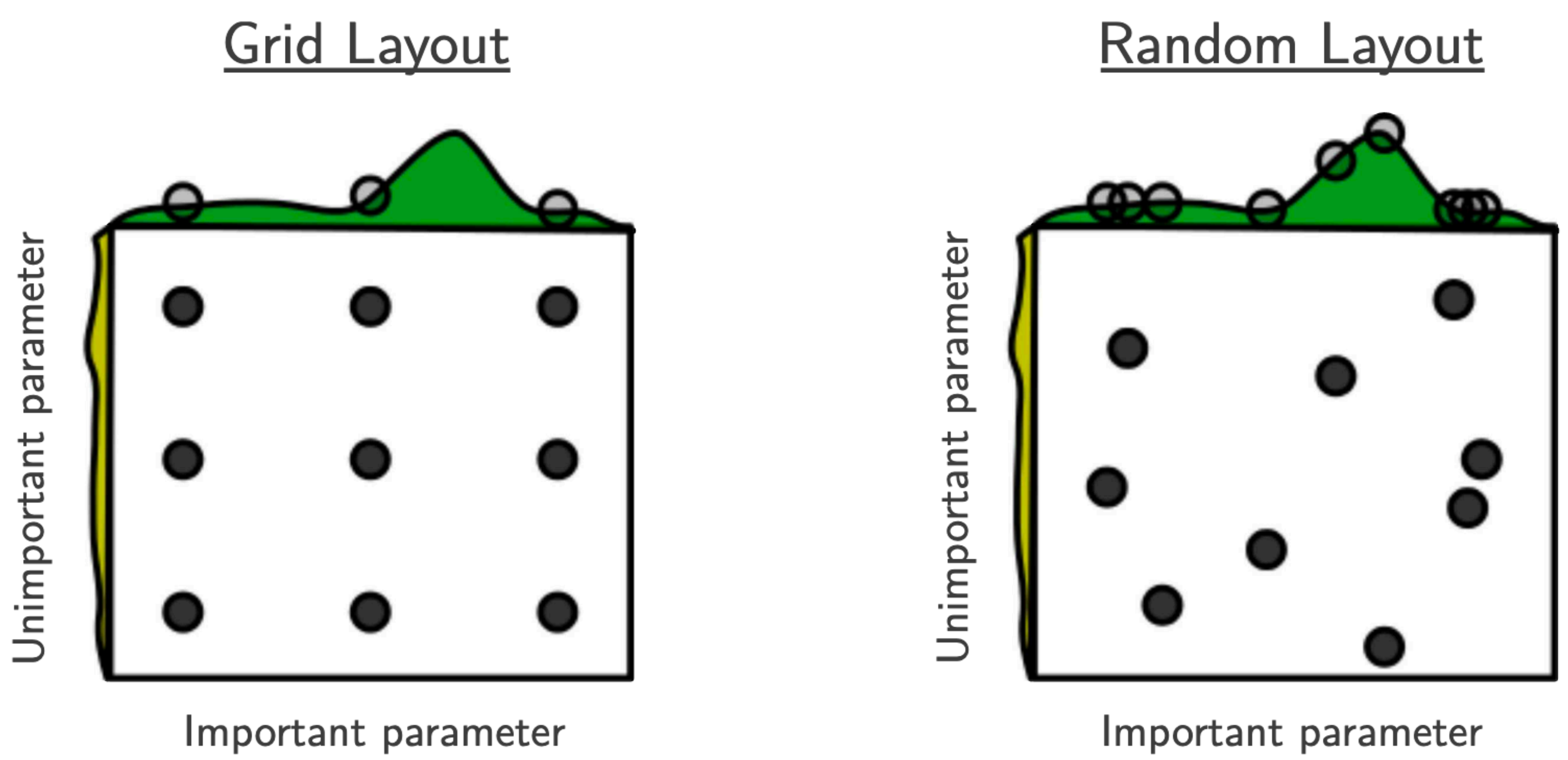
$$y_i \leftarrow \gamma \widehat{x}_i + \beta \equiv \mathrm{BN}_{\gamma,\beta}(x_i) \qquad \text{// scale and shift}$$

Hyper-parameters

- In addition to the model architecture ones mentioned earlier
- **Optimizer**: SGD, Adam, Adagrad, RMSProp, ….
  - Optimizer-specific hyper-parameters: learning rate, alpha, beta, …
  - (Backprop computes gradients; optimizer uses them to update parameters)
- **Regularization**: L1/L2, Dropout, BN, …
  - regularizer-specific ones: e.g. dropout rate
- **Batch size**
- Number of **epochs** to train for
  - Early stopping criterion (e.g. patience)

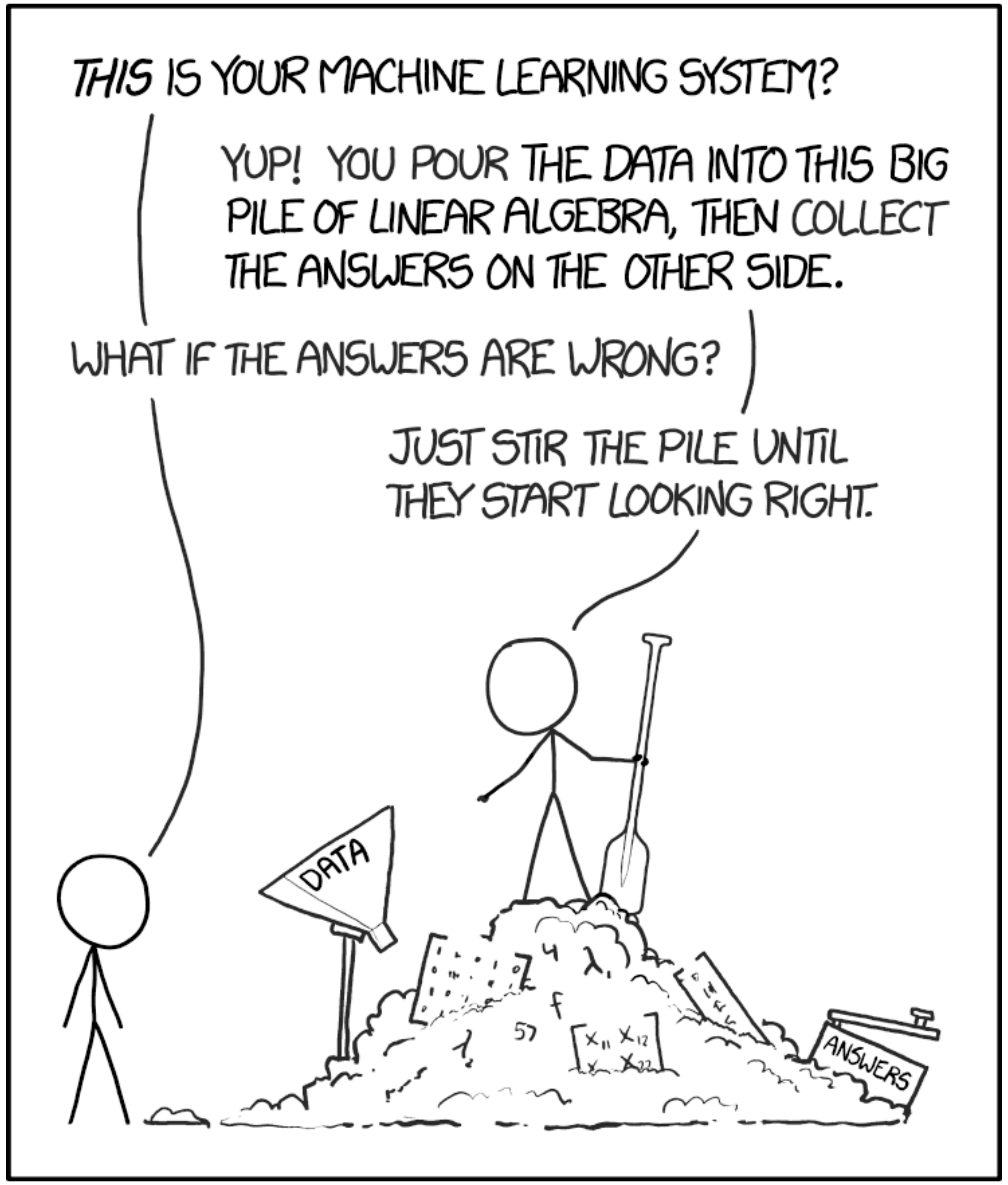
A note on hyper-parameter tuning

- **Grid search**: specify range of values for each hyper-parameter, try all possible combinations thereof
- **Random search**: specify possible values for all parameters, randomly sample values for each, stop when some criterion is met



Bergstra and Bengio 2012

Craft/Art of Deep Learning



https://xkcd.com/1838/

Some Practical Pointers

- Hyper-parameter tuning and the like are not the focus of this course
- For some helpful hand-on advice about training NNs from scratch, debugging under “silent failures”, etc:
  - http://karpathy.github.io/2019/04/25/recipe/

Adagrad

- “Adaptive Gradients”
- Key idea: **adjust the learning rate per parameter**
- Frequent features —> more updates
- Adagrad will make the learning rate **smaller for those**

Adagrad

- Let $g_{t,i} := \nabla_{\theta_{t,i}} \mathscr{L}$
- SGD: $\theta_{t+1,i} = \theta_{t,i} - \alpha g_{t,i}$
- Adagrad: $\theta_{t+1,i} = \theta_{t,i} - \dfrac{\alpha}{\sqrt{G_{t,i} + \epsilon}} g_{t,i}$

$$G_{t,i} = \sum_{k=0}^{t} g_{k,i}^2$$

Accumulated change to parameter i over time

Adagrad

- Pros:
  - “Balances” parameter importance
  - **Less manual tuning** of learning rate needed (0.01 default)
- Cons:
  - $G_{t,i}$ increases monotonically, so **step-size always gets smaller**
- Newer optimizers try to have the pros without the cons
- Resources:
  - Original paper (veeery math-y): https://jmlr.org/papers/volume12/duchi11a/duchi11a.pdf
  - Overview of optimizers: https://ruder.io/optimizing-gradient-descent/index.html#adagrad